

Supporting Information for

**Insights into the Mechanistic Role of Diphenylphosphine
Selenide, Diphenylphosphine, and Primary Amines in the
Formation of CdSe Monomers**

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Catalog

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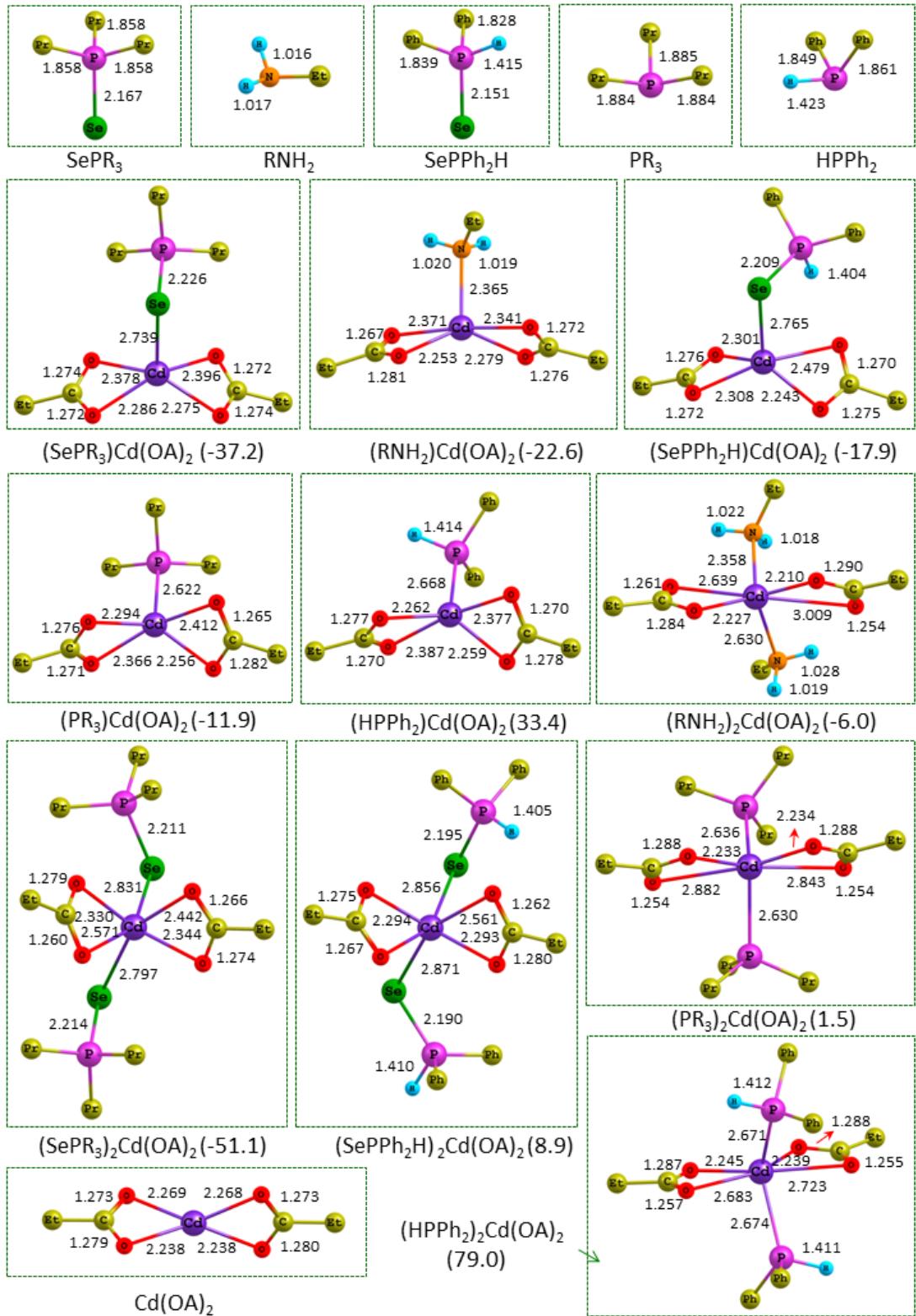


Figure S1a. The geometric structures of various species, and the relative Gibbs free energies (G_r) (kJ mol^{-1}) relative to the discrete reactants calculated at the M06//B3LYP/6-31++G(d, p), SDD level are shown. Bond lengths are reported in \AA .

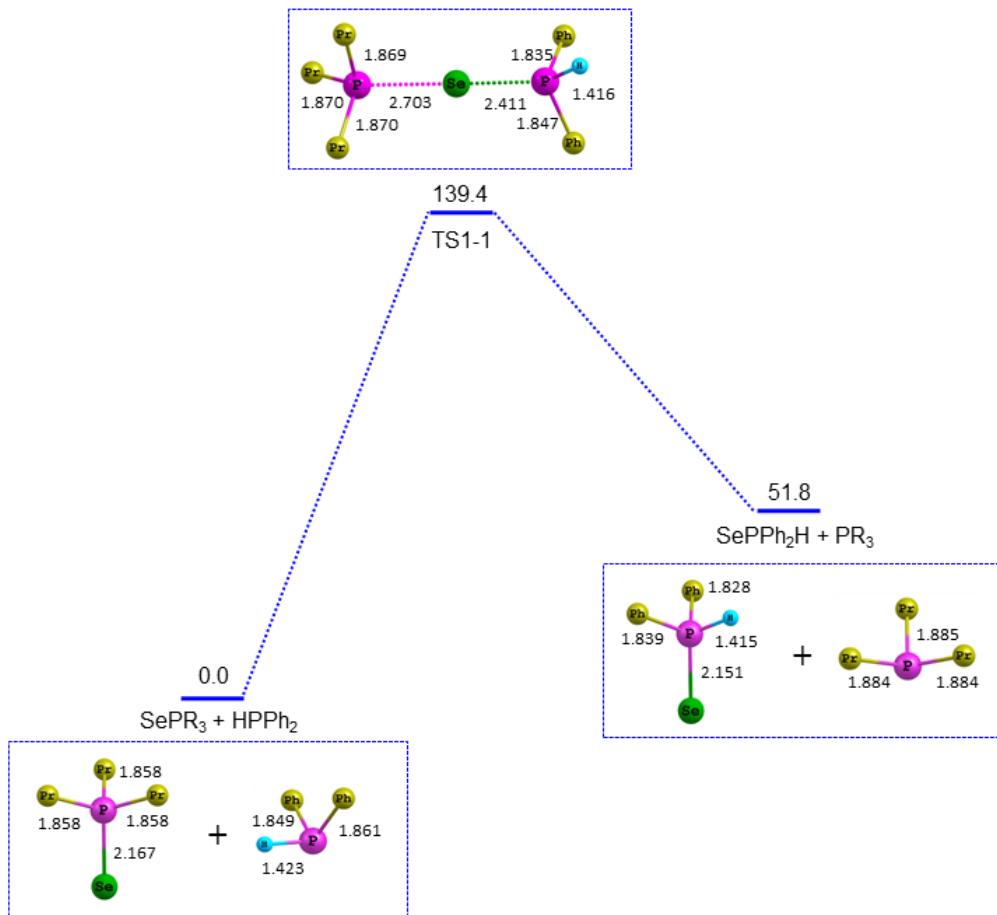
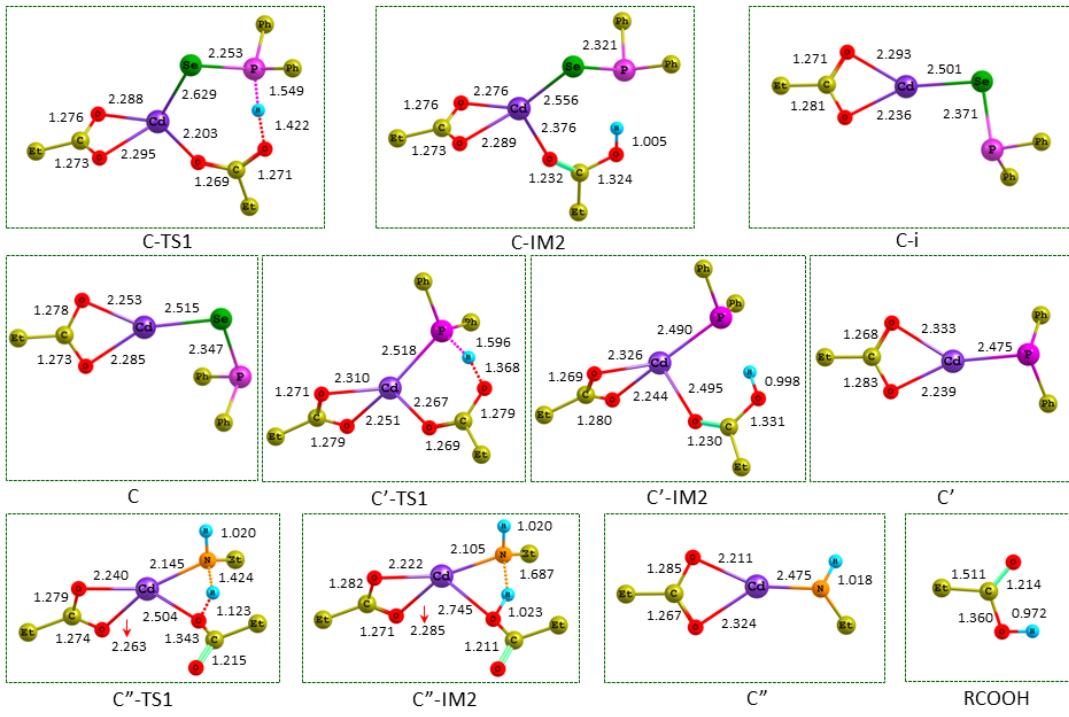
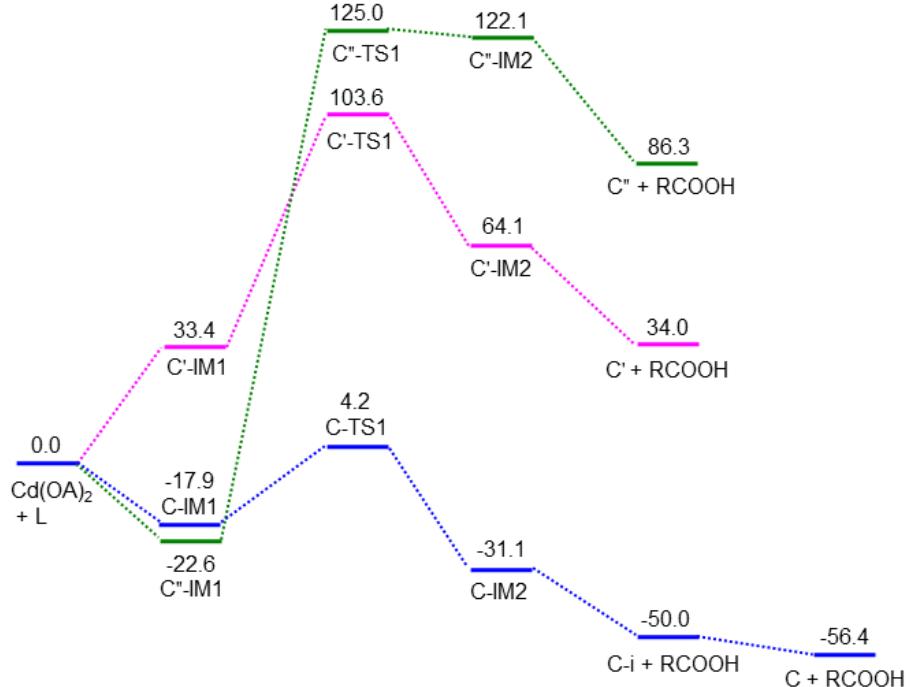


Figure S1b. The geometric structures of various species, and the schematic energy diagrams for the reaction $\text{SePR}_3 + \text{HPPh}_2 \rightarrow \text{SePPh}_2\text{H} + \text{PR}_3$. Bond lengths are reported in Å. Relative Gibbs free energies (G_f) (kJ mol⁻¹) for the corresponding species relative to $\text{SePR}_3 + \text{HPPh}_2$ at the M06//B3LYP/6-31++G(d, p), SDD level are shown.



(a)

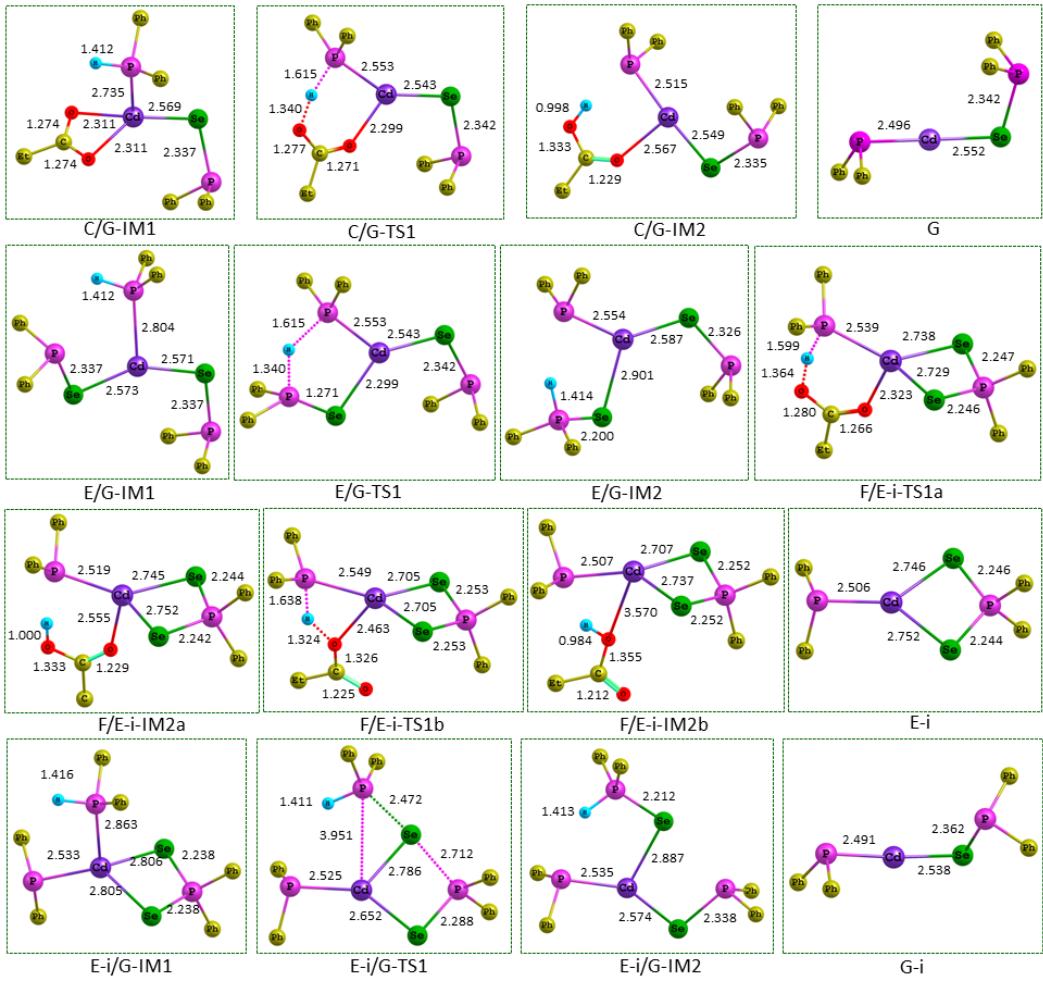


(b)

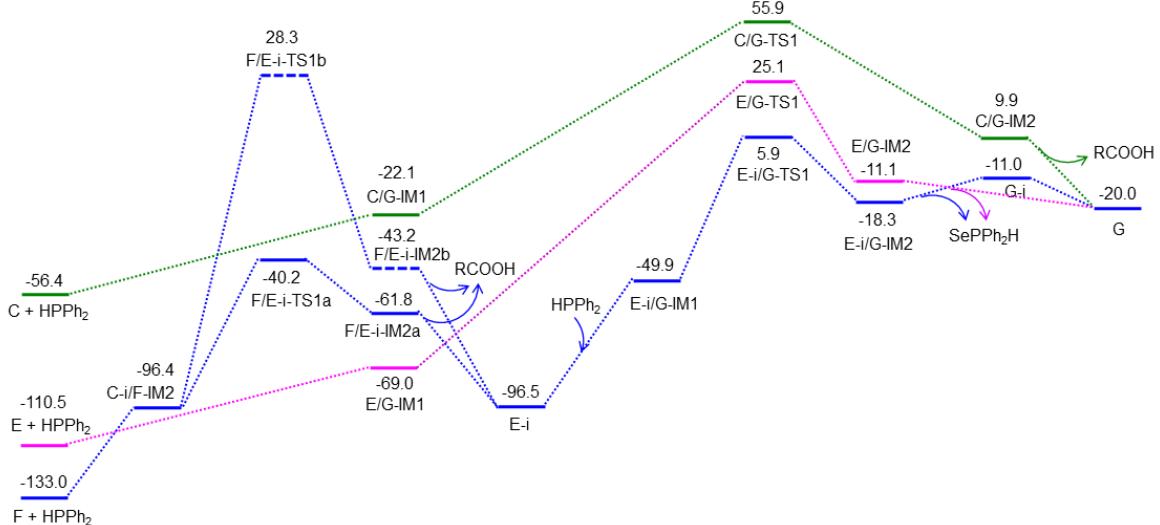
Figure S2. The geometric structures of various species (a), and the schematic energy diagrams (b) for the reaction (3) $\text{Cd(OA)}_2 + \text{SePPh}_2\text{H} \rightarrow \mathbf{C} + \text{RCOOH}$, (4) $\text{Cd(OA)}_2 + \text{HPPH}_2 \rightarrow \mathbf{C}' + \text{RCOOH}$, and (5) $\text{Cd(OA)}_2 + \text{RNH}_2 \rightarrow \mathbf{C}'' + \text{RCOOH}$. Bond lengths are reported in Å. Relative Gibbs free energies (G_r) (kJ mol^{-1}) for the corresponding species relative to $\text{Cd(OA)}_2 + \text{L}$ ($\text{L} = \text{SePPh}_2\text{H}$, HPPH_2 , and RNH_2) at the M06//B3LYP/6-31++G(d, p), SDD level are shown. Blue, red, and green lines represent the reactions (3), (4), and (5), respectively.

As shown in Figures S2a and S2b, for the reaction stage of Cd(OA)_2 with HPPh_2 , to begin, the five-coordination complex $(\text{HPPh}_2)\text{Cd(OA)}_2$ (**C'-IM1**) is generated with the stabilization energy of $-33.4 \text{ kJ mol}^{-1}$. Next, from **C'-IM1**, H-shift from HPPh_2 to carboxylate occurs via a six-membered ring **C'-TS1**, resulting in the carboxylic acid molecular complex **C'-IM2**, with the energy barrier of 70.2 kJ mol^{-1} and the EHHP of $103.6 \text{ kJ mol}^{-1}$ at **C'-TS1**. Then, **C'-IM2** liberates the free carboxylic acid, leaving $\text{RCOO}\text{Cd-PPh}_2$ (**C'**) behind, with the exoergicity of 30.1 kJ mol^{-1} .

As shown in Figures S2a and S2b, for the reaction of Cd(OA)_2 with RNH_2 , first, the five-coordination complex $(\text{RNH}_2)\text{Cd(OA)}_2$ (**C''-IM1**) is engendered with the stabilization energy of 22.6 kJ mol^{-1} . Second, from **C''-IM1**, H-shift from RNH_2 to carboxylate occurs via a four-membered ring **C''-TS1**, yielding the carboxylic acid molecular complex **C''-IM2**, with the energy barrier of $147.6 \text{ kJ mol}^{-1}$ and the EHHP of $125.0 \text{ kJ mol}^{-1}$ at **C''-TS1**. Finally, **C''-IM2** releases the free carboxylic acid, leaving $\text{RCOO}\text{Cd-NHR}$ (**C'**) behind, with the exoergicity of 35.8 kJ mol^{-1} .



(a)

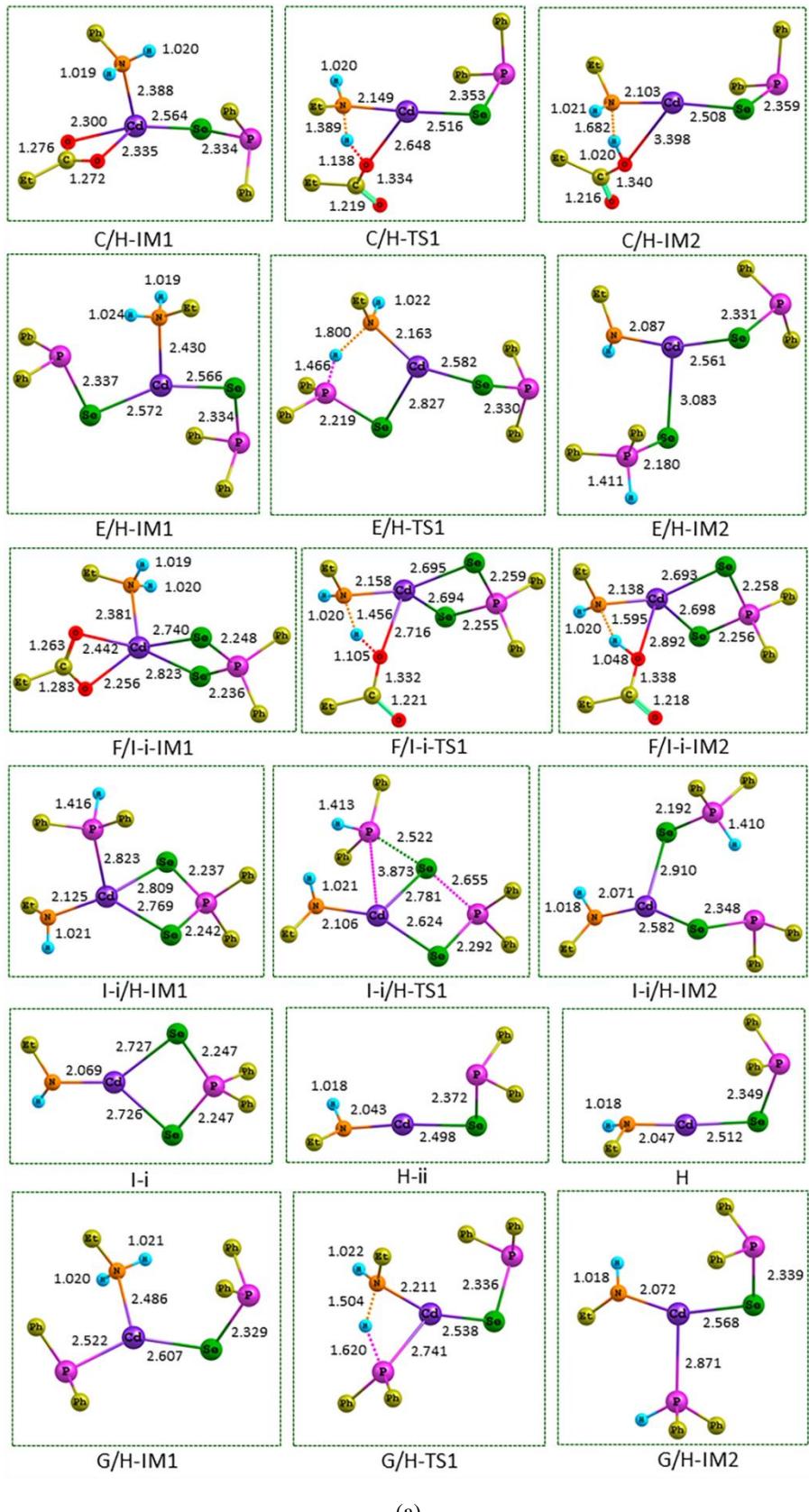


(b)

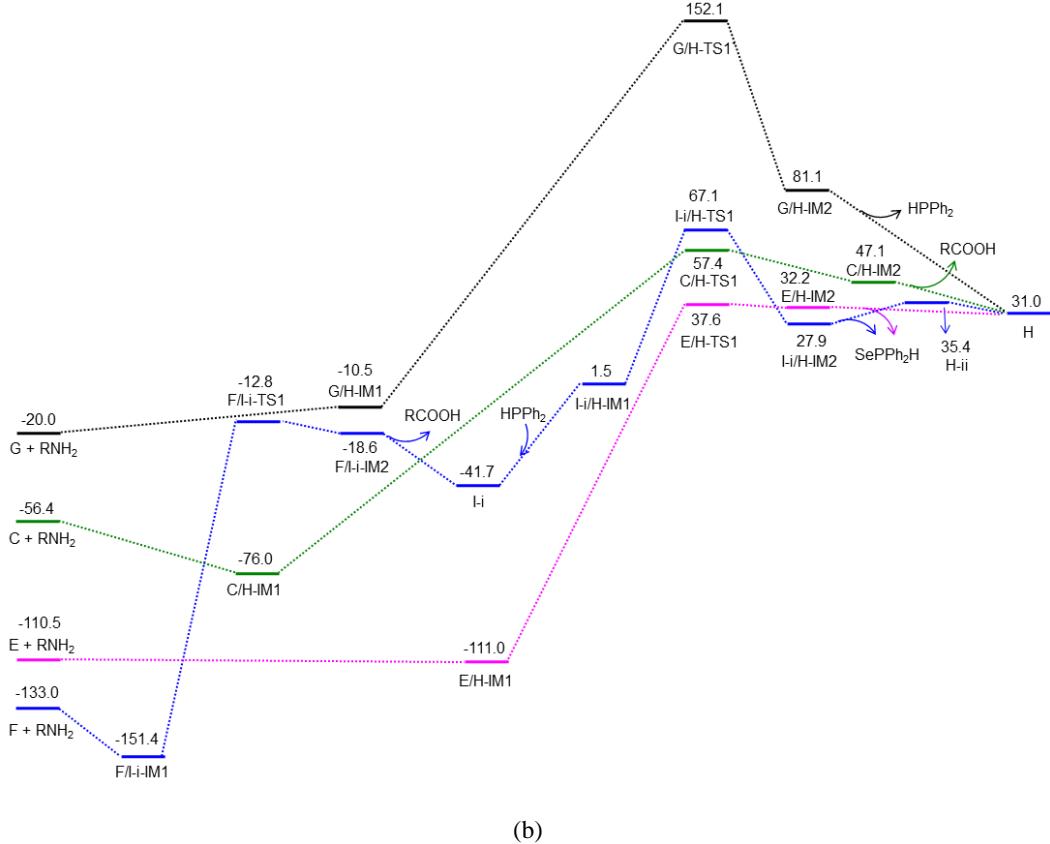
Figure S3. The geometric structures of various species (a), and the schematic energy diagrams (b) for the reaction $\text{Cd(OA)}_2 + \text{SePPh}_2\text{H} + \text{HPPH}_2 \rightarrow \mathbf{G} + 2\text{RCOOH}$ calculated at the M06//B3LYP/6-31++G(d, p), SDD level are shown. Bond lengths are reported in Å. Relative Gibbs free energies (G_r) (kJ mol⁻¹) for the corresponding species plus RCOOH form **C** + HPPh₂ to **G**, for the corresponding species plus HPPH₂ + RCOOH - SePPh₂H from **F** + HPPH₂ to **E-i**, and for the corresponding species plus 2RCOOH - SePPh₂H from **E** and **E-i** to **G** are shown relative to $\text{Cd(OA)}_2 + \text{SePPh}_2\text{H} + \text{HPPH}_2$. Green, red, and blue lines represent the reaction (8) **C** + HPPh₂ → **G** + RCOOH, (9) **E** + HPPh₂ → **G** + SePPh₂H, and (10) **F** + 2HPPH₂ → **G** + RCOOH + SePPh₂H, respectively.

As shown in Figures S3a and S3b, for the reaction of RCOOCdSe- PPh_2 (**C**) with HPPh₂, in the beginning, when the P atom of HPPh₂ interacts with the central Cd atom of **C**, a four-coordination complex **C/G-IM1** is formed. From **C/G-IM1**, H-shift from HPPh₂ to carboxylate occurs via a six-membered ring **C/G-TS1**, leading to a carboxylic acid molecular complex **C/G-IM2**. Then, **C/G-IM2** releases the carboxylic acid, leaving Ph₂P-CdSe-PPh₂ (**G**) monomer behind. This reaction pathway involves the highest energy barrier (HEB) of 78.0 kJ mol⁻¹ at the reaction step of **C/G-IM1** → **C/G-TS1**, the EHHP of 55.9 kJ mol⁻¹ at **C/G-TS1**, and the endoergicity of 36.4 kJ mol⁻¹.

As depicted in Figures S3a and S3b, for the reaction of Ph₂PSe-Cd-SePPh₂ (**E**) with HPPh₂, initially, when the P atom of HPPh₂ coordinates to the central Cd atom of **E**, a three-coordination complex **E/G-IM1** is generated. Next, from **E/G-IM1**, H-shift from HPPh₂ to -PPh₂ group takes place via a five-membered ring **E/G-TS1**, resulting in a SePPh₂H molecular complex **E/G-IM2**. After that, **E/G-IM2** sets the SePPh₂H free, leaving Ph₂P-CdSe-PPh₂ (**G**) monomer behind. This reaction pathway includes the HEB of 94.1 kJ mol⁻¹ at the reaction step of **E/G-IM1** → **E/G-TS1**, the EHHP of 25.1 kJ mol⁻¹ at **E/G-TS1**, and the endoergicity of 90.5 kJ mol⁻¹.



(a)

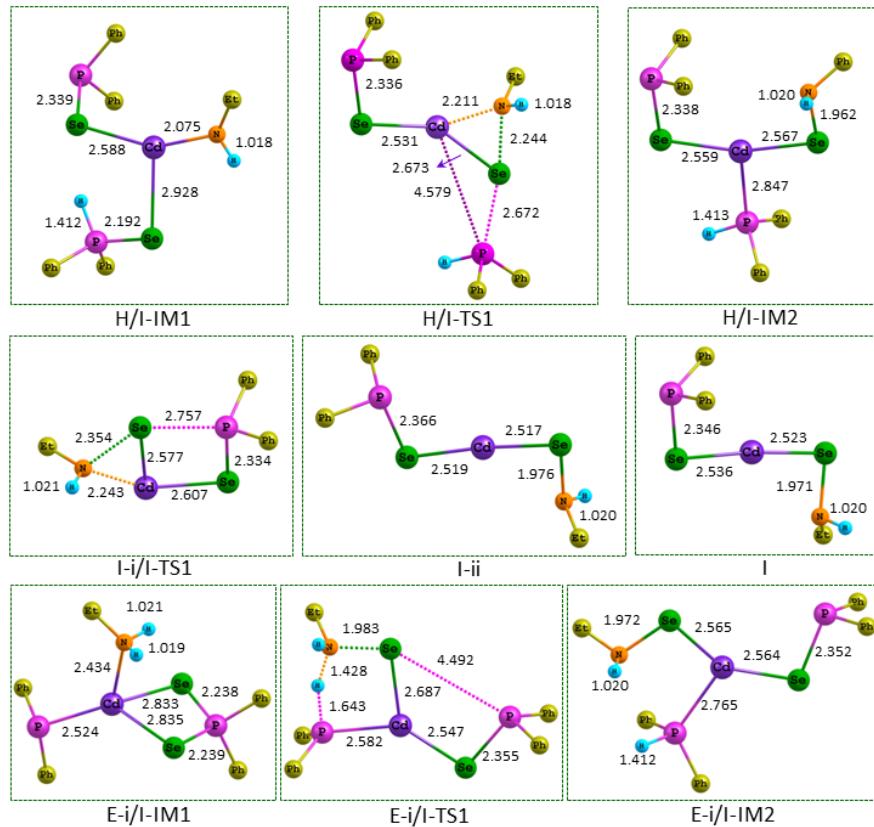


(b)

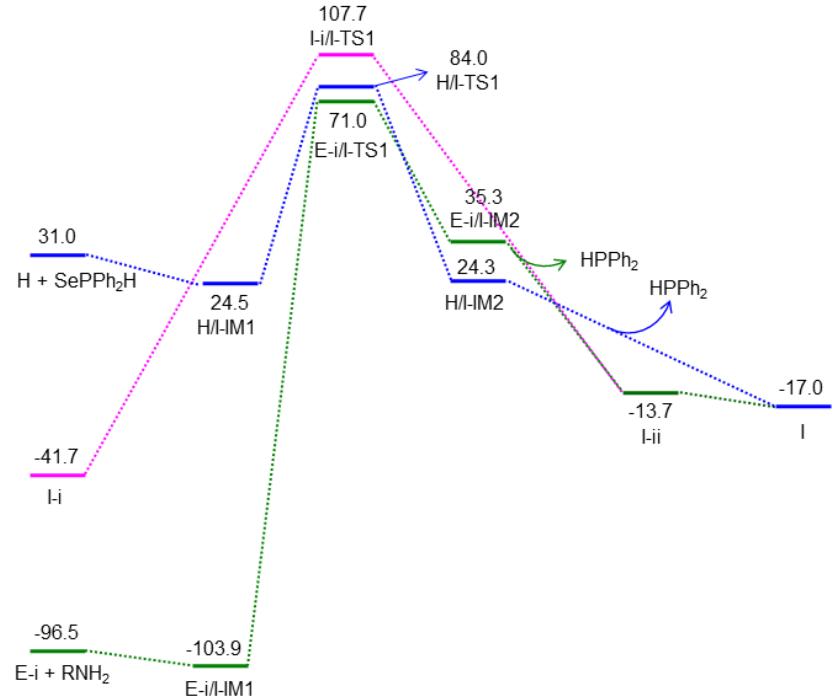
Figure S4. The geometric structures of various species (a), and the schematic energy diagrams (b) for the reaction $\text{Cd(OA)}_2 + \text{SePPh}_2\text{H} + \text{RNH}_2 \rightarrow \text{H} + 2\text{RCOOH}$ calculated at the M06/B3LYP/6-31++G(d, p), SDD level are shown.. Bond lengths are reported in Å. Relative Gibbs free energies (G_r) (kJ mol⁻¹) for the corresponding species plus RCOOH form **C** + RNH₂ to **H**, for the corresponding species plus HPPh₂ + RCOOH - SePPh₂H from **F** + RNH₂ to **I-i**, for the corresponding species plus 2RCOOH - SePPh₂H from **I-i** and **E** to **H**, and for the corresponding species plus 2RCOOH - HPPh₂ from **G** + RNH₂ to **H** are shown relative to $\text{Cd(OA)}_2 + \text{SePPh}_2\text{H} + \text{RNH}_2$. Green, red, blue, and black lines represent the reaction (13) **C** + RNH₂ → **H** + RCOOH, (14) **E** + RNH₂ → **H** + SePPh₂H, (15) **F** + RNH₂ + HPPh₂ → **H** + RCOOH + SePPh₂H, and (16) **G** + RNH₂ → **H** + HPPh₂, respectively.

As shown in Figures S4a and S4b, for the reaction of RCOOCdSe-PPh₂ (**C**) with RNH₂, initially, when the N-end of RNH₂ coordinates to the central Cd atom of **C**, a four-coordination complex **C/H-IM1** is generated. From **C/H-IM1**, H-shift from RNH₂ to carboxylate takes places via a four-membered ring **C/H-TS1**, yielding a carboxylic acid molecular complex **C/H-IM2**. Next, **C/H-IM2** sets the carboxylic acid, leaving RHN-CdSe-PPh₂ (**H**) monomer behind. This reaction pathway includes the highest energy barrier (HEB) of 133.4 kJ mol⁻¹ at the reaction step of **C/H-IM1** → **C/H-TS1**, the EHHP of 57.4 kJ mol⁻¹ at **C/H-TS1**, and the endoergicity of 87.4 kJ mol⁻¹.

As depicted in Figures S4a and S4b, for the reaction of Ph₂P-CdSe-PPh₂ (**G**) with RNH₂, initially, when the N-end of RNH₂ interacts with the central Cd atom of **G**, a three-coordination complex **G/H-IM1** is generated. Next, from **G/H-IM1**, H-shift from RNH₂ to -PPh₂ group takes place via a four-membered ring **G/H-TS1**, resulting in a HPPh₂ molecular complex **G/H-IM2**. Lastly, **G/H-IM2** releases the free HPPh₂, leaving RHN-CdSe-PPh₂ (**H**) monomer behind. This reaction pathway comprises the HEB of 162.6 kJ mol⁻¹ at the reaction step of **G/H-IM1** → **G/H-TS1**, the EHHP of 152.1 kJ mol⁻¹ at **G/H-TS1**, and the endoergicity of 141.5 kJ mol⁻¹.



(a)



(b)

Figure S5. The geometric structures of various species (a), and the schematic energy diagrams (b) for the reaction $\text{Cd(OA)}_2 + 2\text{SePPh}_2\text{H} + \text{RNH}_2 \rightarrow \mathbf{I} + \text{HPPh}_2 + 2\text{RCOOH}$ 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 2RCOOH from **H** + SePPh₂H and **E-i** + RNH₂ to **I**, and for the corresponding species plus HPPh₂ + 2RCOOH from **I-i** to **I** are shown relative to Cd(OA)₂ + 2SePPh₂H + RNH₂. Blue, red, and Green lines represent the reaction (21) **H** + SePPh₂H → **I** + HPPh₂, (22) **I-i** → **I**, and (23) **E-i** + RNH₂ → **I** + HPPh₂, respectively.

As shown in Figures S5a and S5b, for the reaction stage (21) of RHN-CdSe- PPh_2 (**H**) with SePPh_2H , in the beginning, when the Se-end of SePPh_2H interacts with the central Cd atom of **H**, a three-coordination complex **H/I-IM1** is formed. Then, from **H/I-IM1**, Se exchange takes place through the synergistic Se=P bond cleavage of SePPh_2H moiety, Cd-N bond cleavage, and Se-N bond formation via a four-membered plane-like **H/I-TS1**, resulting in a HPPPh_2 molecular complex **H/I-IM2**. Lastly, **H/I-IM2** sets the HPPPh_2 free, leaving $\text{Ph}_2\text{PSe-CdSe-NHR}$ (**I**) monomer behind. Wherein, SePPh_2H serves as Se source for the precursor formation.

For the **I** formation from **E**, this reaction pathway **RP-CEHI** includes the HEB of $148.6 \text{ kJ mol}^{-1}$ at the reaction step of **E/H-IM1** \rightarrow **E/H-TS1**, the EHHP of 84.0 kJ mol^{-1} at **H/I-TS1**, and the endoergicity of 93.5 kJ mol^{-1} , together with the reaction (14) of **E** + $\text{RNH}_2 \rightarrow \text{H} + \text{SePPh}_2\text{H}$.

As shown in Figures S5a and S5b, for the isomerization (22) of RHN-Cd- Se_2PPh_2 (**I-i**), from **I-i**, Se exchange occurs through the synchronous Se-P bond cleavage of $\text{Se}_2\text{PPh}_2\text{H}$ moiety, Cd-N bond cleavage, and Se-N bond formation via a five-membered envelope-like **I-i/I-TS1**, producing an isomer *trans*- $\text{Ph}_2\text{PSe-CdSe-NHR}$ (**I-ii**). Last, **I-ii** can easily isomerize to $\text{Ph}_2\text{PSe-CdSe-NHR}$ (**I**), with the Se-P single bond rotation.

For the **I** formation from **F**, this reaction pathway **RP-CFI-iI** involves the HEB of $149.4 \text{ kJ mol}^{-1}$ at the reaction step of **I-i** \rightarrow **I-i/I-TS1**, the EHHP of $107.7 \text{ kJ mol}^{-1}$ at **I-i/I-TS1**, and the endoergicity of $116.0 \text{ kJ mol}^{-1}$, together with the reaction (17) of **F** + $\text{RNH}_2 \rightarrow \text{I-i} + \text{RCOOH}$.

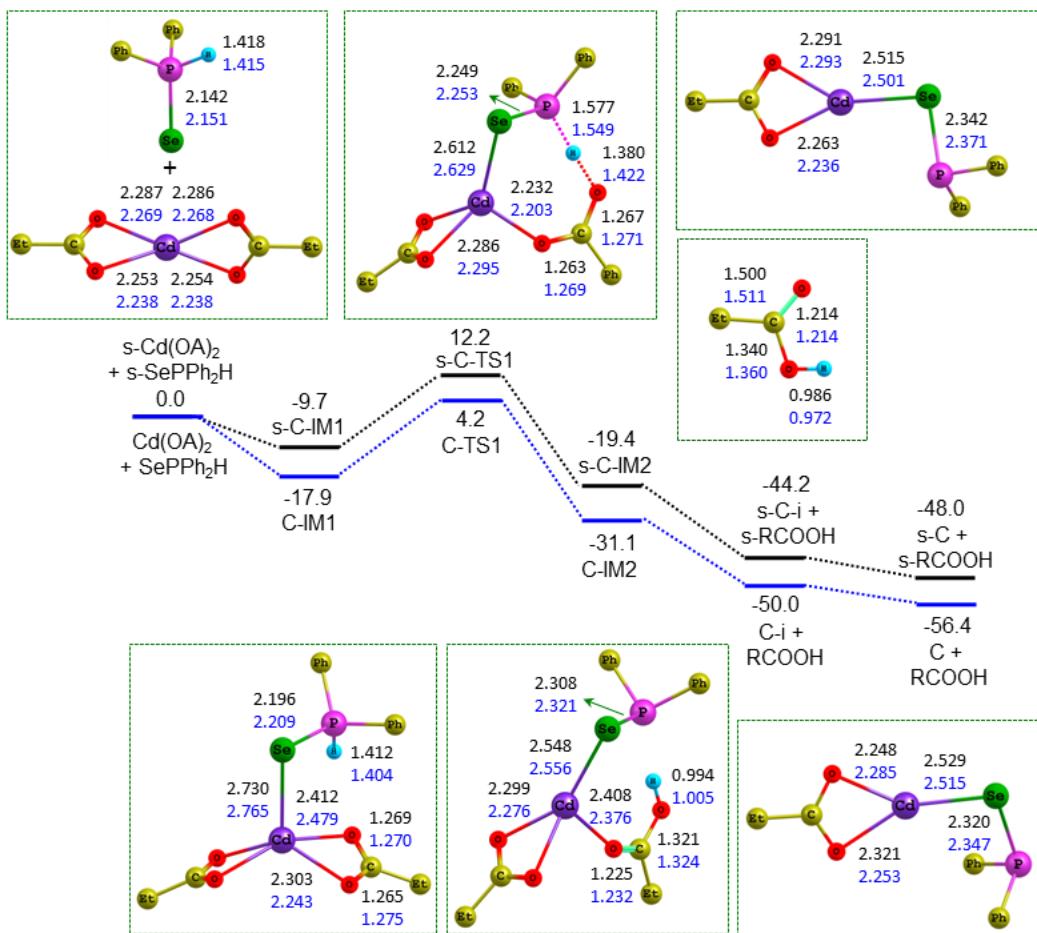


Figure S6. The geometric structures and the schematic energy diagrams for the reaction $\text{Cd(OA)}_2 + \text{SePPh}_2\text{H} \rightarrow \mathbf{C} + \text{RCOOH}$ calculated at the M06/6-31++G(d, p), SDD level in the ODE media under room temperature and atmospheric pressure (298.15 K and 1 atm). Relative Gibbs free energies (G_r) (kJ mol⁻¹) for the corresponding species relative to $\text{Cd(OA)}_2 + \text{SePPh}_2\text{H}$ are shown. Bond lengths are reported in Å. Black and blue lines represent the level of M06/6-31++G(d, p), SDD and M06//B3LYP/6-31++G(d, p), SDD, respectively.

Table S1. 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 + *nL* (*L* = SePR₃, RNH₂, SePPh₂H, PR₃, and HPPh₂; *n* = 1 ~ 2) for all the species in the reaction of Cd(OA)₂ + *nL* → L_{*n*}Cd(OA)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)						
	<i>ZPE</i>	G_0	<i>PCM-E</i>	E_c (<i>PCM-E</i> + <i>ZPE</i>)	E_r	G_c (<i>PCM-E</i> + G_0)	G_r
SePR ₃	0.28681	0.24187	-706.02637	-705.73957		-705.78450	
RNH ₂	0.09263	0.06713	-135.08775	-134.99512		-135.02062	
SePPh ₂ H	0.19343	0.15007	-814.22030	-814.02687		-814.07023	
PR ₃	0.28422	0.24265	-696.66425	-696.38003		-696.42160	
HPPh ₂	0.19113	0.15188	-804.87857	-804.68745		-804.72669	
Cd(OA) ₂	0.15896	0.11333	-703.16954	-703.01058		-703.05621	
SePR ₃ + Cd(OA) ₂	0.44577	0.35520	-1409.19591	-1408.75014	0.0	-1408.84071	0.0
(SePR ₃)Cd(OA) ₂	0.44681	0.37459	-1409.22945	-1408.78264	-85.3	-1408.85486	-37.2
RNH ₂ + Cd(OA) ₂	0.25159	0.18045	-838.25729	-838.00570	0.0	-838.07684	0.0
(RNH ₂)Cd(OA) ₂	0.25398	0.19822	-838.28365	-838.02967	-62.9	-838.08543	-22.6
SePPh ₂ H + Cd(OA) ₂	0.35239	0.26339	-1517.38984	-1517.03744	0.0	-1517.12644	0.0
(SePPh ₂ H)Cd(OA) ₂	0.35320	0.28247	-1517.41571	-1517.06251	-65.8	-1517.13325	-17.9
PR ₃ + Cd(OA) ₂	0.44318	0.35597	-1399.83378	-1399.39060	0.0	-1399.47781	0.0
(PR ₃)Cd(OA) ₂	0.44452	0.37318	-1399.85552	-1399.41100	-53.6	-1399.48234	-11.9
HPPh ₂ + Cd(OA) ₂	0.35009	0.26521	-1508.04811	-1507.69802	0.0	-1507.78290	0.0
(HPPh ₂)Cd(OA) ₂	0.35143	0.28474	-1508.05490	-1507.70346	-14.3	-1507.77016	33.4
2SePR ₃ + Cd(OA) ₂	0.73258	0.59707	-2115.22229	-2114.48971	0.0	-2114.62522	0.0
(SePR ₃) ₂ Cd(OA) ₂	0.73463	0.63899	-2115.28366	-2114.54903	-155.7	-2114.64467	-51.1
2RNH ₂ + Cd(OA) ₂	0.34422	0.24758	-973.34504	-973.00082	0.0	-973.09746	0.0
(RNH ₂) ₂ Cd(OA) ₂	0.34943	0.28819	-973.38793	-973.03850	-98.9	-973.09974	-6.0
2SePPh ₂ H + Cd(OA) ₂	0.54582	0.41346	-2331.61013	-2331.06431	0.0	-2331.19667	0.0
(SePPh ₂ H) ₂ Cd(OA) ₂	0.54723	0.45443	-2331.64770	-2331.10048	-95.0	-2331.19327	8.9
2PR ₃ + Cd(OA) ₂	0.72740	0.59862	-2096.49803	-2095.77063	0.0	-2095.89941	0.0
(PR ₃) ₂ Cd(OA) ₂	0.73095	0.64043	-2096.53926	-2095.80831	-98.9	-2095.89884	1.5
2HPPh ₂ + Cd(OA) ₂	0.54122	0.41709	-2312.92668	-2312.38547	0.0	-2312.50959	0.0
(HPPh ₂) ₂ Cd(OA) ₂	0.54372	0.45988	-2312.93939	-2312.39567	-26.8	-2312.47951	79.0

Table S2. 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 + L(L = SePPh₂H, HPPH₂, RNH₂) for all the species in the reaction of Cd(OA)₂ + SePPh₂H → C + RCOOH, Cd(OA)₂ + HPPH₂ → C' + RCOOH, and Cd(OA)₂ + RNH₂ → C'' + 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)						
	<i>ZPE</i>	G_0	<i>PCM-E</i>	E_c (<i>PCM-E</i> + <i>ZPE</i>)	E_r	G_c (<i>PCM-E</i> + G_0)	G_r
SePPh ₂ H	0.19343	0.15007	-814.22030	-814.02687		-814.07023	
HPPH ₂	0.19113	0.15188	-804.87857	-804.68745		-804.72669	
RNH ₂	0.09263	0.06713	-135.08775	-134.99512		-135.02062	
Cd(OA) ₂	0.15896	0.11333	-703.16954	-703.01058		-703.05621	
RCOOH	0.09058	0.06013	-268.27275	-268.18218		-268.21262	
SePPh ₂ H + Cd(OA) ₂	0.35239	0.26339	-1517.38984	-1517.03744	0.0	-1517.12644	0.0
C-IM1	0.35320	0.28247	-1517.41571	-1517.06251	-65.8	-1517.13325	-17.9
C-TS1	0.35003	0.27966	-1517.40449	-1517.05447	-44.7	-1517.12484	4.2
C-IM2	0.35466	0.28385	-1517.42214	-1517.06748	-78.9	-1517.13829	-31.1
C-i	0.26351	0.20406	-1249.13693	-1248.87342		-1248.93286	
C-i + RCOOH	0.35408	0.26420	-1517.40968	-1517.05560	-47.7	-1517.14548	-50.0
C	0.26354	0.20472	-1249.14001	-1248.87647		-1248.93529	
C + RCOOH	0.35412	0.26486	-1517.41276	-1517.05865	-55.7	-1517.14791	-56.4
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HPPH ₂ + Cd(OA) ₂	0.35009	0.26521	-1508.04811	-1507.69802	0.0	-1507.78290	0.0
C'-IM1	0.35143	0.28474	-1508.05490	-1507.70346	-14.3	-1507.77016	33.4
C'-TS1	0.34809	0.28269	-1508.02614	-1507.67805	52.4	-1507.74345	103.6
C'-IM2	0.35338	0.28580	-1508.04428	-1507.69090	18.7	-1507.75848	64.1
C'	0.26214	0.20651	-1239.76385	-1239.50171		-1239.55734	
C' + RCOOH	0.35272	0.26664	-1508.03660	-1507.68388	37.1	-1507.76996	34.0
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RNH ₂ + Cd(OA) ₂	0.25159	0.18045	-838.25729	-838.00570	0.0	-838.07684	0.0
C''-IM1	0.25398	0.19822	-838.28365	-838.02967	-62.9	-838.08543	-22.6
C''-TS1	0.24905	0.19528	-838.22450	-837.97545	79.4	-838.02922	125.0
C''-IM2	0.25206	0.19646	-838.22681	-837.97474	81.3	-838.03035	122.1
C''	0.16094	0.11845	-569.94980	-569.78886		-569.83135	
C'' + RCOOH	0.25152	0.17858	-838.22256	-837.97104	91.0	-838.04397	86.3

Table S3. 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 + 2SePPh₂H for all the species in the reaction of **C** + SePPh₂H → **E** + RCOOH and **C** + SePPh₂H → **F** + HPPh₂ 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)						
	<i>ZPE</i>	G_0	<i>PCM-E</i>	E_c (<i>PCM-E</i> + <i>ZPE</i>)	E_r	G_c (<i>PCM-E</i> + G_0)	G_r
SePPh ₂ H	0.19343	0.15007	-814.22030	-814.02687		-814.07023	
Cd(OA) ₂	0.15896	0.11333	-703.16954	-703.01058		-703.05621	
RCOOH	0.09058	0.06013	-268.27275	-268.18218		-268.21262	
HPPh ₂	0.19113	0.15188	-804.87857	-804.68745		-804.72669	
Cd(OA) ₂ + 2SePPh ₂ H	0.54582	0.41346	-2331.61013	-2331.06431	0.0	-2331.19667	0.0
C	0.26354	0.20472	-1249.14001	-1248.87647		-1248.93529	
C+ SePPh ₂ H + RCOOH	0.54754	0.41492	-2331.63306	-2331.08551	-55.7	-2331.21813	-56.4
C/E-IM1	0.45782	0.37499	-2063.38419	-2062.92637		-2063.00920	
C/E-IM1 + RCOOH	0.54840	0.43512	-2331.65694	-2331.10855	-116.1	-2331.22182	-66.0
C/E-TS1	0.45450	0.37231	-2063.37266	-2062.91816		-2063.00035	
C/E-TS1 + RCOOH	0.54508	0.43245	-2331.64541	-2331.10033	-94.6	-2331.21297	-42.8
C/E-IM2	0.45934	0.37537	-2063.39037	-2062.93103		-2063.01500	
C/E-IM2 + RCOOH	0.54992	0.43550	-2331.66312	-2331.11321	-128.4	-2331.22762	-81.3
E	0.36828	0.29778	-1795.11131	-1794.74302		-1794.81353	
E + 2RCOOH	0.54944	0.41804	-2331.65681	-2331.10737	-113.1	-2331.23877	-110.5
C-i	0.26351	0.20406	-1249.13693	-1248.87342		-1248.93286	
C-i + SePPh ₂ H + RCOOH	0.54751	0.41427	-2331.62998	-2331.08247	-47.7	-2331.21571	-50.0
C-i/F-IM1	0.45769	0.37420	-2063.38652	-2062.92883		-2063.01232	
C-i/F-IM1 + RCOOH	0.54827	0.43434	-2331.65927	-2331.11101	-122.6	-2331.22494	-74.2
C-i/E-ii-TS1	0.45436	0.37132	-2063.36930	-2062.91494		-2062.99798	
C-i/E-ii-TS1 + RCOOH	0.54494	0.43145	-2331.64205	-2331.09711	-86.1	-2331.21060	-36.6
C-i/E-ii-IM2	0.45923	0.37436	-2063.38619	-2062.92696		-2063.01183	
C-i/E-ii-IM2 + RCOOH	0.54980	0.43449	-2331.65894	-2331.10914	-117.7	-2331.22445	-72.9
E-ii	0.36805	0.29508	-1795.10307	-1794.73502		-1794.80799	
E-ii + 2RCOOH	0.54921	0.41535	-2331.64858	-2331.09937	-92.1	-2331.23323	-96.0
C-i/F-TS1	0.45718	0.37749	-2063.37433	-2062.91715		-2062.99684	
C-i/F-TS1 + RCOOH	0.54776	0.43763	-2331.64708	-2331.09932	-91.9	-2331.20946	-33.6
C-i/F-IM2	0.45770	0.37544	-2063.39623	-2062.93853		-2063.02079	
C-i/F-IM2 + RCOOH	0.54828	0.43558	-2331.66898	-2331.12071	-148.1	-2331.23341	-96.4
F	0.26560	0.20565	-1258.51366	-1258.24806		-1258.30802	
F+ HPPh ₂ + RCOOH	0.54731	0.41766	-2331.66499	-2331.11768	-140.1	-2331.24733	-133.0

Table S4. 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 + SePPh₂H + HPPh₂ for all the species in the reaction of Cd(OA)₂ + SePPh₂H + HPPh₂ → G + 2RCOOH (C + HPPh₂ → G + RCOOH, E + HPPh₂ → G + SePPh₂H, and F + 2HPPh₂ → G + RCOOH + SePPh₂H) 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)						
	<i>ZPE</i>	G_0	<i>PCM-E</i>	E_c (<i>PCM-E</i> + <i>ZPE</i>)	E_r	G_c (<i>PCM-E</i> + G_0)	G_r
Cd(OA) ₂	0.15896	0.11333	-703.16954	-703.01058		-703.05621	
SePPh ₂ H	0.19343	0.15007	-814.22030	-814.02687		-814.07023	
HPPh ₂	0.19113	0.15188	-804.87857	-804.68745		-804.72669	
RCOOH	0.09058	0.06013	-268.27275	-268.18218		-268.21262	
Cd(OA) ₂ + SePPh ₂ H + HPPh ₂	0.54352	0.41528	-2322.26841	-2321.72489	0.0	-2321.85313	0.0
C	0.26354	0.20472	-1249.14001	-1248.87647		-1248.93529	
C + HPPh ₂ + RCOOH	0.54524	0.41674	-2322.29133	-2321.74609	-55.7	-2321.87459	-56.4
C/G-IM1	0.45605	0.37700	-2054.02594	-2053.56989		-2053.64894	
C/G-IM1 + RCOOH	0.54663	0.43713	-2322.29869	-2321.75207	-71.3	-2321.86156	-22.1
C/G-TS1	0.45276	0.37436	-2053.99356	-2053.54080		-2053.61920	
C/G-TS1 + RCOOH	0.54334	0.43449	-2322.26631	-2321.72298	5.0	-2321.83182	55.9
C/G-IM2	0.45813	0.37985	-2054.01660	-2053.55847		-2053.63675	
C/G-IM2 + RCOOH	0.54871	0.43999	-2322.28935	-2321.74065	-41.4	-2321.84937	9.9
G	0.36683	0.29875	-1785.73426	-1785.36743		-1785.43551	
G + 2RCOOH	0.54798	0.41901	-2322.27976	-2321.73178	-18.1	-2321.86075	-20.0
E	0.36828	0.29778	-1795.11131	-1794.74302		-1794.81353	
E+ HPPh ₂ + 2RCOOH - SePPh ₂ H	0.54713	0.41986	-2322.31508	-2321.76795	-113.1	-2321.89523	-110.5
E/G-IM1	0.56051	0.46812	-2599.99251	-2599.43200		-2599.52439	
E/G-IM1 + 2RCOOH - SePPh ₂ H	0.54823	0.43832	-2322.31772	-2321.76948	-117.1	-2321.87940	-69.0
E/G-TS1	0.55691	0.46766	-2599.95623	-2599.39933		-2599.48857	
E/G-TS1 + 2RCOOH - SePPh ₂ H	0.54463	0.43786	-2322.28144	-2321.73681	-31.3	-2321.84358	25.1
E/G-IM2	0.56092	0.46950	-2599.97183	-2599.41091		-2599.50233	
E/G-IM2 + 2RCOOH - SePPh ₂ H	0.54864	0.43970	-2322.29704	-2321.74840	-61.7	-2321.85734	-11.1
F	0.26560	0.20565	-1258.51366	-1258.24806		-1258.30802	
F+2HPPh ₂ + RCOOH - SePPh ₂ H	0.54500	0.41948	-2322.32326	-2321.77826	-140.1	-2321.90379	-133.0
C-i/F-IM2	0.45770	0.37544	-2063.39623	-2062.93853		-2063.02079	
C-i/F-IM2 + HPPh ₂ + RCOOH - SePPh ₂ H	0.54598	0.43739	-2322.32726	-2321.78128	-148.1	-2321.88986	-96.4
F/E-i-TS1a	0.45443	0.37083	-2063.37019	-2062.91576		-2062.99935	
F/E-i-TS1a + HPPh ₂ + RCOOH - SePPh ₂ H	0.54270	0.43278	-2322.30121	-2321.75851	-88.3	-2321.86843	-40.2
F/E-i-IM2a	0.45992	0.37795	-2063.38554	-2062.92562		-2063.00759	

F/E-i-IM2a + HPPh ₂ + RCOOH - SePPh ₂ H	0.54819	0.43989	-2322.31657	-2321.76838	-114.2	-2321.87667	-61.8
F/E-i-TS1b	0.45428	0.37386	-2063.34714	-2062.89286		-2062.97329	
F/E-i-TS1b + HPPh ₂ + RCOOH - SePPh ₂ H	0.54255	0.43581	-2322.27817	-2321.73562	-28.2	-2321.84236	28.3
F/E-i-IM2b	0.45992	0.37639	-2063.37689	-2062.91697		-2063.00050	
F/E-i-IM2b + HPPh ₂ + RCOOH - SePPh ₂ H	0.54819	0.43834	-2322.30792	-2321.75973	-91.5	-2321.86957	-43.2
E-i	0.36870	0.29776	-1795.10594	-1794.73724		-1794.80818	
E-i + HPPh ₂ + 2RCOOH - SePPh ₂ H	0.54755	0.41985	-2322.30972	-2321.76217	-97.9	-2321.88987	-96.5
E-i/G-IM1	0.56055	0.47270	-2599.98984	-2599.42929		-2599.51714	
E-i/G-IM1 + 2RCOOH - SePPh ₂ H	0.54828	0.44289	-2322.31505	-2321.76677	-110.0	-2321.87215	-49.9
E-i/G-TS1	0.56018	0.47263	-2599.96850	-2599.40832		-2599.49587	
E-i/G-TS1 + 2RCOOH - SePPh ₂ H	0.54790	0.44283	-2322.29371	-2321.74581	-54.9	-2321.85088	5.9
E-i/G-IM2	0.56070	0.46717	-2599.97225	-2599.41155		-2599.50508	
E-i/G-IM2 + 2RCOOH - SePPh ₂ H	0.54843	0.43737	-2322.29746	-2321.74903	-63.4	-2321.86009	-18.3
G-i	0.36681	0.29785	-1785.72993	-1785.36312		-1785.43207	
G-i+2RCOOH	0.54796	0.41812	-2322.27543	-2321.72747	-6.8	-2321.85731	-11.0

Table S5. 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 + SePPh₂H + RNH₂ for all the species in the reaction of Cd(OA)₂ + SePPh₂H + RNH₂ → **H** + 2RCOOH ((13) **C** + RNH₂ → **H** + RCOOH , (14) **E** + RNH₂ → **H** + SePPh₂H, (15) **F** + RNH₂ + HPPh₂ → **H** + RCOOH + SePPh₂H, and (16) **G** + RNH₂ → **H** + HPPh₂) 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)						
	<i>ZPE</i>	G_0	<i>PCM-E</i>	E_c (<i>PCM-E</i> + <i>ZPE</i>)	E_r	G_c (<i>PCM-E</i> + G_0)	G_r
Cd(OA) ₂	0.15896	0.11333	-703.16954	-703.01058		-703.05621	
SePPh ₂ H	0.19343	0.15007	-814.22030	-814.02687		-814.07023	
HPPh ₂	0.19113	0.15188	-804.87857	-804.68745		-804.72669	
RNH ₂	0.09263	0.06713	-135.08775	-134.99512		-135.02062	
RCOOH	0.09058	0.06013	-268.27275	-268.18218		-268.21262	
Cd(OA) ₂ + SePPh ₂ H + RNH ₂	0.44502	0.33052	-1652.47759	-1652.03257	0.0	-1652.14707	0.0
C	0.26354	0.20472	-1249.14001	-1248.87647		-1248.93529	
C+RNH ₂ + RCOOH	0.44675	0.33198	-1652.50051	-1652.05377	-55.7	-1652.16853	-56.4
C/H-IM1	0.35888	0.29239	-1384.25580	-1383.89692		-1383.96341	
C/H-IM1 + RCOOH	0.44945	0.35252	-1652.52855	-1652.07910	-122.2	-1652.17603	-76.0
C/H-TS1	0.35333	0.28647	-1384.19907	-1383.84574		-1383.91261	
C/H-TS1 + RCOOH	0.44391	0.34660	-1652.47182	-1652.02792	12.2	-1652.12522	57.4
C/H-IM2	0.35697	0.28850	-1384.20501	-1383.84804		-1383.91652	
C/H-IM2 + RCOOH	0.44755	0.34863	-1652.47776	-1652.03021	6.2	-1652.12914	47.1
H	0.26554	0.21028	-1115.92032	-1115.65477		-1115.71003	
H + 2RCOOH	0.44670	0.33055	-1652.46582	-1652.01912	35.3	-1652.13527	31.0
E	0.36828	0.29778	-1795.11131	-1794.74302		-1794.81353	
E + RNH ₂ + 2RCOOH - SePPh ₂ H	0.44864	0.33510	-1652.52426	-1652.07563	-113.0	-1652.18916	-110.5
E/H-IM1	0.46326	0.38211	-1930.21644	-1929.75317		-1929.83433	
E/H-IM1 + 2RCOOH- SePPh ₂ H	0.45099	0.35231	-1652.54164	-1652.09066	-152.5	-1652.18933	-111.0
E/H-TS1	0.45824	0.38343	-1930.16117	-1929.70293		-1929.77775	
E/H-TS1 + 2RCOOH- SePPh ₂ H	0.44597	0.35363	-1652.48638	-1652.04042	-20.6	-1652.13276	37.6
E/H-IM2	0.45998	0.38144	-1930.16123	-1929.70124		-1929.77979	
E/H-IM2 + 2RCOOH - SePPh ₂ H	0.44771	0.35164	-1652.48643	-1652.03873	-16.2	-1652.13480	32.2
F	0.26560	0.20565	-1258.51366	-1258.24806		-1258.30802	
F+RNH ₂ + HPPh ₂ + RCOOH - SePPh ₂ H	0.44651	0.33472	-1652.53244	-1652.08594	-140.1	-1652.19772	-133.0
F/I-i-IM1	0.36052	0.28819	-1393.62385	-1393.26333		-1393.33566	
F/I-i-IM1+ HPPh ₂ + RCOOH - SePPh ₂ H	0.44879	0.35014	-1652.55487	-1652.10608	-193.0	-1652.20473	-151.4
F/I-i-TS1	0.35625	0.28939	-1393.57228	-1393.21603		-1393.28288	

F/I-i-TS1 + HPPh ₂ + RCOOH - SePPh ₂ H	0.44452	0.35134	-1652.50330	-1652.05878	-68.8	-1652.15196	-12.8
F/I-i-IM2	0.35816	0.28859	-1393.57368	-1393.21552		-1393.28509	
F/I-i-IM2 + HPPh ₂ + RCOOH - SePPh ₂ H	0.44643	0.35054	-1652.50470	-1652.05827	-67.5	-1652.15417	-18.6
I-i	0.26735	0.20908	-1125.29034	-1125.02298		-1125.08126	
I-i+ HPPh ₂ + 2RCOOH - SePPh ₂ H	0.44620	0.33116	-1652.49412	-1652.04791	-40.3	-1652.16295	-41.7
I-i/H-IM1	0.45955	0.38058	-1930.17208	-1929.71253		-1929.79150	
I-i/H-IM1 + 2RCOOH - SePPh ₂ H	0.44727	0.35078	-1652.49729	-1652.05001	-45.8	-1652.14651	1.5
I-i/H-TS1	0.45907	0.38242	-1930.14891	-1929.68984		-1929.76649	
I-i/H-TS1 + 2RCOOH - SePPh ₂ H	0.44680	0.35262	-1652.47412	-1652.02732	13.8	-1652.12150	67.1
I-i/H-IM2	0.45924	0.37728	-1930.15870	-1929.69946		-1929.78142	
I-i/H-IM2 + 2RCOOH - SePPh ₂ H	0.44696	0.34748	-1652.48390	-1652.03694	-11.5	-1652.13643	27.9
H-ii	0.26553	0.20890	-1115.91727	-1115.65173		-1115.70836	
H-ii + 2RCOOH	0.44669	0.32917	-1652.46277	-1652.01608	43.3	-1652.13360	35.4
G	0.36683	0.29875	-1785.73426	-1785.36743		-1785.43551	
G + RNH ₂ + 2RCOOH - HPPh ₂	0.44948	0.33426	-1652.48894	-1652.03946	-18.1	-1652.15469	-20.0
G/H-IM1	0.46200	0.38856	-1920.84108	-1920.37907		-1920.45252	
G/H-IM1 + 2RCOOH - HPPh ₂	0.45203	0.35694	-1652.50801	-1652.05598	-61.5	-1652.15107	-10.5
G/H-TS1	0.45474	0.37634	-1920.76693	-1920.31219		-1920.39058	
G/H-TS1 + 2RCOOH - HPPh ₂	0.44476	0.34473	-1652.43386	-1651.98910	114.1	-1652.08913	152.1
G/H-IM2	0.45770	0.38131	-1920.79895	-1920.34125		-1920.41764	
G/H-IM2 + 2RCOOH - HPPh ₂	0.44772	0.34969	-1652.46588	-1652.01816	37.8	-1652.11619	81.1

Table S6. 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 + 2SePPh₂H + RNH₂ for all the species in the reaction of Cd(OA)₂ + 2SePPh₂H + RNH₂ → **I** + HPPh₂ + 2RCOOH (**H** + SePPh₂H → **I** + HPPh₂, **I-i** → **I**, and **E-i** + RNH₂ → **I** + HPPh₂) 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)						
	<i>ZPE</i>	G_0	<i>PCM-E</i>	E_c (<i>PCM-E</i> + <i>ZPE</i>)	E_r	G_c (<i>PCM-E</i> + G_0)	G_r
Cd(OA) ₂	0.15896	0.11333	-703.16954	-703.01058		-703.05621	
SePPh ₂ H	0.19343	0.15007	-814.22030	-814.02687		-814.07023	
HPPh ₂	0.19113	0.15188	-804.87857	-804.68745		-804.72669	
RNH ₂	0.09263	0.06713	-135.08775	-134.99512		-135.02062	
RCOOH	0.09058	0.06013	-268.27275	-268.18218		-268.21262	
Cd(OA) ₂ + 2SePPh ₂ H + RNH ₂	0.63845	0.48059	-2466.69789	-2466.05943	0.0	-2466.21730	0.0
H	0.26554	0.21028	-1115.92032	-1115.65477		-1115.71003	
H + SePPh ₂ H + 2RCOOH	0.64012	0.48062	-2466.68612	-2466.04599	35.3	-2466.20550	31.0
H/I-IM1	0.45961	0.38025	-1930.16299	-1929.70338		-1929.78275	
H/I-IM1 + 2RCOOH	0.64076	0.50051	-2466.70850	-2466.06774	-21.8	-2466.20798	24.5
H/I-TS1	0.45924	0.37939	-1930.13944	-1929.68019		-1929.76005	
H/I-TS1 + 2RCOOH	0.64040	0.49966	-2466.68494	-2466.04454	39.1	-2466.18528	84.1
H/I-IM2	0.45993	0.38019	-1930.16299	-1929.70306		-1929.78280	
H/I-IM2 + 2RCOOH	0.64108	0.50045	-2466.70849	-2466.06741	-21.0	-2466.20804	24.3
I	0.26729	0.20743	-1125.27927	-1125.01197		-1125.07184	
I+ HPPh₂ + 2RCOOH	0.63957	0.47958	-2466.70334	-2466.06377	-11.4	-2466.22377	-17.0
I-i	0.26735	0.20908	-1125.29034	-1125.02298		-1125.08126	
I-i + HPPh ₂ + 2RCOOH	0.63963	0.48123	-2466.71441	-2466.07478	-40.3	-2466.23318	-41.7
I-i/I-TS1	0.26697	0.21096	-1125.23530	-1124.96833		-1125.02434	
I-i/I-TS1 + HPPh ₂ + 2RCOOH	0.63925	0.48311	-2466.65937	-2466.02013	103.2	-2466.17627	107.7
I-ii	0.26725	0.20530	-1125.27590	-1125.00865		-1125.07060	
I-ii + HPPh ₂ + 2RCOOH	0.63953	0.47745	-2466.69997	-2466.06045	-2.7	-2466.22253	-13.7
E-i	0.26554	0.21028	-1115.92032	-1115.65477		-1115.71003	
E-i + RNH ₂ + 2RCOOH	0.64012	0.48062	-2466.68612	-2466.04599	35.3	-2466.20550	31.0
E-i/I-IM1	0.45961	0.38025	-1930.16299	-1929.70338		-1929.78275	
E-i/I-IM1 + 2RCOOH	0.64076	0.50051	-2466.70850	-2466.06774	-21.8	-2466.20798	24.5
E-i/I-TS1	0.45924	0.37939	-1930.13944	-1929.68019		-1929.76005	
E-i/I-TS1 + 2RCOOH	0.64040	0.49966	-2466.68494	-2466.04454	39.1	-2466.18528	84.1
E-i/I-IM2	0.45993	0.38019	-1930.16299	-1929.70306		-1929.78280	
E-i/I-IM2 + 2RCOOH	0.64108	0.50045	-2466.70849	-2466.06741	-21.0	-2466.20804	24.3

Table S7. Relative Gibbs free energies (G_f , kJ mol⁻¹) for the coordination of RNH₂, SePPh₂H, HPPh₂, and RCOOH ligands towards key intermediates (RCOOCdSe-PPh₂ (**C**), RCOOCdSe₂PPh₂ (**F**), Ph₂PSe-Cd-SePPh₂ (**E**), Ph₂P-CdSe₂PPh₂ (**E-i**), Ph₂P-CdSe-PPh₂ (**G**), RHN-CdSe₂PPh₂(**I-i**), RHN-CdSe-PPh₂ (**H**), and Ph₂PSe-CdSe-NHR (**I**), respectively, relative to the discrete reactants 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).

Key intermediates	Ligands				
	RNH ₂	SePPh ₂ H	HPPh ₂	RCOOH (C=O)	RCOOH (-OH)
C	-19.7	-10.9	34.2	14.0	37.4
F	-18.4	-0.6	36.6	13.0	31.6
E	-0.5	-8.1	41.6	29.3	46.3
E-i	-7.4	-8.4	46.5	34.6	53.3
G	1.5	8.9	33.8	29.9	38.0
I-i	1.1	-8.5	43.2	31.3	23.1
H	3.2	-6.5	50.1	34.5	16.1
I	-3.0	-9.3	30.4	27.2	8.3

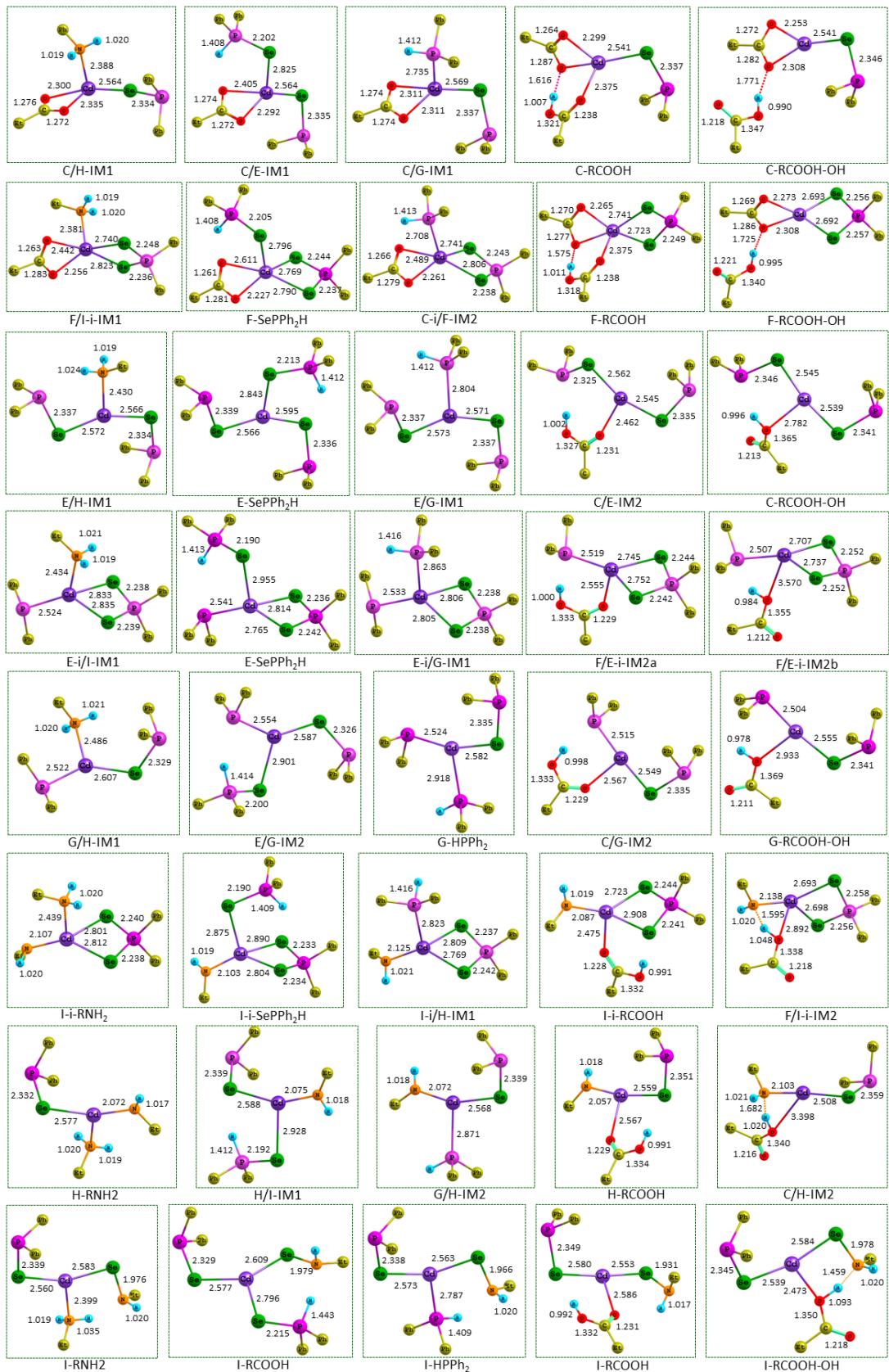
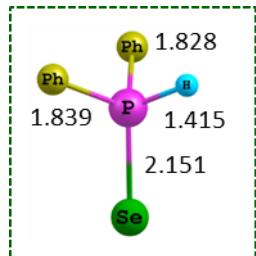


Figure S7. The geometric structures for the coordination of RNH_2 , SePPh_2H , HPPh_2 , and RCOOH toward important intermediates (RCOOCdSe-PPh_2 (**C**), $\text{RCOOCdSe}_2\text{PPh}_2$ (**F**), $\text{Ph}_2\text{PSe-Cd-SePPh}_2$ (**E**), $\text{Ph}_2\text{P-CdSe}_2\text{PPh}_2$ (**E-i**), $\text{Ph}_2\text{P-CdSe-PPh}_2$ (**G**), $\text{RHN-CdSe}_2\text{PPh}_2$ (**I-i**), RHN-CdSe-PPh_2 (**H**), and $\text{Ph}_2\text{PSe-CdSe-NHR}$ (**I**) 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).

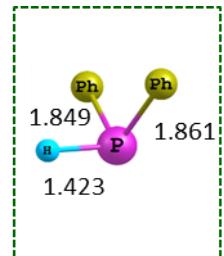
Table S8. Snapshot and standard orientation of all the species in the gas phase calculated at the B3LYP/6-31++G(d, p), SDD level. Distance lengths are reported in Å.

SePPh₂



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

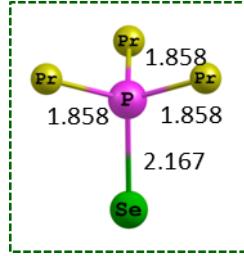
HPPh₂



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

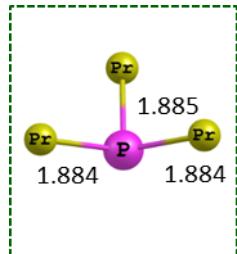
SePR₃



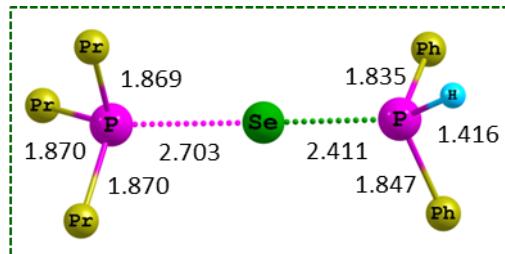
P	-0.47322800	0.00031000	0.00129200
Se	-2.63993800	-0.00271600	0.00281300
C	0.18877700	-0.73179800	1.57562300
C	0.18679400	-0.99575100	-1.42181700
C	0.18251100	1.73204800	-0.15502000
H	-0.53193400	-1.81697900	-1.52152700
H	0.04731400	-0.36733700	-2.31070900
H	-0.53207600	2.22247900	-0.82561100
H	0.03408200	2.19431300	0.82919900
H	0.05135600	-1.81619700	1.47677100
H	-0.52926300	-0.40811500	2.33734500
C	1.61719500	-1.56009400	-1.36774000
C	1.61974800	-0.39995000	2.03227700

C	1.61658200	1.96508300	-0.66058500	H	2.02929700	0.98244100	-0.73204600
H	1.72987600	1.52751000	-1.65953900	C	3.45580600	-0.61431200	-0.99781300
H	2.34306100	1.46178100	-0.01387800	H	3.50909600	-1.70821600	-0.94526900
H	2.34958600	-0.75556700	-1.24251800	H	3.73279400	-0.31537700	-2.01506800
H	1.72100000	-2.21686000	-0.49581500	H	4.21336400	-0.21341000	-0.31400600
H	2.34809400	-0.68850000	1.26702800	C	-2.26706300	-2.67894500	-0.98975000
H	1.72024900	0.68347800	2.16774500	H	-2.30248700	-3.53261800	-0.30260600
C	1.96647700	-1.10381400	3.35212900	H	-3.23811000	-2.17235600	-0.93736100
H	1.91316300	-2.19341200	3.24609300	H	-2.15086900	-3.07284100	-2.00574200
H	2.97998600	-0.84832500	3.67963400	C	-1.20026200	3.29289000	-0.99513100
H	1.27298700	-0.81343000	4.14946400	H	-1.91960500	3.75065100	-0.30578400
C	1.95476800	-2.35694100	-2.63627800	H	-0.27876400	3.88557000	-0.95214100
H	1.25786000	-3.19090800	-2.77667500	H	-1.60676200	3.38132600	-2.00892000
H	1.89898800	-1.72350500	-3.52902500				
H	2.96730200	-2.77130300	-2.58256600				
C	1.95120500	3.46222400	-0.72983500				
H	1.25782300	3.99150400	-1.39313200				
H	1.88626400	3.92943600	0.25952900				
H	2.96624800	3.62156700	-1.10936900				

PR₃



TS1-1

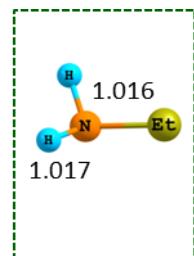


P	0.00421700	0.00063200	1.56483200
C	1.65357900	-0.49824400	0.80334600
C	-1.25538600	-1.17692200	0.80483200
C	-0.38891700	1.67958800	0.80446600
H	-1.28902500	-2.02805100	1.49828600
H	-2.22612100	-0.67455200	0.92484000
H	-1.10631000	2.13590100	1.49983500
H	0.53151300	2.27044500	0.91713000
H	1.70835800	-1.58985600	0.92378400
H	2.40752700	-0.09851400	1.49487300
C	-1.12211900	-1.72179400	-0.62735800
C	2.05291900	-0.10942600	-0.63026800
C	-0.93446700	1.82641100	-0.62513400
H	-1.86927800	1.26040700	-0.71857000
H	-0.23602600	1.39084200	-1.34682000
H	-1.09634300	-0.90029000	-1.35067800
H	-0.16825500	-2.25376900	-0.72868900
H	1.32820500	-0.50269900	-1.35066400

P	-2.64892700	-0.00880500	-0.06076600
Se	0.02453500	-0.00381900	-0.45976100
C	-3.12343100	-0.75878300	1.58469900
C	-3.39435700	1.70552500	-0.10777100
C	-3.51480500	-1.01240800	-1.37866800
H	-2.62950900	2.34631300	0.34957800
H	-3.40936000	1.98769300	-1.16946100
H	-2.91986300	-0.83919100	-2.28445900
H	-3.33184300	-2.06175700	-1.10975300
H	-2.91139800	0.01813300	2.33190800
H	-2.36839700	-1.53700200	1.75447500
C	-4.75625900	2.00187600	0.54357100
C	-4.52399700	-1.35294700	1.81521900
C	-5.00338700	-0.79508400	-1.70127400
H	-5.16599500	0.24992500	-1.99192800
H	-5.61886800	-0.96899200	-0.81202900
H	-5.53751700	1.37431200	0.10166000
H	-4.71609100	1.74309200	1.60868200
H	-5.29423500	-0.58930100	1.66189400
H	-4.71437700	-2.13952000	1.07484200
C	-4.67012500	-1.94619100	3.22430700
H	-4.52088900	-1.17975100	3.99402700
H	-5.66613900	-2.37861400	3.37183200
H	-3.93214700	-2.73796600	3.39840100

C	-5.15010100	3.47947700	0.40177700
H	-4.40103100	4.13431400	0.86226700
H	-5.23688200	3.76658100	-0.65282800
H	-6.11317700	3.68189100	0.88369900
C	-5.48294700	-1.71075600	-2.83720900
H	-4.90621200	-1.53968300	-3.75370100
H	-5.37022800	-2.76761400	-2.56793400
H	-6.53958900	-1.53584300	-3.06906900
P	2.40170800	-0.01444500	-0.85977800
H	2.78506600	-0.08732200	-2.22144200
C	3.37376400	-1.43013200	-0.21444900
C	3.95184400	-2.37075800	-1.08105200
C	3.47804100	-1.62527500	1.17309600
C	4.63267700	-3.48020300	-0.57004600
H	3.87254900	-2.24032100	-2.15724600
C	4.16660900	-2.72727000	1.68099700
H	3.01708700	-0.91576600	1.85507300
C	4.74440300	-3.65890500	0.81093000
H	5.07628100	-4.20074000	-1.25164600
H	4.24644900	-2.86352100	2.75590600
H	5.27576400	-4.51908500	1.20819100
C	3.33124900	1.48311700	-0.30845500
C	2.62699900	2.53218600	0.29682100
C	4.71930200	1.60083500	-0.49328200
C	3.30130200	3.68515100	0.71336600
H	1.55311700	2.43734400	0.43567900
C	5.38939200	2.75360700	-0.08012000
H	5.27899300	0.79022600	-0.95232500
C	4.68042400	3.79806000	0.52488000
H	2.74686800	4.49302800	1.18289900
H	6.46258800	2.83674100	-0.22834800
H	5.20348100	4.69423600	0.84716900

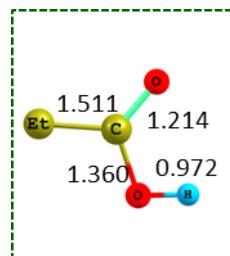
RNH₂



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

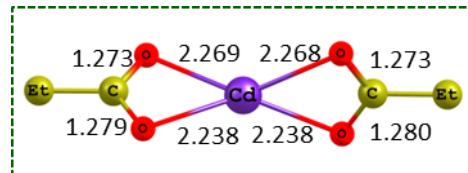
H	-0.06279100	1.12854900	1.00344400
H	-0.07431000	1.30043100	-0.75376000
N	-1.21041600	-0.31956000	-0.11451800
H	-1.26382800	-0.99793800	0.64179300
H	-2.07843800	0.20899100	-0.10711300

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

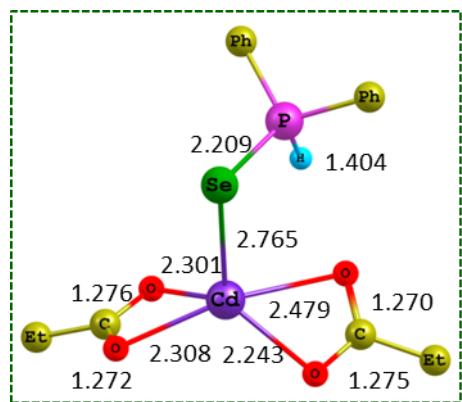
Cd(OA)₂



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

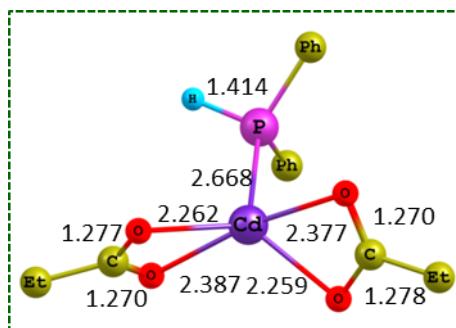
(SePPh₂H)Cd(OA)₂



Cd	1.95606200	0.31923700	0.17437000
O	0.58799400	1.91916100	-1.13562200
O	2.37110200	2.51999300	0.04859400
C	1.40252600	2.80488500	-0.73080600
C	1.20300300	4.24875000	-1.17166800
H	0.94778100	4.22924700	-2.23714900
H	0.30155000	4.60662800	-0.65500500
C	2.38271800	5.18257300	-0.89537300
H	2.14763100	6.20104300	-1.22330900
H	2.62361100	5.20668600	0.17051500
H	3.27996300	4.85147900	-1.42689600
O	3.74476000	-1.03263200	0.72369100
O	2.74689200	-1.31386800	-1.23982000
C	3.64387500	-1.63511700	-0.39177500
C	4.59669000	-2.76765500	-0.74180400
H	5.02792000	-2.52768700	-1.72113300
H	3.97664400	-3.65790900	-0.90764300
C	5.68772300	-3.04183900	0.29392900
H	5.25460000	-3.29681000	1.26525700
H	6.32192900	-3.87384900	-0.03155500
H	6.32233600	-2.16306300	0.44078300
P	-1.61274500	-0.33738900	-0.04055500
C	-2.46693200	-1.89113800	-0.48347000
C	-2.12695400	-3.10264600	0.13079900
C	-3.45155900	-1.86478900	-1.48687300
C	-2.77119300	-4.28227500	-0.25345700
H	-1.36200300	-3.11985100	0.90091200

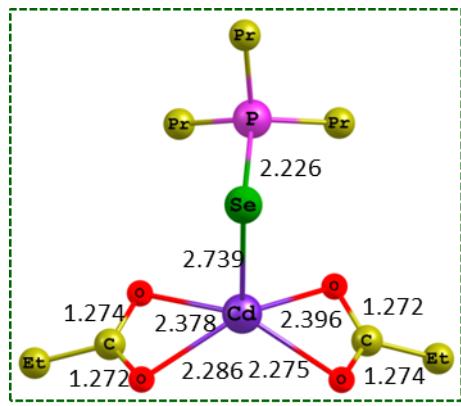
C	-4.08564900	-3.04679300	-1.86951900
H	-3.72647200	-0.92902900	-1.96556600
C	-3.74697200	-4.25610400	-1.25199500
H	-2.50516900	-5.21906600	0.22688200
H	-4.84332800	-3.02342300	-2.64709900
H	-4.24353400	-5.17466500	-1.55094200
C	-2.87949200	0.94701500	0.17150600
C	-2.67511200	2.20343600	-0.42097200
C	-4.02319200	0.70720500	0.94946800
C	-3.62888400	3.20948100	-0.24444500
H	-1.77142100	2.38981000	-0.99606000
C	-4.96681100	1.71997700	1.12216900
H	-4.18074800	-0.26281900	1.41239900
C	-4.77107500	2.96998900	0.52423500
H	-3.47613800	4.18041700	-0.70635100
H	-5.85284600	1.53437400	1.72194600
H	-5.50843700	3.75592300	0.65995800
Se	-0.20732900	-0.57131600	1.64779700
H	-0.92674500	0.08381400	-1.19091500

(HPPh₂)Cd(OA)₂



Cd	-1.31352000	0.45896400	0.09524500
O	-0.42746200	2.65756500	0.27417000
O	-1.33286900	1.63636500	2.02350200
C	-0.77185000	2.65602500	1.49651300
C	-0.53617800	3.87357400	2.37577900
H	-1.52251500	4.18917500	2.73831700
H	0.00155200	3.52628200	3.26621200
C	0.19555500	5.03333200	1.69927200
H	0.30095700	5.87365300	2.39391700
H	1.19619400	4.73436700	1.37235000
H	-0.34766300	5.38107200	0.81620900
O	-3.09028800	0.05043200	-1.24456000
O	-2.53000400	-1.59437900	0.13823300
C	-3.28040000	-1.12067600	-0.77091700
C	-4.43313100	-1.96694600	-1.28865100
H	-5.10842600	-2.11950200	-0.43678100
H	-4.02558500	-2.95898400	-1.51685300

C	-5.18695800	-1.38343400	-2.48454000		H	3.93741500	0.26561100	-1.76441500
H	-4.52541100	-1.25660700	-3.34683200		H	1.96323900	2.16168000	-0.68650900
H	-6.00798800	-2.04682300	-2.77752800		H	1.15281800	1.71493000	0.79500600
H	-5.60390500	-0.40130300	-2.24599800		H	2.05142900	-2.34243600	0.60767300
P	0.86906600	-0.86947200	-0.67379100		H	0.58300300	-1.47940000	1.01647600
H	0.57888500	-1.79677400	-1.70050100		C	4.79863100	-1.03242400	-0.22986100
C	1.48106700	-1.98750900	0.65425200		C	2.21388300	-1.06994000	2.38080900
C	0.54733700	-2.84998800	1.25646200		C	3.31366500	2.04036300	1.01009900
C	2.80625500	-1.96902100	1.11043400		H	4.21600200	1.92930000	0.39680900
C	0.95099700	-3.70000800	2.28767300		H	3.46315000	1.43048800	1.90662800
H	-0.49103300	-2.84926300	0.93214800		H	5.02299900	-0.24310200	0.49482600
C	3.19897500	-2.81686800	2.15107500		H	4.49476500	-1.91192500	0.34932300
H	3.53200300	-1.29873600	0.66085400		H	3.30509600	-0.96705500	2.37106400
C	2.27558900	-3.68551500	2.73714200		H	1.80400900	-0.11367700	2.72486600
H	0.22558100	-4.36554300	2.74643900		C	1.81002900	-2.17232700	3.37026600
H	4.22731400	-2.79554800	2.50053800		H	2.23387700	-3.14092000	3.08040000
H	2.58346100	-4.34325600	3.54486000		H	2.16760800	-1.93863200	4.37862300
C	2.30128700	0.01903900	-1.38218000		H	0.72129400	-2.27927500	3.40926500
C	2.41964500	1.40262800	-1.16949100		C	6.06721400	-1.36712500	-1.02662300
C	3.26588700	-0.64995000	-2.15756600		H	5.88499900	-2.17851800	-1.74018100
C	3.50272200	2.10078700	-1.71396800		H	6.42245700	-0.49830300	-1.59223100
H	1.66306300	1.93808700	-0.60106900		H	6.87439100	-1.68394800	-0.35818400
C	4.34113100	0.05416900	-2.70083500		C	3.16308300	3.51290100	1.41954900
H	3.17777400	-1.71826800	-2.33647800		H	3.04323500	4.15675500	0.54097000
C	4.46184400	1.43036900	-2.47613100		H	2.28646400	3.65549200	2.06014000
H	3.58624600	3.17088800	-1.54899900		H	4.04534300	3.85653000	1.96983800
H	5.08062800	-0.46855600	-3.30060800		Cd	-1.67914700	0.06618400	-0.40689200
H	5.29816700	1.97753700	-2.90180300		O	-1.08289700	1.93514500	0.96788300

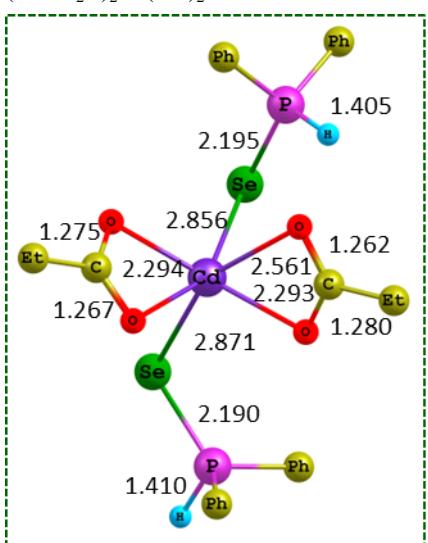
(SePR₃)Cd(OA)₂

P	2.02408700	-0.17732500	-0.38534700
Se	0.50615600	-0.35749900	-2.00294400
C	1.67330600	-1.37836700	0.97247700
C	3.64896700	-0.60338700	-1.16010400
C	2.07822900	1.56275000	0.22506300
H	3.42414800	-1.40948300	-1.86787600

H	3.93741500	0.26561100	-1.76441500
H	1.96323900	2.16168000	-0.68650900
H	1.15281800	1.71493000	0.79500600
H	2.05142900	-2.34243600	0.60767300
H	0.58300300	-1.47940000	1.01647600
C	4.79863100	-1.03242400	-0.22986100
C	2.21388300	-1.06994000	2.38080900
C	3.31366500	2.04036300	1.01009900
H	4.21600200	1.92930000	0.39680900
H	3.46315000	1.43048800	1.90662800
H	5.02299900	-0.24310200	0.49482600
H	4.49476500	-1.91192500	0.34932300
H	3.30509600	-0.96705500	2.37106400
H	1.80400900	-0.11367700	2.72486600
C	1.81002900	-2.17232700	3.37026600
H	2.23387700	-3.14092000	3.08040000
H	2.16760800	-1.93863200	4.37862300
H	0.72129400	-2.27927500	3.40926500
C	6.06721400	-1.36712500	-1.02662300
H	5.88499900	-2.17851800	-1.74018100
H	6.42245700	-0.49830300	-1.59223100
H	6.87439100	-1.68394800	-0.35818400
C	3.16308300	3.51290100	1.41954900
H	3.04323500	4.15675500	0.54097000
H	2.28646400	3.65549200	2.06014000
H	4.04534300	3.85653000	1.96983800
Cd	-1.67914700	0.06618400	-0.40689200
O	-1.08289700	1.93514500	0.96788300
O	-2.71607100	2.08790600	-0.52898600
C	-1.99725100	2.60278600	0.38754100
C	-2.22231400	4.04991600	0.80189300
H	-2.30630700	4.05802700	1.89518600
H	-1.29226800	4.58824100	0.57627900
C	-3.42132000	4.73703000	0.14680400
H	-3.50414800	5.77256800	0.49487700
H	-3.32541900	4.74457900	-0.94245500
H	-4.35356400	4.21827000	0.38830800
O	-3.12175000	-1.70565300	-0.47963200
O	-1.62556300	-1.72008900	1.16134500
C	-2.60189600	-2.25570300	0.54331400
C	-3.15347100	-3.57724000	1.05787500
H	-3.48581500	-3.39666600	2.08810500
H	-2.30347100	-4.26552400	1.14272900
C	-4.27702600	-4.18598600	0.21777500
H	-3.94151400	-4.38854100	-0.80352500
H	-4.61735600	-5.12805000	0.66174000

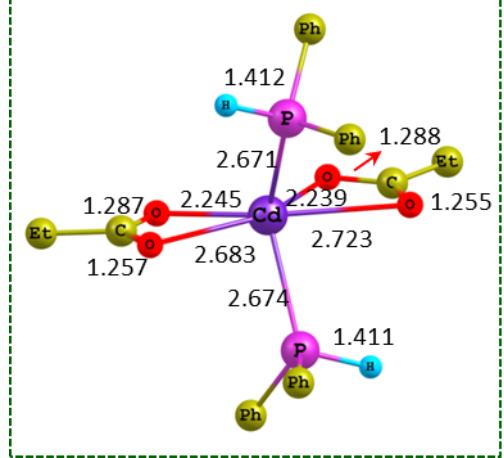
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H	-4.18267000	-2.74591300	0.55085200	H	-6.36608700	-2.50968600	-1.77374500
C	0.66596100	3.46405000	-0.62351700	H	-4.11152300	-3.87475600	1.63251500
H	0.73481600	2.64201700	-1.34365500	H	-5.82078700	-4.28914800	-0.12412800
H	1.66590100	3.63905000	-0.20879100	Se	-1.56846100	1.09785200	-1.29834200
H	0.36958100	4.36488700	-1.16939100	H	-2.64010400	0.72168900	1.46938000
C	-0.34774600	3.16273200	0.47544800	P	3.94244600	0.56872400	-1.21476500
H	-0.42708200	4.01781400	1.16011700	C	3.87368700	2.28994400	-0.62467300
H	-1.33528400	2.98289600	0.04112800	C	4.53764200	3.29060700	-1.35142700
N	0.02719700	1.93196600	1.22510700	C	3.13585700	2.62145200	0.52343300
H	0.96382000	2.02110800	1.61880300	C	4.47437900	4.61996100	-0.92690000
H	-0.60371300	1.79669000	2.01383000	H	5.10175200	3.03925100	-2.24597200

(SePPh₂H)₂Cd(OA)₂



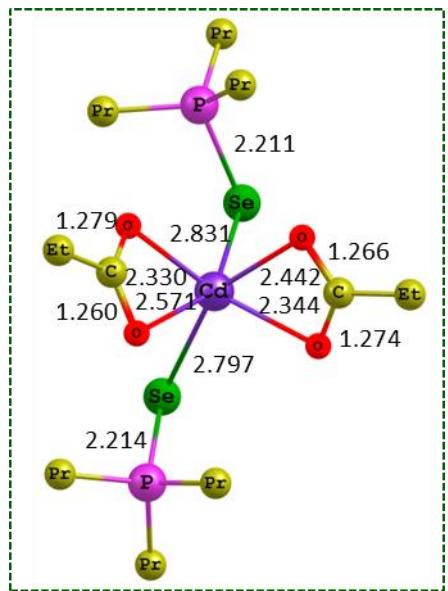
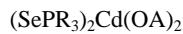
P	-3.16477200	0.74092700	0.16582100	H	7.25245200	-0.41874600	2.31779600
C	-4.44188000	2.05378500	0.15365400	H	6.25975000	-2.62404000	2.90587500
C	-4.29548500	3.19786000	-0.64025200	Se	2.16941800	-0.21270300	-2.23576800
C	-5.56540300	1.92143000	0.98746800	H	4.96467200	0.66016400	-2.18115600
C	-5.26761500	4.20202200	-0.60344000	Cd	0.26389700	-0.77652600	-0.16396900
H	-3.42561100	3.29904900	-1.28223300	O	1.21384800	0.25039200	1.65263300
C	-6.52937900	2.92975200	1.02481000	O	-0.82758200	-0.49066100	2.13485600
H	-5.69359800	1.03233200	1.59867100	C	0.26040700	0.04592700	2.48128900
C	-6.38190300	4.07063600	0.22832600	C	0.49736300	0.46863800	3.92793100
H	-5.15038800	5.08505500	-1.22475800	H	1.36063800	-0.10863500	4.28257800
H	-7.39556300	2.82260200	1.67122700	H	0.83217700	1.51324900	3.91197400
H	-7.13523200	4.85276200	0.25617700	C	-0.69826100	0.28760000	4.86373600
C	-4.03181000	-0.85363400	0.07016900	H	-0.43652700	0.58940300	5.88407000
C	-4.98526600	-1.09089400	-0.93242100	H	-1.55177300	0.89173700	4.53978200
C	-3.70985300	-1.86029000	0.99305700	H	-1.02491400	-0.75591100	4.88580500
C	-5.62814400	-2.32623600	-0.99832400	O	1.16568600	-3.01625000	0.25329800
H	-5.22343500	-0.31730400	-1.65714500	O	-0.72578100	-2.72029700	-0.87446100
C	-4.36183600	-3.09428200	0.92009100	C	0.17189700	-3.47958800	-0.38052400
H	-2.94359100	-1.68861300	1.74379700	C	0.04569500	-4.99081700	-0.54107700

H	-0.07778200	-5.40160200	0.46975700
H	1.01839900	-5.35848400	-0.88873000
C	-1.08423100	-5.45836000	-1.45996100
H	-0.94866900	-5.07710600	-2.47661200
H	-1.11442400	-6.55318700	-1.50515500
H	-2.05372000	-5.09722200	-1.10563900



Cd	-0.00829900	-1.03949700	0.07321900
O	-1.11531000	-0.48205400	-2.35077100
O	-0.81773300	-2.49280700	-1.42639400
C	-1.20871800	-1.73321400	-2.38996000
C	-1.80322400	-2.44295500	-3.60426200
H	-1.05243300	-3.16308300	-3.95279000
H	-2.64027500	-3.05231000	-3.24071500
C	-2.24940300	-1.51971000	-4.73824900
H	-2.66135400	-2.10337300	-5.56919300
H	-3.01714700	-0.81863400	-4.39748700
H	-1.41179900	-0.92628200	-5.11705200
O	1.10373200	-0.35235200	2.41529600
O	0.82672800	-2.42280000	1.63199300
C	1.21815900	-1.59766900	2.53820700
C	1.83108000	-2.21405300	3.79279200
H	2.61650900	-2.90494500	3.46301000
H	1.05745400	-2.85008900	4.24196800
C	2.37117000	-1.20877100	4.81039100
H	1.58407500	-0.52852600	5.14869300
H	2.77801800	-1.72868700	5.68499300
H	3.16732200	-0.59600900	4.37636400
P	-2.11227900	0.31444000	1.00938200
H	-2.03736800	0.57348500	2.39568500
C	-3.73771200	-0.54076800	0.86998900
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C	-4.94536100	0.11113300	1.17177300

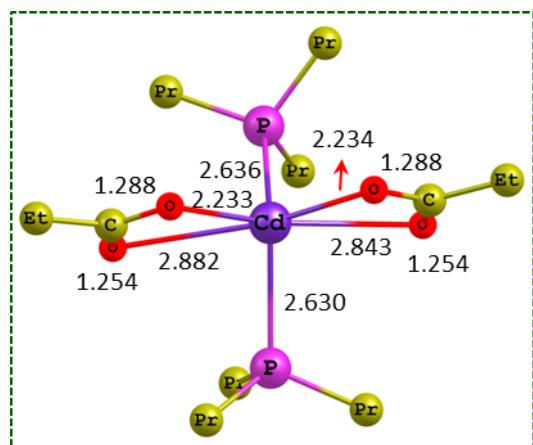
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H	-2.83988300	-2.39903600	0.21009500
C	-6.15601700	-0.57781400	1.08908600
H	-4.94246500	1.15809500	1.46166300
C	-6.17326400	-1.92322100	0.70365500
H	-4.98403700	-3.61597600	0.08844700
H	-7.08479000	-0.06536800	1.32376700
H	-7.11682500	-2.45770500	0.63885200
C	-2.36876200	2.01924400	0.38886300
C	-2.37697500	2.25026700	-0.99838800
C	-2.53366500	3.09884800	1.27206900
C	-2.57189700	3.54466800	-1.48531300
H	-2.21477300	1.42585600	-1.68843900
C	-2.71776100	4.39276400	0.77660900
H	-2.51531500	2.93400600	2.34611400
C	-2.74276600	4.61608600	-0.60264100
H	-2.57972200	3.71594600	-2.55803800
H	-2.84204300	5.22162600	1.46779200
H	-2.88865700	5.62133300	-0.98794000
P	2.06523300	0.26462600	-0.99795700
H	1.92351100	0.47252500	-2.38714200
C	3.68482800	-0.61120300	-0.91411400
C	4.87683200	-0.00590000	-1.34674700
C	3.71718500	-1.92804300	-0.43007600
C	6.07974800	-0.71187300	-1.30506700
H	4.86838600	1.01872900	-1.70757900
C	4.92534000	-2.63262700	-0.39190500
H	2.80974600	-2.40496000	-0.06943100
C	6.10507600	-2.02813700	-0.82967100
H	6.99629600	-0.23563100	-1.64187500
H	4.93890100	-3.65115500	-0.01498900
H	7.04254900	-2.57613200	-0.79738500
C	2.37831600	1.98733400	-0.45637100
C	2.40114800	2.28124800	0.91864500
C	2.57373700	3.01996600	-1.38853600
C	2.64156800	3.58936200	1.34531200
H	2.21501800	1.49519300	1.64636800
C	2.80476900	4.32782600	-0.95350300
H	2.54131900	2.80774500	-2.45391100
C	2.84433000	4.61280100	0.41406200
H	2.66010800	3.80903100	2.40904400
H	2.95259700	5.11990700	-1.68221200
H	3.02567700	5.62914300	0.75237000



Se	1.69094400	-0.66495200	-1.92525900	C	7.33805100	-0.99133600	-2.75375300
Se	-2.16846000	0.49857700	-2.02772600	H	7.01226000	-1.63320000	-3.58017700
Cd	-0.08542600	0.50842200	-0.11089400	H	7.43617700	0.02849700	-3.14302400
O	-0.96949200	-0.96240000	1.46554700	H	8.33229700	-1.32710900	-2.44054500
O	1.17098600	-0.51520700	1.88494600	C	4.98850800	2.75817200	1.48325400
C	0.07391800	-1.04949500	2.20044000	H	4.42647900	3.54894100	0.97549000
C	-0.05404100	-1.85680800	3.49182800	H	4.47613400	2.54111000	2.42686800
H	-1.01139500	-1.58652100	3.95141300	H	5.98516400	3.14647800	1.71996900
H	-0.15493700	-2.91061900	3.19711600	P	-3.77921200	-0.24463000	-0.70761500
C	1.09866200	-1.68325300	4.48210200	C	-3.94441100	0.81452100	0.79665800
H	0.93937300	-2.30237400	5.37224500	C	-5.35817200	-0.14102700	-1.67258700
H	2.05329800	-1.96772700	4.03076800	C	-3.46180900	-2.01053200	-0.26527700
H	1.18773100	-0.64054500	4.80240400	H	-5.27659800	0.78972600	-2.24562000
O	-0.99863700	2.36543900	1.18564600	H	-5.32302500	-0.95658500	-2.40569100
O	0.86824700	2.64565100	0.01248700	H	-3.03535000	-2.43804700	-1.18045900
C	-0.04764700	3.09467900	0.77647600	H	-2.64908800	-1.97546900	0.47024600
C	-0.02142400	4.55758700	1.21035500	H	-4.53890900	1.68048100	0.47734700
H	-0.10917100	4.56929200	2.30359600	H	-2.94047400	1.19809800	1.00623200
H	-0.95070700	5.00785200	0.83835500	C	-6.68490200	-0.15909100	-0.89224400
C	1.19332900	5.36188800	0.74545400	C	-4.53076800	0.17784600	2.06806300
H	1.27584700	5.35475400	-0.34516800	C	-4.62799100	-2.88593500	0.22650500
H	1.11691800	6.40280900	1.08040600	H	-5.41088600	-2.93814100	-0.53960200
H	2.12111600	4.94244600	1.14676300	H	-5.08820500	-2.45155600	1.12008400
P	3.57477000	-0.56389300	-0.76582700	H	-6.77174100	-1.07655400	-0.30102400
C	3.70935700	-2.04414000	0.33085300	H	-6.70274300	0.67335700	-0.17950600
C	4.94173400	-0.59311000	-2.01701900	H	-5.53414500	-0.22381900	1.88263700
C	3.68391200	0.96565800	0.25806800	H	-3.89466700	-0.66096700	2.37065000
H	4.57142600	-1.24731200	-2.81461000	C	-4.59280100	1.20033100	3.21166200
H	4.97045900	0.41686600	-2.44457200	H	-5.24896700	2.04137000	2.95821400
H	3.10946100	1.72615400	-0.28157900	H	-4.97842800	0.73898800	4.12750200

H	-3.59822800	1.60543700	3.42438300
C	-7.89274800	-0.04464000	-1.83265900
H	-7.85339000	0.88104000	-2.41807800
H	-7.92834500	-0.88309800	-2.53776900
H	-8.83043100	-0.04342300	-1.26687100
C	-4.14800300	-4.30902300	0.54749700
H	-3.70654100	-4.78594000	-0.33504800
H	-3.38751600	-4.29922900	1.33586900
H	-4.97955500	-4.93589800	0.88738700

(PR₃)₂Cd(OA)₂

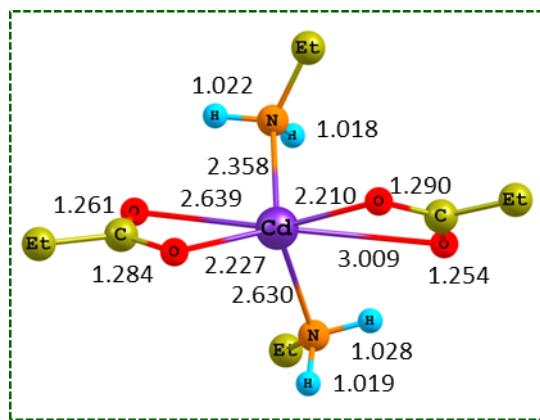


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O	0.43245500	2.73257000	-0.36031300
O	0.27399500	1.78175500	-2.38775400
C	0.43997000	2.79706700	-1.61246800
C	0.65560100	4.13283400	-2.32909300
H	1.52057000	4.00512800	-2.99236100
H	-0.20016900	4.27880800	-3.00018800
C	0.84366600	5.33978600	-1.40953700
H	0.99647000	6.25217200	-1.99737700
H	-0.02988500	5.48782000	-0.76740000
H	1.70803900	5.20583300	-0.75198200
O	-0.41321200	-2.73409200	-0.35918400
O	-0.30254600	-1.80908800	-2.39951300
C	-0.45426800	-2.81533800	-1.61028600
C	-0.69701500	-4.15878400	-2.30249600
H	0.14226100	-4.32187600	-2.99025800
H	-1.57568500	-4.03330900	-2.94784000
C	-0.87411100	-5.35041100	-1.36079700
H	-1.72150500	-5.19844900	-0.68528200
H	-1.04903500	-6.26991000	-1.93108300
H	0.01295800	-5.49702800	-0.73717800
P	2.27022400	-0.21522400	0.22431000
C	2.90087000	-1.96510400	0.28020400
C	3.58626400	0.86185400	-0.53675300

C	2.00663700	0.37553100	1.97043000
H	3.41865200	0.79914900	-1.61926900
H	3.31171400	1.88696500	-0.25758700
H	1.31102800	1.21683300	1.86367900
H	1.44974800	-0.42750400	2.47214600
H	3.33431800	-2.14800800	-0.71304200
H	1.99259500	-2.57864300	0.32337300
C	5.07093000	0.59142600	-0.23957500
C	3.88154900	-2.40611200	1.37977600
C	3.19937800	0.81843500	2.83521600
H	3.72195900	1.64410300	2.33841400
H	3.92526700	0.00513500	2.94027900
H	5.26406500	0.64985100	0.83700600
H	5.32829000	-0.42930300	-0.54739400
H	4.78106100	-1.78126200	1.37118600
H	3.41438900	-2.26735700	2.36229500
C	4.28254600	-3.87994800	1.22167400
H	4.78977400	-4.05166200	0.26502200
H	4.96296300	-4.19247300	2.02145800
H	3.40337600	-4.53338700	1.25312800
C	5.98541500	1.58154200	-0.97543900
H	5.83763200	1.52513300	-2.06010700
H	5.78258200	2.61344500	-0.66636300
H	7.04083000	1.37158100	-0.77014700
C	2.74663400	1.28013500	4.22784800
H	2.04222300	2.11683100	4.15609900
H	2.24812300	0.46920800	4.77204900
H	3.59937100	1.61140400	4.83042500
P	-2.25667900	0.20239500	0.24113400
C	-3.60882800	-0.77772900	-0.58643500
C	-2.04885500	-0.47676200	1.96229800
C	-2.81249200	1.97467400	0.36301500
H	-1.39398700	-1.34645300	1.82836000
H	-1.46080300	0.27481900	2.50649400
H	-1.87795500	2.54571700	0.42482600
H	-3.23632100	2.21168600	-0.62298100
H	-3.39046600	-1.82719000	-0.35063800
H	-3.42024100	-0.67466400	-1.66229600
C	-3.27693600	-0.89265800	2.78996400
C	-5.08217100	-0.44660200	-0.29608200
C	-3.77470600	2.42050900	1.47677300
H	-3.32253900	2.21683400	2.45512800
H	-4.70667100	1.84604300	1.43839000
H	-3.96398500	-0.04889900	2.91291200
H	-3.83017500	-1.67243800	2.25354300
H	-5.29680000	-0.55537800	0.77241500

H	-5.27915200	0.60247200	-0.54753900
C	-6.03528400	-1.34318700	-1.09956300
H	-5.89166100	-2.40035600	-0.84785600
H	-7.08129700	-1.08966900	-0.89530800
H	-5.86809100	-1.23297700	-2.17718500
C	-2.87371800	-1.42735100	4.17168700
H	-2.20518500	-2.29115300	4.08072100
H	-2.35166100	-0.66107200	4.75700400
H	-3.75242000	-1.74310800	4.74461900
C	-4.09599200	3.91896300	1.37860500
H	-3.18400100	4.52298900	1.44352500
H	-4.58489100	4.15743900	0.42674000
H	-4.76615000	4.23309700	2.18643000

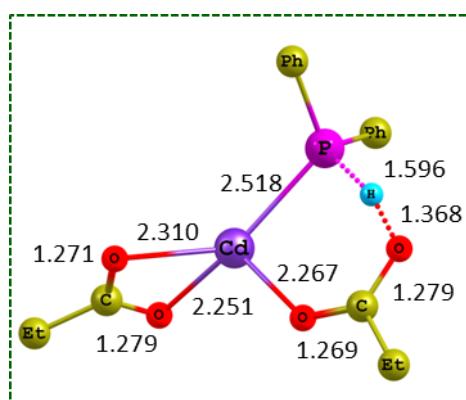
(RNH₂)₂Cd(OA)₂



Cd	-0.04696900	0.12849700	-0.08517700
O	-2.46838400	-0.24527800	0.89423600
O	-1.75818100	-0.83511700	-1.13567400
C	-2.67045700	-0.76789800	-0.23514400
C	-4.05334400	-1.32272600	-0.56030900
H	-4.37401700	-1.91200000	0.30658400
H	-4.73101300	-0.45879100	-0.59010700
C	-4.15436100	-2.13265200	-1.85391900
H	-5.18363800	-2.47382000	-2.01152200
H	-3.85113900	-1.53552300	-2.71817200
H	-3.50445600	-3.01253700	-1.82220900
O	2.65138700	1.45959900	-0.09034900
O	1.91887300	-0.52391500	-0.85619600
C	2.84191000	0.35161300	-0.64558600
C	4.24913100	0.00747100	-1.13738900
H	4.95301400	0.38035000	-0.38523200
H	4.41792600	0.62687200	-2.02911100
C	4.50108000	-1.46647400	-1.46153400
H	3.80149900	-1.82802400	-2.21964300
H	5.52212700	-1.60817700	-1.83341600
H	4.37542100	-2.09559800	-0.57398400

C	0.92547000	-2.71300800	1.94970700
H	1.05456000	-2.61915400	0.86674500
H	-0.08672800	-3.08184300	2.15243100
H	1.63302500	-3.46701900	2.30919800
C	1.18033600	-1.38155600	2.64961400
H	1.13001600	-1.51291500	3.73954200
H	2.18143800	-1.01276100	2.40695200
N	0.21077900	-0.34698000	2.20949500
H	-0.75251900	-0.61886700	2.41391600
H	0.38280000	0.52375300	2.70871800
C	-2.23466700	3.28577900	0.37036700
H	-2.58114800	2.27685600	0.61487800
H	-2.56889400	3.53137000	-0.64522300
H	-2.71308200	3.99427800	1.05469100
C	-0.71619200	3.38794600	0.48445300
H	-0.38729300	4.41688500	0.28300000
H	-0.39508000	3.14532600	1.50327900
N	-0.03133000	2.44321700	-0.43116300
H	-0.27892900	2.65749100	-1.39623000
H	0.99145900	2.50899900	-0.35264300

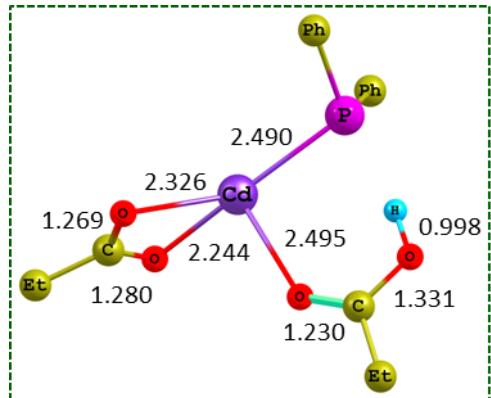
C-TS1



P	1.26554900	0.16792500	-0.29221400
C	2.43255500	0.65730600	1.03272200
C	2.80694500	2.00702600	1.14802700
C	2.93714900	-0.27447800	1.95655200
C	3.66513000	2.41601900	2.17332100
H	2.43356900	2.73624400	0.43440100
C	3.80331500	0.13613500	2.97079400
H	2.65712900	-1.32154800	1.88053500
C	4.16626100	1.48289800	3.08412100
H	3.94701200	3.46213600	2.25215100
H	4.18971200	-0.59390300	3.67641500
H	4.83685700	1.80091300	3.87718100
C	1.97223200	-1.29179500	-1.14600400
C	3.32594300	-1.30350800	-1.52893300

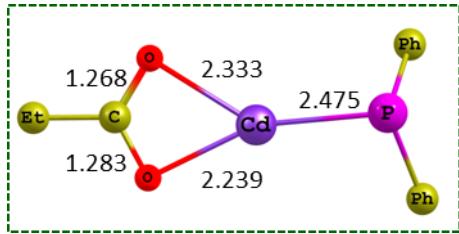
C	1.15860900	-2.38453300	-1.48704600	C	2.99067300	0.03655000	1.73283300
C	3.85052900	-2.38723500	-2.23417000	C	3.34108300	2.75266900	2.28424200
H	3.96970000	-0.46663100	-1.27382900	H	2.12931400	3.10659600	0.53995500
C	1.68491000	-3.46319500	-2.20425000	C	3.76859400	0.43566600	2.82056500
H	0.11340700	-2.40364000	-1.18943800	H	2.85925900	-1.02218300	1.52848000
C	3.03091200	-3.46845500	-2.57662300	C	3.94284600	1.79535100	3.10379700
H	4.89827200	-2.38469500	-2.52118000	H	3.47681400	3.81097800	2.48960400
H	1.04258300	-4.30063200	-2.46094900	H	4.23346700	-0.31599100	3.45284800
H	3.44094600	-4.30977200	-3.12780800	H	4.54518900	2.10317600	3.95370700
Cd	-1.16856300	0.00857100	0.33271800	C	2.14029900	-0.93230400	-1.29093800
H	0.91509700	1.43600000	-1.19594500	C	3.51926600	-0.88479800	-1.57358100
C	-1.62928300	3.82170900	-2.25718600	C	1.41831700	-2.06670700	-1.70087400
H	-1.09818100	4.72173500	-1.92212000	C	4.15303600	-1.94092100	-2.23026300
H	-1.39682400	3.73069700	-3.32542300	H	4.10207100	-0.01742400	-1.27628900
O	0.29306100	2.50708400	-1.77785600	C	2.05063100	-3.11757300	-2.37244700
C	-0.96045200	2.63985300	-1.56377700	H	0.35449200	-2.14606800	-1.49050700
O	-1.67338000	1.88525700	-0.83423400	C	3.42101500	-3.06164700	-2.63630500
C	-3.13483200	3.95183500	-2.02628800	H	5.21969400	-1.88454800	-2.43015400
H	-3.36512600	4.06723600	-0.96337500	H	1.46991800	-3.98444600	-2.67540900
H	-3.52521600	4.82505400	-2.55995200	H	3.91438700	-3.88211800	-3.14931200
H	-3.66847300	3.06579700	-2.38207500	Cd	-0.85341500	-0.21283300	0.39748600
O	-2.82297500	-1.58746600	0.10188100	H	0.06134900	2.10110800	-1.65277700
O	-2.69281000	-0.36355600	1.94614500	C	-2.87537400	3.40550400	-2.18442500
C	-3.26491100	-1.27229800	1.25103100	H	-2.55125600	4.42864100	-1.95532000
C	-4.49169900	-1.95399500	1.82939900	H	-2.80042500	3.31604100	-3.27552700
H	-5.25023200	-1.17038500	1.95308000	O	-0.61435700	2.72196500	-2.04550100
H	-4.23231900	-2.26947900	2.84686000	C	-1.84154800	2.47306300	-1.59374400
C	-5.03696800	-3.11913400	1.00288200	O	-2.11315800	1.58640100	-0.78504500
H	-4.29296400	-3.91479600	0.90044500	C	-4.29964700	3.14564300	-1.69621000
H	-5.92577200	-3.54149700	1.48363100	H	-4.37298200	3.25631600	-0.61082900
H	-5.31063200	-2.79458400	-0.00478000	H	-4.99005700	3.85504600	-2.16238400
				H	-4.62547900	2.13252800	-1.94744800
				O	-2.44477400	-1.90106200	0.23357700
				O	-2.34754800	-0.60083700	2.02661200
				C	-2.88647600	-1.56138200	1.37394900
				C	-4.07488500	-2.27231600	1.99621600
				H	-4.87636200	-1.52590000	2.07123400
				H	-3.80098500	-2.50932800	3.03084800
				C	-4.55292400	-3.51452700	1.24332700
				H	-3.76553200	-4.27231400	1.19010700
				H	-5.41855100	-3.95516000	1.74939700
				H	-4.84022500	-3.26817400	0.21746600

C'-IM2



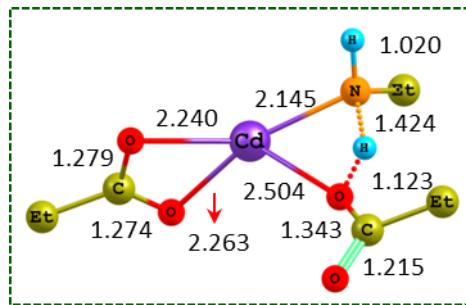
P	1.31951300	0.54814600	-0.55178500
C	2.37937800	0.99064400	0.89881000
C	2.57335600	2.35296600	1.18548800

C'



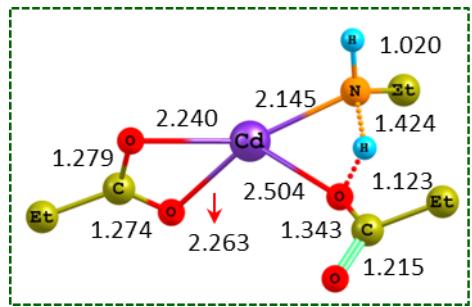
P	-1.17887600	0.10705000	-1.21886700
C	-2.22908100	-1.13309200	-0.31941300
C	-3.19881000	-1.80823200	-1.08130100
C	-2.11368100	-1.45688400	1.04592800
C	-4.02674000	-2.77554200	-0.50065600
H	-3.30584100	-1.57345600	-2.13694800
C	-2.94007200	-2.41937000	1.62844500
H	-1.37637700	-0.94841900	1.66201700
C	-3.89861000	-3.08389000	0.85485800
H	-4.76850100	-3.28521800	-1.10926400
H	-2.83155100	-2.65522300	2.68352200
H	-4.53764500	-3.83671900	1.30750800
C	-1.50438200	1.70666800	-0.33116400
C	-2.58052800	1.90344800	0.55010400
C	-0.70077700	2.81688300	-0.65815600
C	-2.83446700	3.16636900	1.09659600
H	-3.22744800	1.07314600	0.81341600
C	-0.95035800	4.07313700	-0.10637600
H	0.13066600	2.69997100	-1.35070700
C	-2.02074500	4.25490700	0.77692000
H	-3.67287200	3.29390700	1.77632900
H	-0.30947800	4.91073600	-0.36786700
H	-2.21695300	5.23282600	1.20680100
Cd	1.08652600	-0.41706500	-0.36963600
O	3.23117200	0.47083000	-0.13606900
O	2.81003500	-1.64682700	0.35974200
C	3.62904200	-0.66402300	0.26545600
C	5.07924200	-0.90322700	0.64190900
H	5.44159100	-1.70912600	-0.00875400
H	5.07711800	-1.32795100	1.65314100
C	5.98257100	0.32718000	0.55476300
H	5.63533000	1.12153800	1.22167000
H	7.00728500	0.06437800	0.83763700
H	5.99929400	0.73498500	-0.45980900

C''-TS1



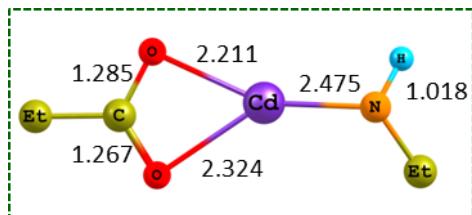
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C	-1.46442000	2.77117400	0.55137200
H	-1.29350400	2.39399100	1.56702900
H	-0.75596300	3.59824400	0.39953900
C	-2.89527300	3.30399700	0.43791900
H	-3.08755300	3.70389800	-0.56516000
H	-3.62590500	2.51173700	0.63232200
H	-3.06553800	4.11305300	1.15733400
O	-2.10043200	-2.84699200	0.34218500
C	-2.41988000	-1.68541600	0.18780700
C	-3.86442500	-1.21950600	0.02147100
H	-4.07694900	-0.50598700	0.82910500
H	-3.92700000	-0.64104800	-0.91023600
C	-4.88056000	-2.36120700	0.02378000
H	-5.89612000	-1.96906100	-0.09429700
H	-4.68288900	-3.06337600	-0.79087000
H	-4.83249200	-2.92569100	0.95886600
N	-1.21376700	1.66056300	-0.39075500
H	-1.40560900	1.97692200	-1.34103100
O	-1.50957000	-0.69896700	0.16024600
H	-1.73923600	0.37308600	-0.08319100
O	2.34316200	-0.46191800	-1.29940400
O	2.50539700	0.04086900	0.84892000
C	3.00451500	-0.47106100	-0.20508200
C	4.37522100	-1.11570200	-0.18621000
H	4.91824600	-0.74001700	-1.06093200
H	4.21076600	-2.18333800	-0.38167900
C	5.17060400	-0.91176000	1.10392800
H	4.62884200	-1.30503800	1.96814200
H	6.13475100	-1.42602400	1.03648500
H	5.36197000	0.14945300	1.28909400

C"-IM2



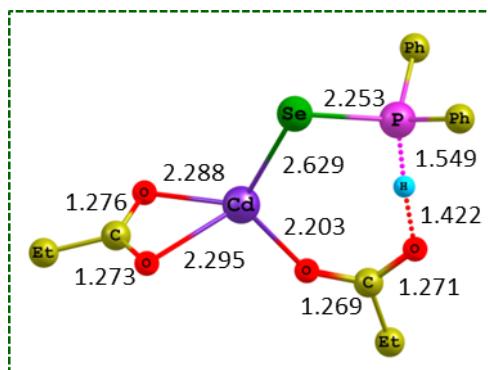
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H	-0.64083900	3.56550300	0.50629900
C	-2.77359400	3.26210300	0.59519800
H	-2.99927100	3.70133200	-0.38428700
H	-3.49780600	2.46201700	0.78153200
H	-2.91869000	4.04206600	1.35162900
O	-2.40701900	-2.92663700	0.24487300
C	-2.59598600	-1.73731100	0.11646500
C	-3.97526300	-1.09244300	0.03137500
H	-4.05211500	-0.36047200	0.84679500
H	-4.01874100	-0.50833000	-0.89771800
C	-5.12167900	-2.10120300	0.09649500
H	-6.08573900	-1.58599600	0.03594200
H	-5.05932100	-2.81874100	-0.72616300
H	-5.08959800	-2.67032600	1.02938900
N	-1.13234100	1.65453000	-0.35992900
H	-1.32452800	2.03174700	-1.28820100
O	-1.55664700	-0.87575700	0.04282600
H	-1.76882700	0.11538900	-0.09337900
O	2.41286200	-0.45364800	-1.28482600
O	2.51909500	-0.00239900	0.87778500
C	3.03068900	-0.51987200	-0.16369400
C	4.36663600	-1.23224200	-0.11456900
H	4.98549800	-0.80238800	-0.91118700
H	4.17451600	-2.26759000	-0.42331400
C	5.07699300	-1.18203400	1.23843600
H	4.46272000	-1.63047400	2.02384300
H	6.02430400	-1.72851400	1.18682400
H	5.29181100	-0.15153500	1.53593900

C''



Cd	0.40971000	-0.38276300	0.03041200
C	3.21856200	0.82047700	0.31481800
H	2.71790900	1.73715000	-0.02114800
H	3.27647400	0.88314900	1.41485900
C	4.64207200	0.79377200	-0.25282600
H	5.17709400	-0.10562400	0.07652900
H	4.62019200	0.79144200	-1.34726000
H	5.21386900	1.66563800	0.08794000
N	2.44271900	-0.33256000	-0.16551100
H	2.87527900	-1.19790500	0.15171700
O	-1.61149600	-1.27825400	-0.01018700
O	-1.50660300	0.93094700	-0.00812600
C	-2.19357000	-0.13315600	-0.02156800
C	-3.70866700	-0.09944500	-0.05279200
H	-4.05483300	-0.69982600	0.79743900
H	-4.01647400	-0.65839100	-0.94528600
C	-4.32295600	1.30051400	-0.03441600
H	-3.99447100	1.88825000	-0.89610300
H	-5.41557200	1.23382000	-0.05916000
H	-4.03245500	1.84834500	0.86646900

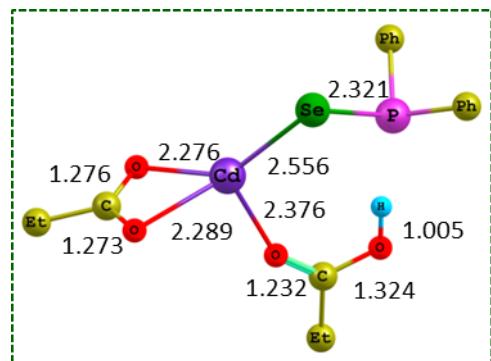
A/C-TS1



Cd	-1.88464300	-0.15020200	-0.20405800
O	0.42307300	2.26571400	1.34007000
O	-1.70862000	1.51694800	1.22540100
C	-0.81498000	2.32725800	1.62054800
C	-1.24674700	3.48241600	2.51935700
H	-0.67392300	3.38112100	3.44993600
H	-0.87428300	4.40099200	2.04938100
C	-2.74603300	3.57281400	2.80265200

H	-2.95598800	4.42580700	3.45691800
H	-3.31792900	3.70052800	1.87904900
H	-3.11225000	2.66579000	3.29152800
O	-3.95075500	-0.01444800	-1.19361800
O	-3.64131800	-1.45279400	0.46735400
C	-4.39512800	-0.91199400	-0.40805800
C	-5.84476200	-1.35997700	-0.49115800
H	-6.29390600	-1.14334800	0.48636500
H	-5.83443000	-2.45371400	-0.56993500
C	-6.65653700	-0.72735500	-1.62216400
H	-6.22312200	-0.96160700	-2.59889300
H	-7.68658300	-1.09976600	-1.60496000
H	-6.68152400	0.36190100	-1.52871700
P	1.74430900	0.00228600	-0.05329400
C	2.53601400	-1.19321000	1.08831000
C	2.14335900	-2.53557200	1.16044200
C	3.53269100	-0.71235400	1.95694200
C	2.74578400	-3.39165800	2.08777500
H	1.37160800	-2.90811300	0.49393700
C	4.13007000	-1.57120700	2.87957700
H	3.84367900	0.32803200	1.91329200
C	3.73752500	-2.91284600	2.94630600
H	2.43666800	-4.43171600	2.13597900
H	4.89890800	-1.19254300	3.54674900
H	4.20286400	-3.57954800	3.66653900
C	3.08455500	0.74447500	-1.03975100
C	3.07722500	2.13550500	-1.23341100
C	4.09183300	-0.03727000	-1.62808500
C	4.07343400	2.73639000	-2.00774100
H	2.30276300	2.74547400	-0.77668100
C	5.08326900	0.56906200	-2.39977200
H	4.10422600	-1.11340300	-1.48069900
C	5.07429100	1.95544500	-2.59127000
H	4.06662100	3.81283800	-2.15156700
H	5.86096800	-0.03897400	-2.85261400
H	5.84739100	2.42446600	-3.19307200
Se	0.27614000	-1.02451800	-1.41982000
H	1.01348900	1.14191200	0.69888700

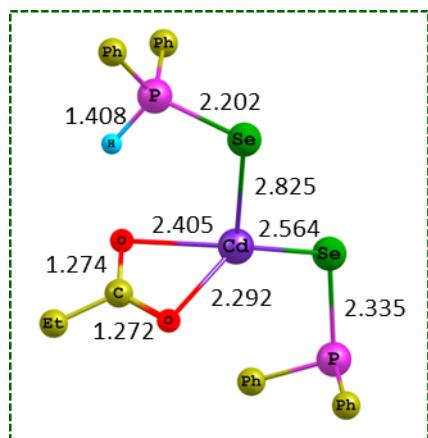
A/C-IM1



Cd	-1.76143500	-0.29681300	-0.57212800
O	0.01781500	2.34564000	1.91953600
O	-1.85507300	1.49331600	0.98751800
C	-1.29298100	2.28840800	1.74265000
C	-2.04364300	3.30694400	2.57053000
H	-1.75917900	3.13716700	3.61671300
H	-1.63252000	4.29178800	2.31508800
C	-3.56002000	3.26623400	2.38821300
H	-4.03161500	4.02809200	3.01610700
H	-3.83988800	3.45589400	1.34836800
H	-3.96617200	2.29028900	2.66765800
O	-3.92561100	-0.19715900	-1.31247700
O	-3.42833800	-1.48367000	0.42342500
C	-4.28046200	-1.01160000	-0.40125900
C	-5.72960900	-1.44828000	-0.27564600
H	-6.03125200	-1.24774600	0.75960600
H	-5.73613700	-2.54119800	-0.37254100
C	-6.69219200	-0.79989000	-1.27127200
H	-6.40120200	-1.01917300	-2.30236500
H	-7.70988800	-1.17270000	-1.11307700
H	-6.70348900	0.28815700	-1.15934900
P	1.76663400	0.24654100	0.20499600
C	2.39910500	-1.25724100	1.08015200
C	2.14098200	-2.57579200	0.68312600
C	3.13696800	-1.03384000	2.25773100
C	2.62223900	-3.65014100	1.43952000
H	1.56307200	-2.76145600	-0.21707200
C	3.62342500	-2.10632100	3.00653100
H	3.33642200	-0.01753100	2.59025900
C	3.36548000	-3.41988900	2.59903700
H	2.41376900	-4.66692500	1.11813400
H	4.19602100	-1.91667900	3.91016400
H	3.73731400	-4.25557200	3.18506600
C	3.28055300	0.91141000	-0.61195700
C	3.34860900	2.29727100	-0.83276100
C	4.34943900	0.10205300	-1.03029000

C	4.46027300	2.86310900	-1.46150300
H	2.52993700	2.93684800	-0.51295200
C	5.46181500	0.66936900	-1.65541000
H	4.31482800	-0.97032700	-0.86436100
C	5.51948400	2.04966500	-1.87364200
H	4.49955600	3.93631500	-1.62543200
H	6.28239600	0.03268300	-1.97426000
H	6.38606500	2.48839800	-2.36011500
Se	0.55770900	-0.51193500	-1.62575200
H	0.51207500	1.66452300	1.37060200

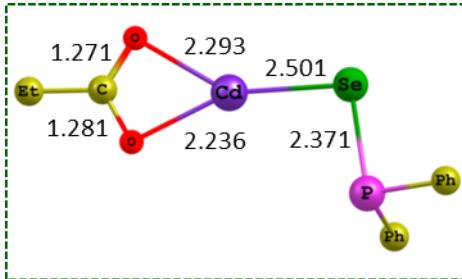
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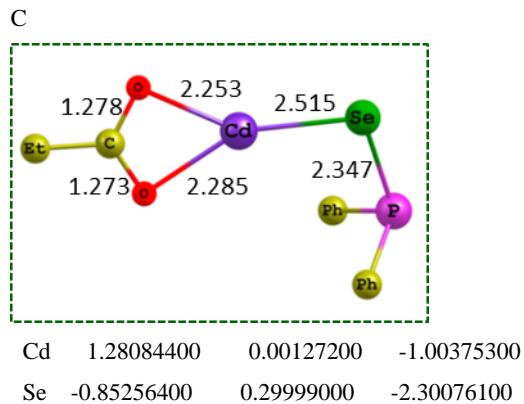
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C	-3.94033600	0.96159800	1.36647100
C	-4.99408800	0.19191000	1.89768200
C	-2.93642600	1.40587200	2.24213100
C	-5.02670400	-0.14003100	3.25329400
H	-5.79107300	-0.15961000	1.24848100
C	-2.97030200	1.07401400	3.60018500
H	-2.12065800	2.01105300	1.85849500
C	-4.01301100	0.29833200	4.11186800
H	-5.84486200	-0.74331800	3.63787900
H	-2.17596300	1.42217100	4.25513800
H	-4.03854300	0.03954100	5.16680100
C	-4.51201000	-0.02080600	-1.27869900
C	-4.04025800	-1.30201800	-0.94382800
C	-5.37594700	0.11353000	-2.37835800
C	-4.42282500	-2.41637900	-1.69265700
H	-3.37189500	-1.44027000	-0.09939600
C	-5.75815900	-1.00226400	-3.13009600
H	-5.74921200	1.09854100	-2.64745800
C	-5.28176600	-2.27004800	-2.78826500
H	-4.04428800	-3.39819900	-1.42144700

H	-6.42690500	-0.87957800	-3.97778500
H	-5.57698200	-3.13928600	-3.36973600
O	0.50393000	-0.87570700	1.67437400
O	-1.00849100	-2.07422400	0.57807900
C	-0.24018800	-1.90570700	1.57715700
C	-0.20098800	-2.94114500	2.69144600
H	0.84386700	-3.26167600	2.79323100
H	-0.43312200	-2.40667700	3.62080600
C	-1.12855700	-4.14158000	2.49986500
H	-1.03453800	-4.83373800	3.34375000
H	-2.17252800	-3.82363500	2.43158800
H	-0.88961500	-4.68423200	1.58069500
Se	1.94230200	-0.29008800	-1.81760100
P	3.24541500	-0.10803000	-0.05236200
H	2.59566100	-0.63986200	1.07799500
C	3.69790500	1.60909800	0.38012000
C	4.55373200	1.83436900	1.47245800
C	3.17232000	2.69308600	-0.33274200
C	4.87760700	3.13929100	1.84312800
H	4.96916900	0.99914300	2.02995600
C	3.50353900	3.99856900	0.04250900
H	2.50802700	2.51546700	-1.17304900
C	4.35280600	4.22213500	1.12795300
H	5.53690000	3.31086900	2.68882500
H	3.09125200	4.83593700	-0.51214400
H	4.60580500	5.23731400	1.41961700
C	4.78257200	-1.06904600	-0.17937700
C	4.89357900	-2.28618600	0.51004200
C	5.83249400	-0.63207200	-1.00244500
C	6.05410800	-3.05399400	0.38579200
H	4.08061000	-2.63573400	1.14045800
C	6.98873800	-1.40312100	-1.12191000
H	5.75004700	0.30633000	-1.54337100
C	7.10042400	-2.61354300	-0.42892500
H	6.13833000	-3.99349200	0.92371400
H	7.80050000	-1.06134500	-1.75698200
H	8.00148900	-3.21208400	-0.52533400

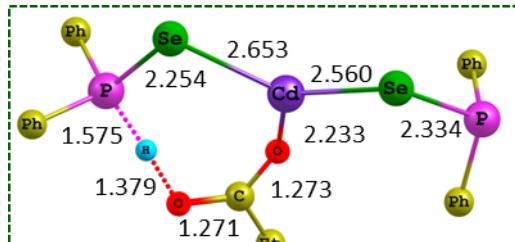
C-i



Cd	2.04989000	-0.36284700	-0.19688900	P	-2.46655800	0.40479600	-0.59992400
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O	4.30665100	-0.48756800	-0.58033900	C	-2.13959400	2.92271900	0.53884900
C	4.51668700	0.05146300	0.55121600	C	-0.74074800	1.23883800	1.56726600
C	5.92462300	0.31919500	1.04483500	C	-1.59818500	3.89301500	1.38722900
H	6.02669400	-0.21244000	1.99916100	H	-2.89498000	3.20478500	-0.19018500
H	5.96961500	1.38453700	1.30175400	C	-0.20045600	2.20804800	2.41571400
C	7.03775000	-0.06823900	0.07102800	H	-0.41088300	0.20830900	1.66528400
H	6.94845300	0.47980700	-0.87117500	C	-0.62646600	3.53789700	2.32647800
H	8.01589100	0.15708000	0.50832700	H	-1.93779700	4.92245100	1.31547300
H	7.00404500	-1.13543300	-0.16515600	H	0.55142000	1.92161300	3.14564000
P	-1.43828800	-0.07812900	0.78065600	H	-0.20572900	4.29022800	2.98759600
C	-2.98800500	-1.05128500	0.50185100	C	-2.35015800	-1.20693300	0.30868300
C	-3.11562300	-2.25605500	1.21598000	C	-2.92458800	-1.28117200	1.59314500
C	-4.02967400	-0.65849800	-0.35472700	C	-1.88194000	-2.39081600	-0.28222700
C	-4.25219500	-3.05430200	1.07067600	C	-2.99948000	-2.49751500	2.27332500
H	-2.32112700	-2.56816000	1.88931900	H	-3.30877600	-0.38403300	2.07130400
C	-5.16870700	-1.45487700	-0.49555400	C	-1.96157800	-3.60983500	0.39939000
H	-3.95475900	0.27180800	-0.90884600	H	-1.45422300	-2.36155700	-1.27966600
C	-5.28203800	-2.65459700	0.21365100	C	-2.51569200	-3.66801000	1.67960700
H	-4.33511300	-3.98283900	1.62857800	H	-3.43600500	-2.52968300	3.26781400
H	-5.96708700	-1.13832900	-1.16118100	H	-1.58785900	-4.51326300	-0.07482000
H	-6.16912600	-3.27174400	0.10219500	H	-2.57464200	-4.61451200	2.20918200
C	-1.97176900	1.63306100	0.29481900	O	3.53333700	0.01822700	-0.93858500
C	-1.83585800	2.21230500	-0.97506200	O	2.43002200	-0.58516000	0.88220400
C	-2.52520000	2.40584500	1.33271600	C	3.53011400	-0.37654200	0.27722100
C	-2.25687500	3.52621700	-1.20574000	C	4.85924300	-0.59479300	0.97354600
H	-1.39454700	1.63826500	-1.78416900	H	5.40236000	-1.33962600	0.37844300
C	-2.95562200	3.71371300	1.09957000	H	5.42950300	0.33528000	0.86182500
H	-2.61933700	1.98336100	2.33077200	C	4.76341400	-1.01982400	2.43908400
C	-2.82053100	4.27890000	-0.17237700	H	5.76543100	-1.16452400	2.85603400
H	-2.14347300	3.95936500	-2.19594200	H	4.24921400	-0.26313500	3.03857200
H	-3.38436500	4.29282200	1.91272900	H	4.20816800	-1.95594800	2.54452000
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Se	-0.22737400	-0.86362400	-1.10086400				

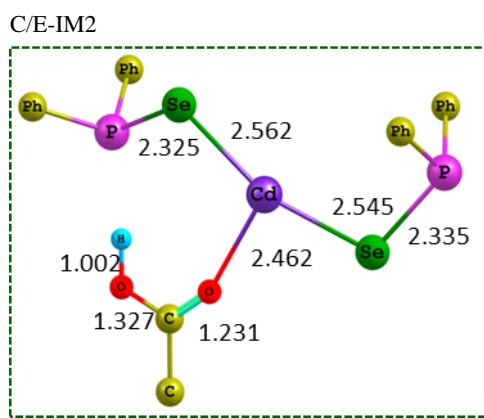


C/E-TS1



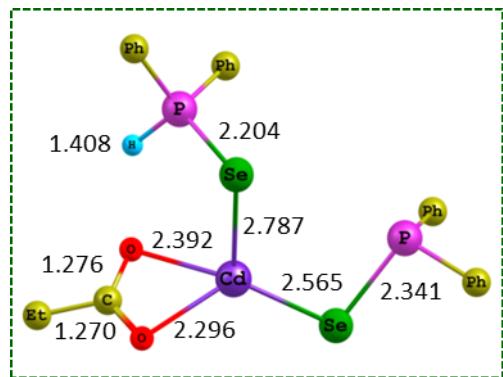
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P	-4.46754300	0.07694500	-1.03932500
C	-4.19073600	1.53354600	0.07177900

C	-3.23958000	1.58193100	1.10614800	C	4.38848700	-2.41748400	-0.22725700
C	-4.98567900	2.66613900	-0.16940800	C	5.62234100	-0.49109400	-1.04333600
C	-3.08850300	2.73847900	1.87372500	C	5.44211200	-3.25102400	-0.61326400
H	-2.61248800	0.71952500	1.31358600	H	3.50572800	-2.84336700	0.24175000
C	-4.83313800	3.82501200	0.59913600	C	6.67086400	-1.32777400	-1.42569100
H	-5.72653600	2.64012500	-0.96453500	H	5.69645400	0.57946700	-1.21157500
C	-3.88341400	3.86331200	1.62240000	C	6.58134800	-2.70825200	-1.21254500
H	-2.34717300	2.76238300	2.66834800	H	5.37109900	-4.32144600	-0.44384500
H	-5.45604400	4.69237300	0.39840300	H	7.55566000	-0.90435400	-1.89206700
H	-3.76274700	4.76150900	2.22191000	H	7.39879700	-3.35743200	-1.51281600
C	-4.24634500	-1.35397800	0.11919000				
C	-3.63268000	-2.54987700	-0.28915400				
C	-4.88691100	-1.32814600	1.37302600				
C	-3.64377800	-3.67896400	0.53498600				
H	-3.14063400	-2.59532800	-1.25624100				
C	-4.89650500	-2.45625300	2.19653100				
H	-5.37875900	-0.42160800	1.71402600				
C	-4.27423700	-3.63803500	1.78179700				
H	-3.15993600	-4.59225400	0.19846300				
H	-5.39246900	-2.41038100	3.16254000				
H	-4.28518100	-4.51686000	2.42052900				
O	1.28293900	-1.63943300	1.72823300				
O	-0.55017100	-0.47178600	1.12185000				
C	0.07501100	-1.27575200	1.88489600				
C	-0.70226100	-1.81899800	3.07619300				
H	-1.03935800	-0.94619000	3.65016900				
H	-1.61706300	-2.27039600	2.67461600				
C	0.05837800	-2.80053700	3.96765700				
H	-0.57872300	-3.12791200	4.79611000				
H	0.37017200	-3.68633800	3.40650300				
H	0.95912800	-2.34345300	4.38741300				
Se	1.96747900	0.69642900	-1.80831000				
P	3.05750700	0.01069100	0.04123800				
H	2.08452200	-0.85148300	0.92987300				
C	3.76141300	1.44083100	0.94944400				
C	4.61328800	1.18122000	2.03852800				
C	3.42335000	2.76393000	0.63777600				
C	5.12026800	2.23553500	2.79857300				
H	4.88387800	0.15987100	2.29241600				
C	3.93508600	3.81695100	1.40269800				
H	2.76656400	2.96792000	-0.20225000				
C	4.78214200	3.55596200	2.48176600				
H	5.77810700	2.02585000	3.63704300				
H	3.67030200	4.83979100	1.15084000				
H	5.17804200	4.37546100	3.07464100				
C	4.47548400	-1.03207800	-0.43974500				
				Se	-2.91040200	1.71434800	-0.86296600
				P	-4.41691200	0.11707700	-0.06744900
				C	-3.87088100	-0.15994500	1.68242700
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				C	-2.48741700	-1.16805100	3.41457700
				H	-2.33074300	-1.63861700	1.32403400
				C	-4.17210300	0.45703400	4.02110100
				H	-5.33392000	1.25933900	2.39389100
				C	-3.14755600	-0.41765500	4.39342700
				H	-1.69113800	-1.85203400	3.69512900
				H	-4.69403100	1.03932700	4.77550800
				H	-2.86681800	-0.51741700	5.43815300
				C	-3.94264500	-1.48947700	-0.86715800
				C	-4.52354800	-2.66629800	-0.35392900
				C	-3.18015500	-1.58075500	-2.04086700
				C	-4.32151500	-3.89674100	-0.98029500
				H	-5.13205400	-2.62447600	0.54603000
				C	-2.98223700	-2.81426600	-2.67149900
				H	-2.74061300	-0.68306700	-2.46480000
				C	-3.54750300	-3.97625800	-2.14331500
				H	-4.77032300	-4.79309500	-0.56073500
				H	-2.38305500	-2.86219800	-3.57691300
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				Cd	-0.63369100	0.97336200	-0.00002900



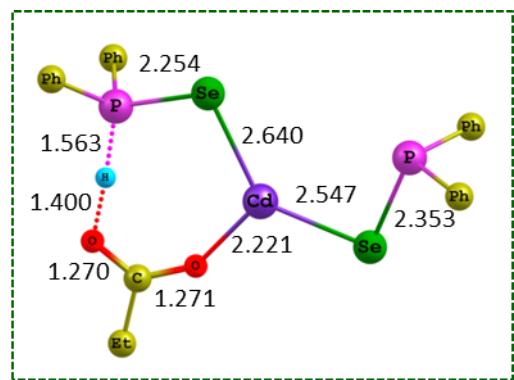
Se	1.13036500	-0.36191200	1.29271400	Cd	0.24814000	1.85472700	-0.27266500
H	2.71661200	1.83710600	-1.33201400	Se	-2.28848700	1.72007400	-0.62903900
C	1.44977500	4.61369600	-2.47276300	P	-2.68517500	-0.30164100	0.48231300
H	1.75840300	4.42882300	-3.50950100	C	-3.41826500	-1.39303000	-0.83422600
H	2.24022000	5.24278200	-2.04389100	C	-4.11246200	-2.54519100	-0.41322800
O	2.69363200	2.69837400	-1.84381300	C	-3.19366000	-1.21634000	-2.20761300
C	1.50672700	3.28514000	-1.75260500	C	-4.57845200	-3.48039100	-1.33894600
O	0.55089000	2.80170600	-1.14674000	H	-4.30111400	-2.70868400	0.64511700
C	0.08704600	5.30150800	-2.40652400	C	-3.65733300	-2.15647300	-3.13518700
H	0.12154900	6.25146800	-2.94831200	H	-2.66594500	-0.33236200	-2.55272300
H	-0.69440100	4.67970300	-2.85169900	C	-4.35157400	-3.29000500	-2.70719400
H	-0.20410800	5.50611400	-1.37267500	H	-5.12247600	-4.35498200	-0.99179100
P	2.93815600	-0.04889200	-0.13587500	H	-3.47942100	-1.99406500	-4.19504800
C	3.09545700	-1.64749900	-1.04389700	H	-4.71655800	-4.01573200	-3.42873500
C	3.16418600	-2.89606100	-0.40191800	C	-4.20021200	0.12675400	1.45862500
C	3.12115900	-1.60227000	-2.44637100	C	-5.45489700	0.39327200	0.88405800
C	3.26267200	-4.06957800	-1.14861300	C	-4.06506700	0.20906100	2.85388800
H	3.13247000	-2.94873400	0.68240000	C	-6.54582400	0.72885500	1.68686000
C	3.22040800	-2.78001700	-3.19614000	H	-5.57784100	0.33795300	-0.19363700
H	3.06551700	-0.64442500	-2.95771500	C	-5.15729800	0.54744100	3.65943500
C	3.29087400	-4.01421200	-2.54796800	H	-3.09979500	0.00620300	3.31121000
H	3.31321300	-5.02878600	-0.64090900	C	-6.39982500	0.80751300	3.07696500
H	3.24061000	-2.72954500	-4.28114800	H	-7.50964100	0.93364700	1.22848200
H	3.36459500	-4.93049200	-3.12690800	H	-5.03620600	0.60598800	4.73771600
C	4.37705600	-0.08889100	1.02575200	H	-7.25036100	1.07012200	3.70001400
C	5.59692200	-0.65619400	0.61512500	O	2.12744100	1.86572700	-1.75304800
C	4.32473200	0.57350300	2.26392500	O	1.51431300	3.72171900	-0.69884900
C	6.73002200	-0.57077700	1.42806100	C	2.27306300	3.11079500	-1.51343800
H	5.66555900	-1.17303800	-0.33717500	C	3.37885300	3.86490900	-2.23819100
C	5.45931700	0.65547400	3.07473400	H	4.31296200	3.31896600	-2.05496000
H	3.39038800	1.01018200	2.60281700	H	3.18235200	3.75024500	-3.31168600
C	6.66583700	0.08396500	2.66106400	C	3.51707300	5.33972000	-1.85848300
H	7.66151900	-1.02136400	1.09660400	H	4.32789300	5.80587200	-2.42896500
H	5.39625700	1.16306000	4.03333900	H	2.59262800	5.88663000	-2.06312600
H	7.54650000	0.14625900	3.29391100	H	3.73478200	5.45524900	-0.79276900
Se	1.54094100	0.32558600	1.66635900	Se	2.79217800	-0.76441300	0.21593200

C-i/F-IM1



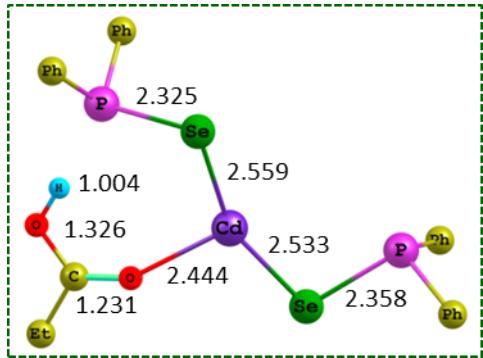
H	2.68197900	-4.71678600	-2.75011800	C	-6.42934000	2.53895400	3.01538400
H	-1.04154800	-3.74537100	-0.81156900	H	-7.79569100	2.50967200	1.34383300
H	0.27207600	-5.19162000	-2.35224900	H	-4.86979300	2.38366000	4.50010600
C	4.36977400	-1.32331800	0.92157800	H	-7.08080900	3.14168900	3.64215700
C	5.54318900	-0.60625200	0.64262700	O	3.28663200	1.51907400	-1.82930100
C	4.41251100	-2.42866300	1.78584400	O	1.09438300	1.88067100	-2.24126700
C	6.75394200	-1.00129400	1.21663100	C	2.32709000	2.17493700	-2.34046400
H	5.51485400	0.25657300	-0.01716500	C	2.65149200	3.42347200	-3.15366000
C	5.62468500	-2.81766700	2.35612200	H	2.19699000	3.27732800	-4.14148900
H	3.50632700	-2.98467500	2.00859700	H	2.08864800	4.24738000	-2.69774200
C	6.79505000	-2.10525400	2.07237500	C	4.13607500	3.76758600	-3.27366300
H	7.66093800	-0.44673600	0.99546900	H	4.26618100	4.67377200	-3.87482900
H	5.65568700	-3.67449300	3.02243500	H	4.58427200	3.94166700	-2.29110500
H	7.73694700	-2.41036000	2.51872300	H	4.69486600	2.95710300	-3.75053700

C-i/E-ii-TS1



Cd	-0.31495700	0.70156400	-0.99297000	H	5.40847400	-3.46103200	-4.21020800
Se	-2.70049300	1.59233700	-1.04460000	H	1.59221600	-5.23364500	-3.29428500
P	-3.55847400	-0.05141500	0.40334600	H	3.69741500	-5.22186000	-4.61938800
C	-4.73496700	-1.02520700	-0.65741500	C	4.13779400	-1.41645200	0.59974000
C	-5.50128500	-2.00620200	0.00178600	C	4.81010000	-0.28703400	1.09442900
C	-4.83889500	-0.92117000	-2.05113300	C	4.44516300	-2.68835200	1.10887100
C	-6.36326400	-2.84029400	-0.71104000	C	5.78137400	-0.43220500	2.08845200
H	-5.42793100	-2.11590800	1.08154000	H	4.58167000	0.69969400	0.70119600
C	-5.69756900	-1.76368800	-2.76737000	C	5.41652500	-2.82695400	2.10088600
H	-4.25142500	-0.17496900	-2.57724100	H	3.93176700	-3.56694600	0.72898400
C	-6.46416400	-2.72218900	-2.10209300	C	6.08418000	-1.69974500	2.59252100
H	-6.95195200	-3.58487400	-0.18183400	H	6.30111200	0.44402800	2.46474000
H	-5.76720600	-1.66357700	-3.84742600	H	5.65111000	-3.81303700	2.49111400
H	-7.13159100	-3.37393700	-2.65907800	H	6.83962600	-1.81092500	3.36503900
C	-4.74768400	0.97263700	1.38939200				
C	-5.99722400	1.40675100	0.91597800				
C	-4.35539500	1.33443200	2.68909700				
C	-6.83166100	2.18194700	1.72371000				
H	-6.31998400	1.13516800	-0.08463200				
C	-5.18829900	2.11390800	3.49683200				
H	-3.39289700	1.00193600	3.07027700				

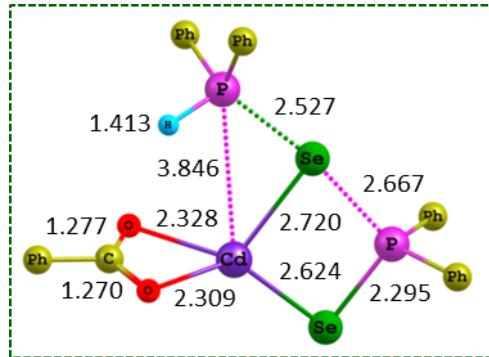
C-i/E-ii-IM2



Se	-2.50642500	-0.90676300	0.88931000
P	-3.40169100	0.48069500	-0.79433800
C	-4.30687600	1.73123700	0.22971300
C	-5.45874500	1.44903700	0.98396600
C	-3.78515700	3.03483200	0.25510200
C	-6.07193400	2.44714600	1.74224700
H	-5.87728800	0.44686100	0.97589500
C	-4.39714700	4.03540700	1.01715600
H	-2.89629200	3.26724600	-0.32638800
C	-5.54217900	3.74296700	1.76159500
H	-6.96230500	2.21470300	2.32034500
H	-3.98211500	5.03959900	1.02448200
H	-6.02190300	4.51845000	2.35240200
C	-4.81659600	-0.52347400	-1.45690900
C	-5.78893200	0.15731100	-2.21597400
C	-4.89600100	-1.92108500	-1.37074700
C	-6.81712600	-0.53890000	-2.85239400
H	-5.74846600	1.23997300	-2.30588100
C	-5.92555900	-2.61868700	-2.01260100
H	-4.15767000	-2.46614900	-0.79101900
C	-6.88976200	-1.93279300	-2.75349500
H	-7.56083800	0.00769900	-3.42603500
H	-5.97205600	-3.70113200	-1.92682000
H	-7.68915700	-2.47571500	-3.24993500
Cd	-0.11338300	-0.74981700	0.07292200
Se	1.77088600	-0.09860000	-1.53172300
H	3.10159900	-1.11290900	1.84362000
C	1.60956100	-3.10281600	3.95128400
H	1.87427100	-2.51128100	4.83701900
H	2.38283200	-3.87810000	3.87997400
O	3.00156500	-1.68709600	2.66055700
C	1.78137100	-2.19755100	2.75212300
O	0.87852900	-1.96127300	1.94896300
C	0.21371400	-3.71062500	4.08018700
H	0.16409200	-4.34727100	4.96866500
H	-0.55116300	-2.93457800	4.16983100

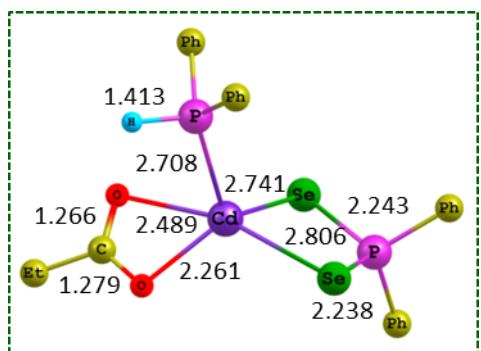
H	-0.03540200	-4.32018100	3.20720500
P	3.49800400	0.09819300	0.01296600
C	3.73659800	1.91719400	0.20858500
C	3.95479200	2.78514600	-0.87514700
C	3.67127600	2.45086500	1.50487800
C	4.11088700	4.15437000	-0.66246600
H	3.99571200	2.38836500	-1.88527100
C	3.82824300	3.82509000	1.71863400
H	3.49846900	1.79272600	2.35283000
C	4.04823800	4.67752100	0.63539700
H	4.27789500	4.81555400	-1.50824700
H	3.77652700	4.22423100	2.72767200
H	4.16813600	5.74499700	0.79758100
C	4.98385700	-0.40482100	-0.96710500
C	6.23289100	0.17347700	-0.67512300
C	4.92914400	-1.45821000	-1.89465900
C	7.39298400	-0.28501700	-1.30341900
H	6.30355500	0.98893200	0.03847500
C	6.09169900	-1.91284200	-2.52278400
H	3.97421400	-1.91267600	-2.13952200
C	7.32713800	-1.32928700	-2.23035900
H	8.34730200	0.17900600	-1.06993900
H	6.02760500	-2.72160100	-3.24550000
H	8.22943200	-1.68253400	-2.72130400

C-i/F-TS1



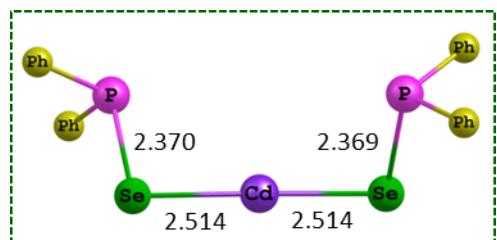
Cd	0.03011800	1.98446500	-0.25455400
P	2.52043900	-0.20994100	0.08240300
Se	2.63283400	2.08179200	0.06472500
C	3.61385300	-0.85601100	-1.25058300
C	3.89449900	-2.23543000	-1.26808100
C	4.08569300	-0.05217400	-2.29809900
C	4.64525800	-2.79147600	-2.30419100
H	3.53256300	-2.87602000	-0.46830100
C	4.83643200	-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	-2.32496100	-5.00199100	-2.82409000
H	5.20167200	0.02265000	-4.13687900	H	-6.26385400	-3.28991600	-2.50934400
H	5.70363800	-2.41522700	-4.14889500	H	-4.75333900	-5.07667000	-3.35544700
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	Cd	-0.61416500	1.23748500	-0.28026600
O	-1.38414000	3.24310300	-1.57576800	P	2.34759000	-0.30053100	0.08076400
C	-2.15375900	3.47068700	-0.59144400	Se	1.09800800	0.53943200	1.74312300
C	-3.37756000	4.35771000	-0.75923600	C	3.97409500	0.55143300	-0.00611800
H	-4.23061500	3.81664900	-0.33210000	C	4.98363600	0.00889500	-0.81919500
H	-3.22460000	5.22229500	-0.10052500	C	4.20746200	1.74824900	0.68219100
C	-3.66214700	4.80630400	-2.19323500	C	6.21303200	0.65701800	-0.93446200
H	-4.54760700	5.45043200	-2.22189400	H	4.81253100	-0.91636600	-1.36160000
H	-2.81624500	5.36208100	-2.60654300	C	5.44155000	2.39457400	0.56206100
H	-3.84036400	3.94882400	-2.84902200	H	3.42845600	2.16893500	1.31031700
P	-2.61353900	-0.80819200	-0.20082200	C	6.44413400	1.85243800	-0.24451300
H	-3.19207400	0.32946100	-0.80612700	H	6.98863300	0.23074600	-1.56421900
C	-3.46877400	-0.81919600	1.41719600	H	5.61482400	3.32179800	1.10061600
C	-3.93284200	-2.01194700	1.99291700	H	7.40182600	2.35679100	-0.33671000
C	-3.56759500	0.38600500	2.13554300	C	2.78282400	-2.05206000	0.43377400
C	-4.50704200	-1.99747800	3.26686100	C	3.40236000	-2.36106600	1.65650400
H	-3.85655500	-2.94912300	1.44942300	C	2.51221300	-3.07495500	-0.48299600
C	-4.14559600	0.39073700	3.40666600	C	3.75084200	-3.67886600	1.95072100
H	-3.18682000	1.31329300	1.71228500	H	3.60625900	-1.57660100	2.37959800
C	-4.61694800	-0.79745500	3.97466900	C	2.86392000	-4.39545800	-0.18336000
H	-4.86862400	-2.92434400	3.70313800	H	2.02770300	-2.83712600	-1.42513000
H	-4.22356600	1.32609300	3.95346900	C	3.48192500	-4.69929000	1.03103100
H	-5.06452100	-0.78815200	4.96440300	H	4.22743900	-3.90999400	2.89897500
C	-3.31930000	-2.17770500	-1.19420400	H	2.65291200	-5.18301300	-0.90126000
C	-2.47102200	-3.18340500	-1.67877800	H	3.75239300	-5.72539300	1.26343600
C	-4.69143300	-2.22326700	-1.49876100	Se	1.26564000	-0.10987000	-1.86919800
C	-2.98924200	-4.22747400	-2.45201800	O	-2.08990100	2.95556300	0.75126100
H	-1.40766200	-3.14134500	-1.46157400	O	-1.01657400	3.27763800	-1.16804700
C	-5.20357000	-3.26365200	-2.27472500	C	-1.79333700	3.68718200	-0.23852100
H	-5.35864700	-1.45015800	-1.12763500	C	-2.36925500	5.09548000	-0.31456700
C	-4.35266900	-4.26816000	-2.75062400	H	-3.44970700	5.00923200	-0.14718400
				H	-1.98238000	5.63392500	0.56031900



C	-2.06554500	5.86078400	-1.60353400	H	-7.31859400	-2.28755000	1.45891600
H	-2.50680600	6.86300400	-1.56521600	H	-3.99349600	-3.35183800	3.97853300
H	-0.98772000	5.96291300	-1.75669100	H	-6.37743900	-3.64242800	3.32094800
H	-2.47040300	5.34155200	-2.47746400	C	-4.15175500	1.33958300	-0.12461300
P	-2.97428600	-0.09055700	-0.31383000	C	-4.57951500	2.36457200	0.74031200
H	-3.99512100	0.79048400	-0.73570500	C	-4.59804100	1.35230800	-1.45350200
C	-3.57367500	-0.54499500	1.36809500	C	-5.45146100	3.35945200	0.29414200
C	-3.92976800	-1.85756600	1.70824200	H	-4.22932400	2.38549100	1.77010200
C	-3.61798200	0.46480200	2.34613800	C	-5.46356300	2.35540500	-1.90325700
C	-4.33756100	-2.15737600	3.01187400	H	-4.26411900	0.58088000	-2.14059700
H	-3.89390800	-2.64656000	0.96367100	C	-5.89565000	3.35824700	-1.03220400
C	-4.03525400	0.15723300	3.64270300	H	-5.77419200	4.13940100	0.97826300
H	-3.32152400	1.48046800	2.09636000	H	-5.79910200	2.34961400	-2.93685400
C	-4.39455100	-1.15190700	3.97955400	H	-6.56676500	4.13667200	-1.38405200
H	-4.61093600	-3.17753500	3.26654100	Cd	0.00654600	-0.22399600	-1.33115000
H	-4.07105600	0.94305300	4.39188300	Se	2.30622100	0.77911400	-1.48534600
H	-4.71252600	-1.38682800	4.99137200	P	2.99230200	-0.14574900	0.58508600
C	-3.29970900	-1.52790000	-1.40119100	C	3.87461900	1.31254300	1.30424900
C	-2.23360300	-2.36339200	-1.77126000	C	5.16024000	1.72565400	0.91606600
C	-4.58930700	-1.80061700	-1.89122500	C	3.19835300	2.04279000	2.29612700
C	-2.45828000	-3.46332100	-2.60448600	C	5.75274500	2.84326800	1.50668400
H	-1.22635900	-2.14580800	-1.42729600	H	5.70024300	1.17095900	0.15460900
C	-4.80815000	-2.89574200	-2.72883800	C	3.79020900	3.16366700	2.88471000
H	-5.42266100	-1.15937300	-1.61713400	H	2.20501900	1.73111500	2.60954100
C	-3.74294500	-3.73067600	-3.08354100	C	5.06912600	3.56584800	2.49068000
H	-1.62637000	-4.10185000	-2.88689500	H	6.74755400	3.15191700	1.19718000
H	-5.80741800	-3.09591500	-3.10481500	H	3.25509400	3.71736400	3.65115600
H	-3.91437600	-4.58159800	-3.73665000	H	5.53270100	4.43509100	2.94870100

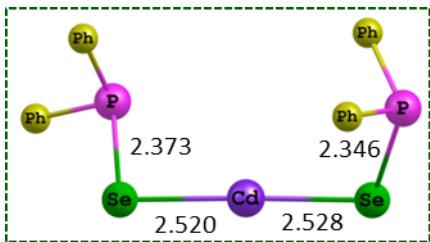
E-ii



Se	-2.29681100	-1.22427600	-1.121880600
P	-2.97041800	0.11447100	0.61675300
C	-4.12748300	-1.07774400	1.43147100
C	-5.47407000	-1.24805700	1.06994300
C	-3.60746900	-1.84469000	2.48905800
C	-6.27833000	-2.16671000	1.74872000
H	-5.89726000	-0.66042700	0.26124700
C	-4.41071300	-2.76634000	3.16399300
H	-2.56880800	-1.71838000	2.78452200
C	-5.74931000	-2.92912700	2.79473700

H	-7.31859400	-2.28755000	1.45891600
H	-3.99349600	-3.35183800	3.97853300
H	-6.37743900	-3.64242800	3.32094800
C	-4.15175500	1.33958300	-0.12461300
C	-4.57951500	2.36457200	0.74031200
C	-4.59804100	1.35230800	-1.45350200
C	-5.45146100	3.35945200	0.29414200
H	-4.22932400	2.38549100	1.77010200
C	-5.46356300	2.35540500	-1.90325700
H	-4.26411900	0.58088000	-2.14059700
C	-5.89565000	3.35824700	-1.03220400
H	-5.77419200	4.13940100	0.97826300
H	-5.79910200	2.34961400	-2.93685400
H	-6.56676500	4.13667200	-1.38405200
Cd	0.00654600	-0.22399600	-1.33115000
Se	2.30622100	0.77911400	-1.48534600
P	2.99230200	-0.14574900	0.58508600
C	3.87461900	1.31254300	1.30424900
C	5.16024000	1.72565400	0.91606600
C	3.19835300	2.04279000	2.29612700
C	5.75274500	2.84326800	1.50668400
H	5.70024300	1.17095900	0.15460900
C	3.79020900	3.16366700	2.88471000
H	2.20501900	1.73111500	2.60954100
C	5.06912600	3.56584800	2.49068000
H	6.74755400	3.15191700	1.19718000
H	3.25509400	3.71736400	3.65115600
H	5.53270100	4.43509100	2.94870100
C	4.41769600	-1.24325300	0.12753200
C	5.11681800	-1.82423400	1.20367500
C	4.77668100	-1.60442600	-1.17806900
C	6.16048000	-2.72183200	0.97665000
H	4.84844300	-1.57003000	2.22660800
C	5.81949600	-2.51044600	-1.40462600
H	4.24563700	-1.17451900	-2.02151900
C	6.51572500	-3.06932000	-0.33158200
H	6.69212300	-3.15313700	1.82039600
H	6.08593000	-2.77483500	-2.42444700
H	7.32496000	-3.77177800	-0.50982800

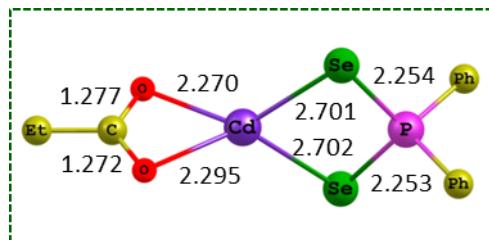
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Cd	0.03011800	1.98446500	-0.25455400
P	2.52043900	-0.20994100	0.08240300
Se	2.63283400	2.08179200	0.06472500
C	3.61385300	-0.85601100	-1.25058300
C	3.89449900	-2.23543000	-1.26808100
C	4.08569300	-0.05217400	-2.29809900
C	4.64525800	-2.79147600	-2.30419100
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

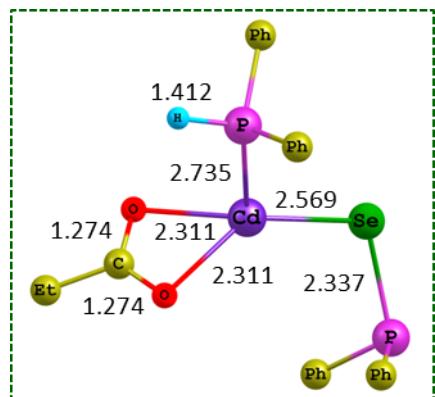
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Se	-0.03648500	-0.16190800	1.83337000
Se	-0.03590500	-0.05525100	-1.83706900
C	-2.30983100	1.56615800	0.06119300
C	-3.32398600	1.69020100	1.02668000
C	-2.03084500	2.63769600	-0.79625300
C	-4.05520600	2.87358800	1.12198700
H	-3.54410200	0.86784900	1.70119300
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

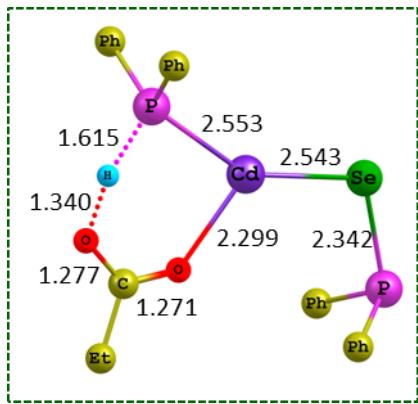
C/G-IM1



Cd	-0.02464100	-0.94571700	0.06282500
Se	0.57218100	-0.00265400	-2.25150200
P	2.64783100	1.03618800	-1.97777100
C	3.74068900	-0.23017100	-1.17619300
C	4.89793300	0.21045700	-0.50460700
C	3.56277900	-1.61060300	-1.36046900
C	5.83252000	-0.70319400	-0.01444100
H	5.06910500	1.27300800	-0.35472400
C	4.50101000	-2.52497500	-0.87067300
H	2.68491800	-1.97358900	-1.88633400
C	5.63762800	-2.07667000	-0.19444200
H	6.71319100	-0.34061600	0.50902600
H	4.33702900	-3.58910800	-1.01795300
H	6.36517400	-2.78750200	0.18718700
C	2.37450000	2.23499400	-0.58892200

C	2.27429900	1.88295400	0.76868800
C	2.24136600	3.58766100	-0.94579300
C	2.03906800	2.85870400	1.73937500
H	2.37921000	0.84779700	1.08011400
C	2.00574400	4.56568500	0.02617000
H	2.32419300	3.87512400	-1.99115900
C	1.90325700	4.20243000	1.37140200
H	1.95984900	2.56565800	2.78260500
H	1.90971900	5.60752700	-0.26793400
H	1.72241500	4.95970700	2.12939300
P	-2.62910400	-0.42342000	0.71248500
H	-3.05811600	-0.95378100	1.94876300
C	-3.04627700	1.35122000	0.92865900
C	-2.33415900	2.31139700	0.19230400
C	-4.05564000	1.76811500	1.81314600
C	-2.63843200	3.66869900	0.33067300
H	-1.53966700	2.00807000	-0.48488600
C	-4.34966600	3.12512800	1.95449700
H	-4.61262600	1.03648500	2.39216900
C	-3.64342300	4.07668200	1.21052600
H	-2.07962000	4.40272300	-0.24195900
H	-5.12830800	3.43906700	2.64380300
H	-3.87344600	5.13244300	1.32176600
C	-3.90678100	-1.13607800	-0.39574100
C	-4.96347300	-1.91225000	0.10640000
C	-3.80328000	-0.92927800	-1.78167700
C	-5.90713000	-2.46435600	-0.76401200
H	-5.05203200	-2.09089600	1.17444900
C	-4.75430400	-1.47357500	-2.64665500
H	-2.98097300	-0.34677400	-2.18956100
C	-5.80674200	-2.24238900	-2.13994900
H	-6.71923200	-3.06566500	-0.36549200
H	-4.66629500	-1.30475500	-3.71581900
H	-6.54155200	-2.67108100	-2.81509400
O	0.21293100	-2.91418600	1.24982400
O	0.92825500	-1.02509100	2.16718400
C	0.77187100	-2.28879400	2.20888800
C	1.25231800	-3.08476700	3.41149600
H	0.38255600	-3.63024300	3.79868100
H	1.92904800	-3.85644300	3.02465400
C	1.92480900	-2.26220400	4.51140800
H	2.23962700	-2.91306700	5.33431000
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H	1.24439900	-1.50544100	4.91278300

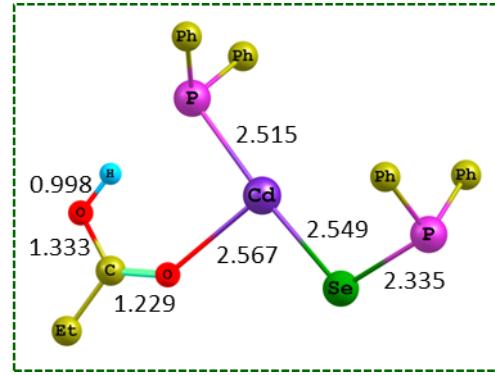
C/G-TS1



Se	-1.34913200	0.56901200	-2.45075700
P	-3.54363900	0.29622500	-1.68090100
C	-3.72634500	1.53986200	-0.32138900
C	-3.11724500	1.44541500	0.94249400
C	-4.51824900	2.66394400	-0.60895900
C	-3.29865800	2.45493800	1.88968200
H	-2.49938000	0.58700000	1.19095900
C	-4.69805000	3.67564100	0.34034000
H	-4.99530500	2.74750200	-1.58227300
C	-4.08755200	3.57278800	1.59204900
H	-2.82091900	2.37061100	2.86241500
H	-5.31417500	4.53805300	0.10117400
H	-4.22518200	4.35578500	2.33277300
C	-3.55591500	-1.31217600	-0.75978100
C	-2.79416000	-2.41147600	-1.19159200
C	-4.48850300	-1.51357700	0.27530500
C	-2.94076100	-3.66511400	-0.59221300
H	-2.07905900	-2.28408400	-1.99891900
C	-4.63357200	-2.76714300	0.87432800
H	-5.10129300	-0.68785700	0.62448200
C	-3.85860800	-3.84877100	0.44557700
H	-2.33677300	-4.49912500	-0.93999600
H	-5.35413900	-2.89631100	1.67762900
H	-3.97256800	-4.82360200	0.91146200
P	2.62520200	-0.04261900	0.37542400
C	3.74629800	-1.21135300	-0.48511200
C	3.65628200	-2.58069200	-0.17758900
C	4.66404400	-0.79070000	-1.46178400
C	4.46236500	-3.50879900	-0.84060700
H	2.96484000	-2.92176400	0.58868300
C	5.47515300	-1.72138800	-2.11522800
H	4.75040300	0.26336500	-1.70903100
C	5.37442300	-3.08229500	-1.81057000
H	4.38373200	-4.56324200	-0.59124500
H	6.18345600	-1.38182100	-2.86579100

H	6.00446900	-3.80403300	-2.32220000
C	3.50662400	1.55855000	0.51911400
C	4.54187200	1.69886200	1.46217000
C	3.15226800	2.66565300	-0.26946900
C	5.21009500	2.91607200	1.60371400
H	4.82215000	0.85520900	2.08655200
C	3.81945500	3.88587900	-0.12244300
H	2.35520300	2.57761300	-1.00269300
C	4.84937700	4.01224400	0.81250100
H	6.00696500	3.01046700	2.33594200
H	3.53278800	4.73319800	-0.73862700
H	5.36719700	4.96011900	0.92762100
Cd	0.23795700	0.11131300	-0.51731100
H	2.07916400	-0.64348300	1.77134300
C	-0.85156700	-1.58342200	3.67798800
H	-1.48537400	-0.73815000	3.97568600
H	-1.53314500	-2.30134600	3.20590200
O	1.32574300	-1.13407700	2.76429100
C	0.06470100	-1.06724300	2.57526600
O	-0.50313300	-0.60041000	1.53893200
C	-0.14938200	-2.19488100	4.89077300
H	0.51289500	-1.47094600	5.37374200
H	-0.88891600	-2.52936800	5.62615500
H	0.46083500	-3.05631200	4.60388400

C/G-IM2

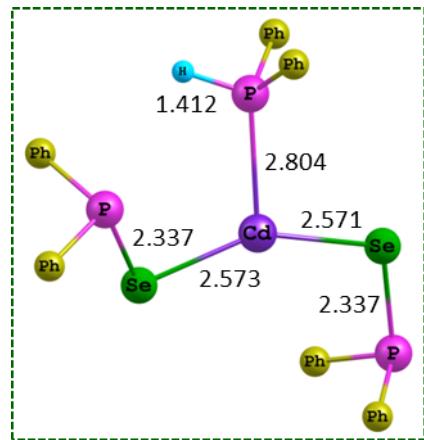


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P	3.15880000	-1.69666500	-0.48595100
C	3.03908200	-1.01675100	1.23392100
C	2.39184200	0.18059900	1.58429500
C	3.62661700	-1.78465300	2.25299400
C	2.32202000	0.59255700	2.91622400
H	1.94674400	0.80326700	0.81326600
C	3.55800700	-1.37542700	3.58851400
H	4.13656500	-2.71027700	1.99818100
C	2.90403700	-0.18717800	3.92244900
H	1.80760200	1.51546700	3.16790600

H	4.01676500	-1.98342300	4.36342400
H	2.84782200	0.13327200	4.95905900
C	3.22172900	-0.15220500	-1.51375500
C	4.15126200	0.85121900	-1.17507400
C	2.52448600	-0.02894400	-2.72690900
C	4.35733000	1.94989900	-2.01157900
H	4.71666600	0.77888200	-0.25010200
C	2.73634400	1.06889900	-3.56748200
H	1.81392100	-0.79751500	-3.01583100
C	3.65055300	2.06410300	-3.21343100
H	5.07306600	2.71554800	-1.72439500
H	2.18544600	1.14076700	-4.50165400
H	3.81673500	2.91548400	-3.86756000
P	-2.18358500	1.05120800	0.34424800
C	-1.54598800	1.84960700	1.88397800
C	-1.75325600	1.17923500	3.10526900
C	-0.92590200	3.11025100	1.91329500
C	-1.34539200	1.74485900	4.31344700
H	-2.24458600	0.20855000	3.11337900
C	-0.52712700	3.68097300	3.12667000
H	-0.75870600	3.65433700	0.98916000
C	-0.73201000	3.00265900	4.33090700
H	-1.51498300	1.20729400	5.24244600
H	-0.05522000	4.66006300	3.12613500
H	-0.42353000	3.44924100	5.27181600
C	-1.94468000	2.32009700	-0.97944100
C	-3.05649800	3.10145100	-1.34609300
C	-0.72947800	2.53348500	-1.65490500
C	-2.95445100	4.07112600	-2.34760200
H	-4.00714300	2.94746100	-0.84281800
C	-0.62690100	3.49933500	-2.65995000
H	0.14712100	1.94548500	-1.39836900
C	-1.73872800	4.27194500	-3.00731100
H	-3.82500600	4.66405000	-2.61420000
H	0.32236400	3.64352000	-3.16783400
H	-1.65917100	5.02195900	-3.78921600
Cd	-0.63761700	-0.84821000	-0.22956700
H	-3.90647400	-0.43871200	0.25358100
C	-4.84038600	-3.49229100	-0.37168200
H	-5.38372700	-3.60073900	0.57551200
H	-5.59939100	-3.19898000	-1.10816900
O	-4.53967800	-1.20405800	0.15787900
C	-3.90355900	-2.31530100	-0.21240800
O	-2.69097100	-2.37963400	-0.40423700
C	-4.14388900	-4.79201000	-0.77211300
H	-3.40154100	-5.09004500	-0.02661600

H	-4.87910100	-5.59684100	-0.86710000
H	-3.62475200	-4.68520000	-1.72844400

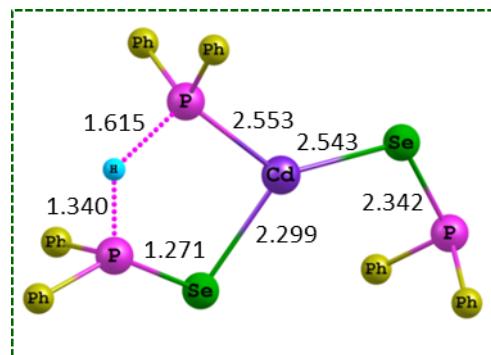
E/G-IM1



Se	2.71834400	1.64129800	0.71291100
P	4.59220900	0.40097300	0.07116300
C	4.13386100	-0.24656300	-1.60408800
C	3.36523800	-1.40173800	-1.83010500
C	4.58601900	0.48914300	-2.71314000
C	3.04836600	-1.80220200	-3.13039200
H	3.01728700	-1.99614700	-0.99038700
C	4.26642700	0.09117200	-4.01426000
H	5.18974000	1.37930500	-2.55428600
C	3.49568500	-1.05563900	-4.22562400
H	2.44823200	-2.69446600	-3.28543000
H	4.62376600	0.67242600	-4.85998500
H	3.24798600	-1.36880100	-5.23606800
C	4.55500900	-1.14848300	1.09240900
C	5.43150900	-2.18781200	0.72232400
C	3.83198900	-1.28006700	2.28679200
C	5.55695000	-3.33314800	1.50951400
H	6.01496900	-2.10756400	-0.19158400
C	3.96255200	-2.42640100	3.07847700
H	3.16280300	-0.48422800	2.59866800
C	4.82053000	-3.45782900	2.69273100
H	6.23029500	-4.12750000	1.19883700
H	3.38778400	-2.51041400	3.99700800
H	4.91800700	-4.34882200	3.30656200
Cd	0.63695600	0.29687300	0.02704200
Se	-0.44408600	-1.88623600	-0.80162300
P	-1.40847900	2.18569400	0.36134700
H	-2.65202000	1.73630000	-0.13431400
C	-1.87715000	2.63139200	2.08757600
C	-1.58994500	3.88867600	2.63698700
C	-2.47473500	1.64557100	2.89153300

C	-1.90606900	4.15969000	3.97188500
H	-1.12692900	4.65965400	2.02891200
C	-2.79460100	1.92518200	4.22129400
H	-2.68895100	0.66208000	2.47912800
C	-2.51001800	3.18192100	4.76561600
H	-1.68033200	5.13764800	4.38743300
H	-3.26367700	1.15919300	4.83241400
H	-2.75560100	3.39562500	5.80182100
C	-1.24042900	3.76405100	-0.55567600
C	-2.36846900	4.42761400	-1.07021200
C	0.03496300	4.31573700	-0.76072600
C	-2.22152100	5.62599000	-1.77087300
H	-3.36047300	4.00974400	-0.92294400
C	0.17609500	5.52108100	-1.45511200
H	0.92083800	3.80646200	-0.38987800
C	-0.94925600	6.17595800	-1.96111200
H	-3.09879200	6.12869400	-2.16789300
H	1.16708500	5.93898700	-1.60609700
H	-0.83679900	7.10856100	-2.50661800
P	-2.53267300	-1.58465300	0.20342900
C	-3.00195900	-3.34531100	0.52940000
C	-3.47514600	-4.22571700	-0.45780000
C	-2.86084700	-3.81727900	1.84513000
C	-3.80069800	-5.54442100	-0.13403900
H	-3.59143200	-3.87961400	-1.48040400
C	-3.18216400	-5.13829100	2.16859900
H	-2.49560000	-3.14720600	2.61953900
C	-3.65438900	-6.00461300	1.17897300
H	-4.16593300	-6.21404000	-0.90804200
H	-3.06696200	-5.48761200	3.19099500
H	-3.90800600	-7.03118000	1.42833100
C	-3.68283500	-1.15570900	-1.19371600
C	-5.04530900	-1.01740300	-0.86303900
C	-3.28098400	-0.87027500	-2.50591800
C	-5.97920100	-0.62476700	-1.82268000
H	-5.38048100	-1.22461400	0.15104800
C	-4.21670100	-0.46778300	-3.46672500
H	-2.23439200	-0.97167500	-2.77767700
C	-5.56655400	-0.34626200	-3.13106500
H	-7.02697500	-0.53368500	-1.54917100
H	-3.88565200	-0.25568500	-4.47997600
H	-6.29161900	-0.03643200	-3.87845500

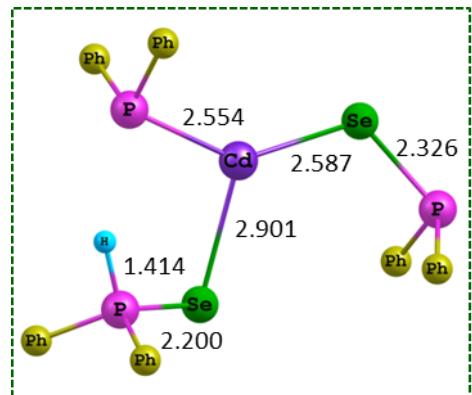
E/G-TS1



Se	-2.71797400	-2.37865700	0.00516200
P	-4.59852300	-1.00592900	-0.12992800
C	-4.34236200	-0.00357200	-1.66657800
C	-3.63373200	1.20776300	-1.73418800
C	-4.91292000	-0.51512000	-2.84545700
C	-3.49205800	1.88276000	-2.94915400
H	-3.19593700	1.63247900	-0.83621100
C	-4.76635500	0.15571000	-4.06228700
H	-5.47187100	-1.44686500	-2.80789900
C	-4.05488700	1.35768800	-4.11688400
H	-2.93552300	2.81536700	-2.98225900
H	-5.21208200	-0.25693100	-4.96327900
H	-3.94155200	1.88338000	-5.06097100
C	-4.42176700	0.26944000	1.20629400
C	-5.26948600	1.39435500	1.16112000
C	-3.62282600	0.08633000	2.34509300
C	-5.29388100	2.31685100	2.20813200
H	-5.91164500	1.55613400	0.29922100
C	-3.65230000	1.00758600	3.39772100
H	-2.97848800	-0.78501400	2.41048200
C	-4.48352900	2.12779500	3.33311900
H	-5.94850500	3.18209500	2.14590900
H	-3.02363800	0.84424500	4.26934400
H	-4.50673900	2.84291100	4.15076100
Cd	-0.55237400	-1.01049800	-0.16388800
Se	-0.11187300	1.60868600	-0.83416600
P	1.90521600	-1.62898100	0.29677000
H	2.33634700	0.15374200	0.28768700
C	2.22274900	-2.55726100	1.84904500
C	1.24155500	-3.38483200	2.42383800
C	3.45476200	-2.41141400	2.51425900
C	1.48845700	-4.05272300	3.62686800
H	0.28255800	-3.50944900	1.92924100
C	3.70337800	-3.08480200	3.71262600
H	4.22112400	-1.76786700	2.09088700
C	2.71924600	-3.90573200	4.27241100

H	0.71836000	-4.68720900	4.05647000
H	4.66106200	-2.96283400	4.21114400
H	2.90986000	-4.42504800	5.20737200
C	2.66882100	-2.56717400	-1.08000400
C	3.40775000	-3.74801000	-0.88749800
C	2.53520700	-2.06562600	-2.39099800
C	3.99486600	-4.40381400	-1.97322100
H	3.52101100	-4.16045300	0.11000900
C	3.12400900	-2.72395400	-3.47124500
H	1.95946700	-1.16044700	-2.57274600
C	3.85882300	-3.89723500	-3.26853800
H	4.55687400	-5.31825600	-1.80263100
H	3.00209700	-2.32192100	-4.47343100
H	4.31328700	-4.41184800	-4.11002100
P	1.96950700	1.75232200	0.02424700
C	1.99629700	2.84957400	1.49229300
C	0.82451200	3.14897300	2.20341900
C	3.23365000	3.31393500	1.97758200
C	0.88825400	3.90788600	3.37542000
H	-0.13446400	2.80148600	1.83166500
C	3.29041400	4.07149500	3.14796000
H	4.15074100	3.09300200	1.43871200
C	2.11776900	4.37061300	3.85033500
H	-0.02726000	4.14002800	3.91194200
H	4.25018500	4.42956700	3.50956000
H	2.16418400	4.96178200	4.76037100
C	3.10913100	2.50700600	-1.18920100
C	4.03674100	1.68264000	-1.84685200
C	3.06093600	3.87674900	-1.49912300
C	4.90735000	2.22285100	-2.79789100
H	4.08210400	0.62076900	-1.62215700
C	3.93184300	4.41142200	-2.44880500
H	2.34390000	4.52195800	-1.00012000
C	4.85594500	3.58574300	-3.09958300
H	5.62252500	1.57760100	-3.29971800
H	3.88742900	5.47099200	-2.68400400
H	5.53215900	4.00499000	-3.83910200

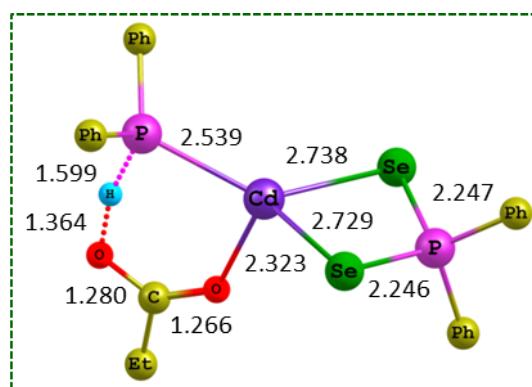
E/G-IM2



Se	-2.36398700	-2.50649300	0.15796900
P	-4.30029700	-1.23300500	-0.03720000
C	-4.17083800	-0.39960400	-1.68668500
C	-3.59723200	0.86075100	-1.92197800
C	-4.70619400	-1.10677600	-2.77823300
C	-3.55155000	1.39352800	-3.21309200
H	-3.19015100	1.43461000	-1.09575100
C	-4.65331700	-0.57936300	-4.07052900
H	-5.16270900	-2.07948700	-2.61264000
C	-4.07552900	0.67429900	-4.29174400
H	-3.09889400	2.36815100	-3.37479000
H	-5.06823800	-1.14388500	-4.90112900
H	-4.03614700	1.08892500	-5.29525400
C	-4.14299300	0.18350100	1.15103900
C	-5.05428900	1.25277100	1.03701700
C	-3.29168200	0.15537100	2.26632900
C	-5.08871800	2.27174500	1.99031900
H	-5.74102300	1.29379700	0.19558200
C	-3.33215400	1.17180900	3.22686600
H	-2.59926300	-0.67224900	2.38684200
C	-4.22643600	2.23620000	3.09187700
H	-5.79447200	3.09021900	1.87551300
H	-2.66538200	1.12394700	4.08415000
H	-4.26259500	3.02299700	3.84055000
Cd	-0.14503600	-1.18745300	-0.00758900
Se	-0.21253100	1.54190100	-0.98716800
P	2.34513900	-1.53543500	0.44011400
H	2.35410100	1.13031800	0.47593400
C	2.37572900	-2.63543900	1.93372100
C	1.46943200	-3.68884000	2.16000400
C	3.34673700	-2.37623300	2.91777900
C	1.53484800	-4.45625500	3.32494800
H	0.70434500	-3.91140600	1.42155100
C	3.41300500	-3.14101400	4.08760600
H	4.05865800	-1.56980900	2.76202400

C	2.50643400	-4.18323000	4.29413000
H	0.82142200	-5.26132200	3.47834400
H	4.17208600	-2.92130700	4.83371800
H	2.55305100	-4.77705000	5.20278200
C	2.79948400	-2.65691300	-0.96282400
C	3.34410400	-3.94123100	-0.78681500
C	2.68673100	-2.16236200	-2.27872100
C	3.75180800	-4.70402400	-1.88607900
H	3.44944900	-4.35263000	0.21193800
C	3.09045200	-2.92590600	-3.37396900
H	2.27097400	-1.17120800	-2.45123500
C	3.62712500	-4.20468600	-3.18447300
H	4.16601500	-5.69553600	-1.72157900
H	2.98199200	-2.52277200	-4.37756500
H	3.93980600	-4.80137400	-4.03650300
P	1.64343800	2.24088900	-0.03580600
C	1.37890700	3.40141300	1.35293200
C	0.11447300	3.52302000	1.94456100
C	2.46508500	4.13447100	1.86201700
C	-0.06174900	4.37360500	3.03940100
H	-0.72660900	2.96195700	1.54860300
C	2.28145300	4.97955300	2.95712900
H	3.44692400	4.05333100	1.40467800
C	1.01810000	5.10026100	3.54621600
H	-1.04508900	4.46623400	3.49033100
H	3.12272800	5.54492400	3.34709000
H	0.87758800	5.76127700	4.39659200
C	2.84827600	2.99341600	-1.16904300
C	4.03047000	2.29799600	-1.46774200
C	2.58710000	4.22987000	-1.78097200
C	4.95114900	2.84625600	-2.36517000
H	4.23187100	1.33378300	-1.00853800
C	3.51076800	4.77060000	-2.67511500
H	1.66799200	4.76624100	-1.56224500
C	4.69262700	4.07978000	-2.96771800
H	5.86503600	2.30610500	-2.59356200
H	3.30761700	5.72767400	-3.14629700
H	5.40836800	4.50265700	-3.66665200

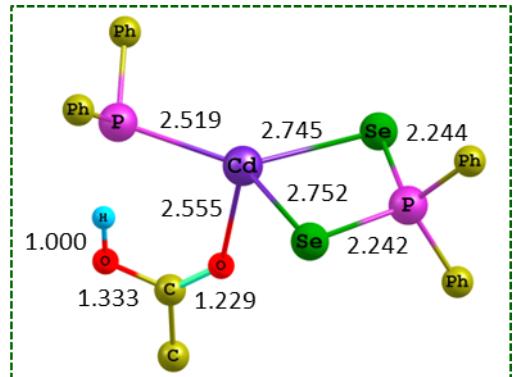
F/E-i-TS1a



Cd	0.62319800	0.22256800	-0.10700700
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C	1.70871000	3.28454700	-0.72371000
C	1.42967200	4.76169600	-0.98955700
H	1.97229600	5.32625400	-0.22083700
H	1.92624400	5.01022300	-1.93553300
C	-0.04659800	5.15648800	-1.02093900
H	-0.14849300	6.23044300	-1.21193800
H	-0.58274600	4.61708000	-1.80759500
H	-0.53630000	4.92967600	-0.06925000
O	2.94539000	2.95333000	-0.72274500
H	3.22599800	1.63445700	-0.51631000
P	-2.60365500	-0.39347800	0.07006300
Se	-1.35503200	-0.66735400	-1.77769500
Se	-1.26264200	-0.07041300	1.84305700
C	-3.69144600	-1.84703500	0.33192000
C	-4.02963800	-2.25544100	1.63051100
C	-4.20698200	-2.54343100	-0.77241100
C	-4.88851300	-3.34101600	1.82033600
H	-3.61443000	-1.73689200	2.48912300
C	-5.06496100	-3.62758700	-0.57652100
H	-3.93024100	-2.24855400	-1.78003200
C	-5.40768300	-4.02698400	0.71893600
H	-5.14333800	-3.65327900	2.82888600
H	-5.45772900	-4.16335200	-1.43578200
H	-6.07030400	-4.87458900	0.86899700
C	-3.71948400	1.04787100	-0.14171000
C	-5.11265700	0.92339400	-0.04496000
C	-3.14819000	2.30558800	-0.40045300
C	-5.92805600	2.04837100	-0.20785400
H	-5.56707200	-0.04079400	0.15573500
C	-3.96801800	3.42118800	-0.56138400
H	-2.06991800	2.41517300	-0.47539400
C	-5.35906800	3.29624100	-0.46621500
H	-7.00655700	1.94323000	-0.13215200

H	-3.51896600	4.38956200	-0.76143000	H	-0.66454700	5.05255400	-0.57488800
H	-5.99374100	4.16869000	-0.59295000	O	3.07061800	3.45688100	-0.66420200
P	3.15678400	0.07506000	-0.16821700	H	3.27978500	2.50133000	-0.45434500
C	3.99527300	-0.24127100	1.43167400	P	-2.41995900	-0.18188000	0.04866900
C	4.28257600	0.84539400	2.27615500	Se	-1.14477900	-0.53199100	-1.76386200
C	4.32672100	-1.53968400	1.85455700	Se	-1.12303400	0.36778200	1.79337600
C	4.88222400	0.63440000	3.52071900	C	-3.41782400	-1.67854300	0.41290400
H	4.04631800	1.85705700	1.95737800	C	-3.15456700	-2.46525200	1.54234200
C	4.93647300	-1.74493100	3.09374700	C	-4.42829200	-2.06528600	-0.48372700
H	4.11295400	-2.39039100	1.21371100	C	-3.89963600	-3.62463100	1.77570900
C	5.21260000	-0.65974800	3.93205500	H	-2.37014000	-2.17223000	2.23331000
H	5.09935200	1.48358300	4.16264100	C	-5.16957100	-3.22283900	-0.24461100
H	5.19102400	-2.75386100	3.40647000	H	-4.63641300	-1.46754200	-1.36623100
H	5.68402100	-0.82230900	4.89705300	C	-4.90650400	-4.00476800	0.88521900
C	3.90918300	-1.05472300	-1.40111700	H	-3.69002300	-4.22855500	2.65379500
C	5.28323600	-0.96203600	-1.69129700	H	-5.94974300	-3.51472300	-0.94170500
C	3.12927800	-1.98890300	-2.10164300	H	-5.48376200	-4.90662600	1.06810800
C	5.86049700	-1.79059600	-2.65407300	C	-3.65256800	1.14130100	-0.26990500
H	5.90031500	-0.24060600	-1.16313200	C	-4.78094900	1.25287600	0.55969100
C	3.70854300	-2.81244200	-3.07259700	C	-3.46044900	2.06434700	-1.30662500
H	2.06781200	-2.07952900	-1.88806500	C	-5.70848000	2.27346400	0.34572700
C	5.07398200	-2.71670900	-3.34881400	H	-4.93699600	0.54877900	1.37124200
H	6.92264300	-1.70865200	-2.86725600	C	-4.39200200	3.08493200	-1.51492200
H	3.09128700	-3.52970100	-3.60604300	H	-2.58831600	1.98173800	-1.94763700
H	5.52473900	-3.35795100	-4.10089400	C	-5.51641400	3.19060500	-0.69253900
				H	-6.57892800	2.35227100	0.99063300
				H	-4.23801600	3.79420700	-2.32300100
				H	-6.23960600	3.98418200	-0.85783600

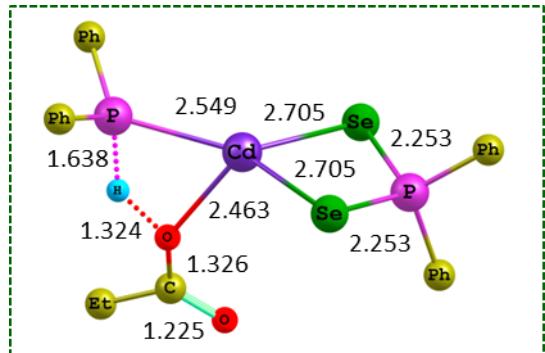
F/E-i-IM2a



Cd	0.87473500	0.29587600	-0.09863000	H	3.68418900	0.29302900	4.92751500
O	0.91705400	2.76317800	-0.76234000	H	5.46046900	-3.13643300	3.02831300
C	1.76412700	3.64981000	-0.84163000	H	4.90608500	-1.87424300	5.10248300
C	1.43521500	5.09528400	-1.14772400	C	3.96651800	-0.91598700	-1.29471400
H	1.78973700	5.68796600	-0.29456200	C	5.15807600	-0.63248500	-1.98658600
H	2.06372500	5.39957100	-1.99366000	C	3.26186500	-2.08506300	-1.63601900
C	-0.04529500	5.35088500	-1.42515700	C	5.63327700	-1.49032600	-2.98338000
H	-0.21270000	6.41491500	-1.61902400	H	5.71598600	0.26737900	-1.74202900
H	-0.38615500	4.78554200	-2.29734200	C	3.73381200	-2.94286500	-2.63296400

H	2.33730000	-2.32778700	-1.11970500
C	4.92124100	-2.64730700	-3.30995400
H	6.55584500	-1.25124800	-3.50539700
H	3.17140100	-3.83851500	-2.88220900
H	5.28615500	-3.31228300	-4.08774100

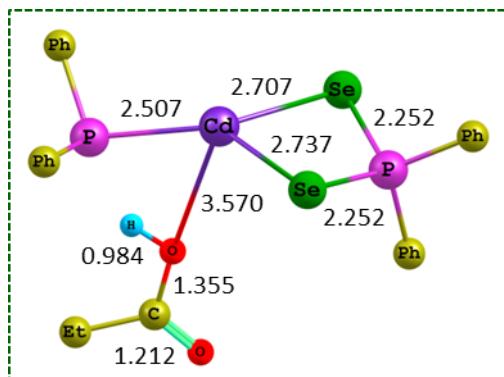
F/E-i-TS1b



Cd	0.55705700	-0.17796400	0.05342400
O	0.02517800	3.75624800	-0.27328700
C	1.18055100	3.36072300	-0.18258200
C	2.38525300	4.27769400	-0.38966300
H	3.00280200	4.22199900	0.51652400
H	2.99694100	3.84165900	-1.19099800
C	2.01800000	5.72579400	-0.71202600
H	2.92194800	6.32846000	-0.85206500
H	1.41790900	5.78444400	-1.62447600
H	1.42796600	6.16982900	0.09478000
O	1.48494900	2.10270200	0.10559800
H	2.63687800	1.45439400	0.03792000
P	-2.71392200	-0.37750500	0.03734500
Se	-1.40353400	-0.41685000	-1.79533700
Se	-1.41225600	-0.55996300	1.86753400
C	-3.93068900	-1.74707000	-0.03909600
C	-4.20307800	-2.53689900	1.08600500
C	-4.60561600	-1.99853000	-1.24550200
C	-5.15453900	-3.55845600	1.00922000
H	-3.66843700	-2.36195400	2.01428500
C	-5.55354800	-3.01977000	-1.31631200
H	-4.38700600	-1.40570400	-2.12872000
C	-5.83017500	-3.80075200	-0.18886400
H	-5.35953200	-4.16661700	1.88542700
H	-6.06979600	-3.20922700	-2.25288200
H	-6.56495500	-4.59864000	-0.24760800
C	-3.68439200	1.17346500	0.09554000
C	-5.07375400	1.15666100	0.29676700
C	-3.00875000	2.39906200	-0.03190400
C	-5.78241100	2.35962300	0.36421100

H	-5.60608200	0.21726700	0.40021300
C	-3.72577900	3.59334800	0.03819700
H	-1.93347400	2.44661200	-0.18117600
C	-5.11092400	3.57754100	0.23435200
H	-6.85762800	2.33966100	0.51774000
H	-3.19057100	4.53269100	-0.06128300
H	-5.66423600	4.51113900	0.28633300
P	3.10485600	-0.11490500	0.03549900
C	4.02389700	-0.64868300	1.52487700
C	3.88289900	0.09807900	2.70885100
C	4.83469000	-1.79589100	1.53761600
C	4.53505900	-0.29792300	3.87797000
H	3.26388000	0.99167500	2.71683300
C	5.49373700	-2.18232300	2.70740400
H	4.95422600	-2.38696900	0.63461000
C	5.34488200	-1.43808600	3.88122500
H	4.41524100	0.28934500	4.78407900
H	6.12008800	-3.07014900	2.70062000
H	5.85567600	-1.74266000	4.79004400
C	3.99373300	-0.73707400	-1.43872400
C	5.32171300	-0.33912300	-1.68421600
C	3.35399900	-1.57113600	-2.37026300
C	5.99141100	-0.77314200	-2.82887900
H	5.83092100	0.31032900	-0.97762400
C	4.02272300	-1.99438300	-3.52339500
H	2.33234800	-1.89528000	-2.19389000
C	5.34225100	-1.59943100	-3.75333300
H	7.01685400	-0.45971300	-3.00355100
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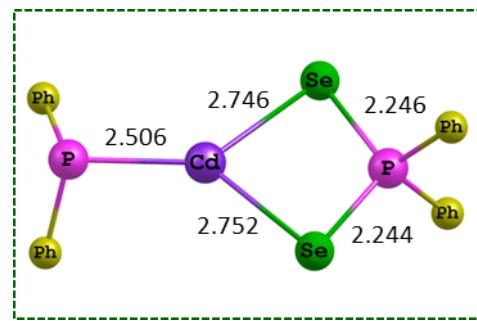


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C	2.97350500	4.39469200	-0.56368800

H	3.24943500	3.85463700	0.35183800
H	3.64539900	4.01426500	-1.34515600
C	3.14791100	5.90249700	-0.38406900
H	4.18454300	6.13451100	-0.12062700
H	2.89401900	6.43864000	-1.30238000
H	2.49618200	6.28070400	0.40829300
O	1.33453900	2.66095700	-1.06714800
H	2.12735900	2.11544700	-0.86215200
P	-2.67588300	-0.32807600	0.02695200
Se	-1.50090100	-0.86393100	-1.81838300
Se	-1.37554600	-0.67543800	1.83251300
C	-4.20549500	-1.33147400	0.09746100
C	-4.42651100	-2.25305500	1.12851100
C	-5.14789900	-1.20293400	-0.93790800
C	-5.58902300	-3.03024900	1.13235300
H	-3.69203300	-2.36538200	1.91994800
C	-6.30423700	-1.98224500	-0.92920800
H	-4.98019100	-0.49988700	-1.74869700
C	-6.52705200	-2.89671300	0.10674100
H	-5.75580800	-3.74061700	1.93679700
H	-7.02851000	-1.87788200	-1.73172700
H	-7.42789000	-3.50365800	0.11059900
C	-3.20589300	1.42394600	-0.02649200
C	-4.42575400	1.81686200	0.54834100
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C	-2.69643700	3.74428400	-0.51981300
H	-1.39782000	2.11072200	-1.00967400
C	-3.91563300	4.13162500	0.04498900
H	-5.72570400	3.46495400	1.01705200
H	-2.00509700	4.47815800	-0.92272500
H	-4.19134200	5.18203800	0.07413900
P	2.99141500	-0.02781600	-0.16204200
C	3.62528800	-0.33485600	1.54662600
C	2.95566300	0.26127400	2.63352100
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C	3.45308700	0.15115000	3.93231800
H	2.03204800	0.81213500	2.46786900
C	5.31161600	-1.14690800	3.10807000
H	5.36029400	-1.50141700	0.98956700
C	4.63524400	-0.55603900	4.17771000
H	2.91277000	0.61415900	4.75359000
H	6.23214300	-1.69765600	3.28285200
H	5.02132900	-0.64515700	5.18895200
C	3.81330100	-1.30499500	-1.21833000

C	4.56901000	-0.86624500	-2.31876700
C	3.70138500	-2.69073100	-0.99600100
C	5.19054900	-1.78145000	-3.17577100
H	4.67310800	0.19926600	-2.50452300
C	4.32712800	-3.60489700	-1.84479800
H	3.12440600	-3.05604000	-0.15057400
C	5.07183500	-3.15233900	-2.94034000
H	5.76755600	-1.42036500	-4.02261100
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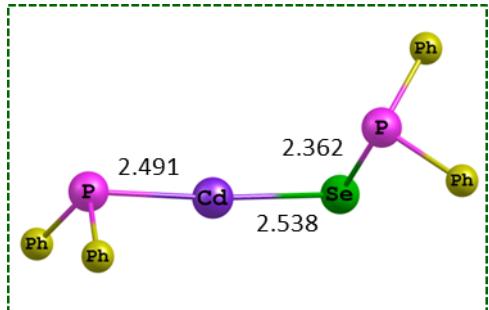
E-i



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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	3.43399600	1.42429200	0.40529300
C	3.74928700	-0.71721500	-0.91889100	C	4.51716200	1.97010400	-0.31117600
C	4.70473200	-1.50441900	-0.25351000	C	3.09001000	1.99816000	1.63791700
C	3.85249200	-0.52031500	-2.30143000	C	5.24286200	3.04634600	0.20096100
C	5.75515000	-2.07962000	-0.96779600	H	4.80232300	1.54840900	-1.27168100
H	4.63182200	-1.66732200	0.81788200	C	3.81681300	3.07941600	2.14849300
C	4.90701400	-1.10128100	-3.01263600	H	2.26027300	1.59230900	2.20812400
H	3.11414600	0.08661700	-2.81607800	C	4.89478800	3.60667200	1.43490600
C	5.85778500	-1.87946700	-2.34918500	H	6.08023300	3.44657400	-0.36420100
H	6.49095600	-2.68558400	-0.44723900	H	3.53867700	3.50414300	3.10932800
H	4.98237800	-0.94170100	-4.08431400	H	5.45919500	4.44482900	1.83370800
H	6.67613700	-2.32955200	-2.90382900	P	-2.98698700	-0.35209600	-1.24944100
C	3.16469900	0.83029200	1.46577900	C	-4.22053300	-1.08853900	-0.06913800
C	4.19387200	1.75178100	1.20696100	C	-4.96564500	-2.18740200	-0.53114900
C	2.74995100	0.60423600	2.78384600	C	-4.43640000	-0.64631100	1.25058700
C	4.80311000	2.43207900	2.26074000	C	-5.89159900	-2.83017900	0.29840700
H	4.51943100	1.93872000	0.18774400	H	-4.82174400	-2.53861700	-1.54960900
C	3.36342000	1.29077000	3.83640000	C	-5.36570300	-1.28031700	2.07643400
H	1.95396300	-0.10626900	2.98359100	H	-3.87918700	0.20511500	1.63276500
C	4.38820400	2.20315700	3.57768000	C	-6.09459700	-2.37822400	1.60351000
H	5.59862000	3.14201700	2.05400300	H	-6.45532900	-3.67856400	-0.07973800
H	3.03868900	1.10819300	4.85662600	H	-5.51625400	-0.92260200	3.09143500
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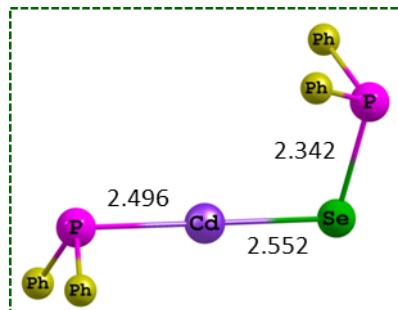
G-i



Se	1.28064700	-0.92852700	1.34198200
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C	4.78724000	-1.47642000	0.06232200
C	3.64053700	-1.83116500	-2.03795700
C	5.72084900	-2.45326500	-0.28474000
H	4.87629000	-0.96156100	1.01449000
C	4.57548400	-2.81162600	-2.38588500
H	2.83291000	-1.58895900	-2.72441400
C	5.61684300	-3.12400400	-1.50937300
H	6.52897400	-2.69410800	0.40058100
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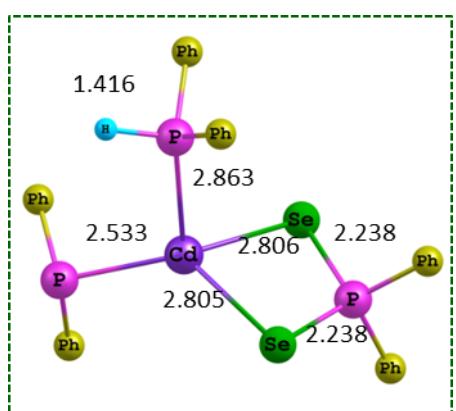
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C	3.09001000	1.99816000	1.63791700
C	5.24286200	3.04634600	0.20096100
H	4.80232300	1.54840900	-1.27168100
C	3.81681300	3.07941600	2.14849300
H	2.26027300	1.59230900	2.20812400
C	4.89478800	3.60667200	1.43490600
H	6.08023300	3.44657400	-0.36420100
H	3.53867700	3.50414300	3.10932800
H	5.45919500	4.44482900	1.83370800
P	-2.98698700	-0.35209600	-1.24944100
C	-4.22053300	-1.08853900	-0.06913800
C	-4.96564500	-2.18740200	-0.53114900
C	-4.43640000	-0.64631100	1.25058700
C	-5.89159900	-2.83017900	0.29840700
H	-4.82174400	-2.53861700	-1.54960900
C	-5.36570300	-1.28031700	2.07643400
H	-3.87918700	0.20511500	1.63276500
C	-6.09459700	-2.37822400	1.60351000
H	-6.45532900	-3.67856400	-0.07973800
H	-5.51625400	-0.92260200	3.09143500
H	-6.81387100	-2.87431800	2.24890200
C	-3.27520800	1.47719500	-1.12656400
C	-4.52742800	2.02534800	-0.79723000
C	-2.25315200	2.35836600	-1.53075900
C	-4.74229700	3.40617100	-0.85517600
H	-5.34278200	1.37570800	-0.49508900
C	-2.46807500	3.73574500	-1.58752000
H	-1.27520000	1.96788700	-1.80659900
C	-3.71599200	4.26872000	-1.24682400
H	-5.71874100	3.80496500	-0.59296200
H	-1.65863600	4.39237100	-1.89467300
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G



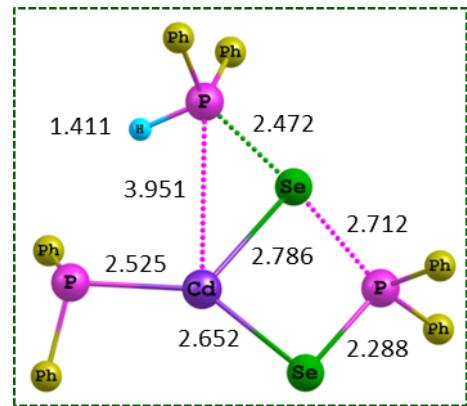
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C	2.06822000	1.43338200	-1.36882000	E-i/G-IM1			
C	2.55918900	3.07989200	0.33209100				
C	1.48075300	2.42629700	-2.15856200				
H	2.12000100	0.41565200	-1.74536800				
C	1.96807500	4.07180900	-0.45491300				
H	2.98200400	3.34012400	1.29918800				
C	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				
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H	3.53267100	-4.18975500	-0.76798600				
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H	-2.94459800	-2.51750800	-2.62426800				
C	-4.29271300	-3.09378800	0.96420400				
H	-3.45111200	-1.17486000	1.43556800				
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H	-4.16021000	-4.60497600	-2.08313000				
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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				
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H	-5.26118300	4.40140000	0.37272300				



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H	-5.86380100	1.36580600	-3.19460100
H	-6.09873700	-0.45811300	0.69977100
H	-7.13840300	0.05982500	-1.50090400
C	-1.83938300	3.64228200	-0.77847100
C	-2.85180200	4.44550400	-0.22631600
C	-0.83851900	4.22926500	-1.56247900
C	-2.86281800	5.81943100	-0.46580300
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H	-0.05324000	3.61065300	-1.98566000
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H	-3.64934500	6.43374900	-0.03704000
H	-0.07402200	6.05481200	-2.40767000
H	-1.87246300	7.47381800	-1.43627500
P	-0.02484800	-2.69634100	0.89191500
H	0.89427500	-3.41495400	1.69494400
C	0.06349400	-3.72420900	-0.62435300
C	-0.53619500	-3.25549100	-1.80620200
C	0.74286400	-4.95408600	-0.64207000
C	-0.47268700	-4.01503200	-2.97670200
H	-1.03953600	-2.29278000	-1.81789300
C	0.81370500	-5.70533700	-1.81796300
H	1.21983800	-5.32551700	0.26058000
C	0.20231200	-5.23926100	-2.98538000
H	-0.94050100	-3.64246300	-3.88341600
H	1.34625000	-6.65213800	-1.82072900
H	0.25773200	-5.82425800	-3.89905100
C	-1.61017500	-3.15489200	1.72453300
C	-2.40466400	-4.23570000	1.31266800
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C	-3.58625000	-4.54128900	1.99389100
H	-2.10403100	-4.84008400	0.46278400
C	-3.20084900	-2.69315300	3.50454600
H	-1.44176000	-1.51596800	3.12881500
C	-3.98416700	-3.77544000	3.09343500
H	-4.19295800	-5.38056100	1.66530700
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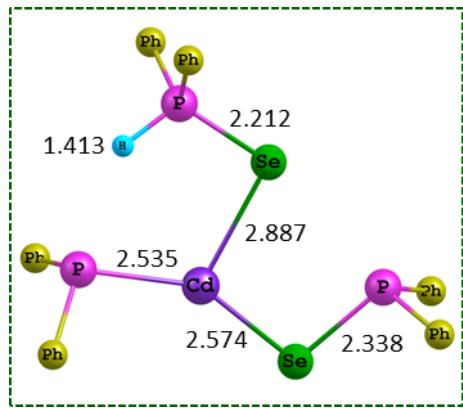
E-i/G-TS1



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Se	0.45240400	-1.27217100	0.06812700
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Cd	-0.05736500	1.41643700	-0.45656900
C	4.15477200	-0.75404800	-1.12216100
C	4.37214100	-0.09494600	-2.34100700
C	4.81411600	-1.97416900	-0.88102300
C	5.23940400	-0.63782700	-3.29425100
H	3.87173900	0.84878400	-2.53526300
C	5.67992700	-2.51226500	-1.83397000
H	4.65738700	-2.50231200	0.05559600
C	5.89572400	-1.84544800	-3.04509700
H	5.40446000	-0.11013500	-4.22971400
H	6.18694300	-3.45133100	-1.62958500
H	6.57115600	-2.26423100	-3.78582200
C	3.84749800	-0.24804700	1.70730200
C	3.18838000	-0.76477600	2.83309500
C	5.16964200	0.21097400	1.83596400
C	3.84147900	-0.82471700	4.06855000
H	2.16574800	-1.11998400	2.74002800
C	5.81899500	0.14928200	3.06924600
H	5.68891700	0.61689400	0.97278500
C	5.15612300	-0.36874800	4.18834700
H	3.32261300	-1.22912900	4.93327800
H	6.84062300	0.50824200	3.15879400
H	5.66396700	-0.41499500	5.14772900
C	-2.24990000	-3.42566500	1.10566800
C	-1.67064900	-4.69013700	0.90859900
C	-3.04625100	-3.20062600	2.23992000
C	-1.89779000	-5.71637500	1.82626200
H	-1.04481000	-4.87434800	0.03964400
C	-3.26574100	-4.23042300	3.15905700
H	-3.49728800	-2.22590800	2.40562200

C	-2.69415200	-5.48877300	2.95386400
H	-1.44993300	-6.69239300	1.66314500
H	-3.88560100	-4.04814600	4.03235100
H	-2.86702000	-6.28850200	3.66818500
C	-2.43412600	-2.62382600	-1.71376800
C	-1.50962500	-2.67408600	-2.76573200
C	-3.77050300	-2.99356000	-1.94597700
C	-1.91575500	-3.09273200	-4.03719200
H	-0.47875100	-2.38070700	-2.58899900
C	-4.17208000	-3.40627800	-3.21676900
H	-4.49428800	-2.96350400	-1.13608800
C	-3.24437300	-3.45675300	-4.26393200
H	-1.19319700	-3.12833800	-4.84729500
H	-5.20699800	-3.68685400	-3.39064500
H	-3.55973100	-3.77719200	-5.25281800
P	-2.28500200	2.47144700	-1.00490500
C	-3.38302800	1.77309500	0.32696300
C	-3.07097900	1.76210700	1.70088800
C	-4.59978300	1.19173300	-0.07443600
C	-3.94032100	1.19487800	2.63496800
H	-2.14159700	2.20942100	2.04321600
C	-5.47106300	0.61425500	0.85764100
H	-4.86675900	1.19903100	-1.12800000
C	-5.14457300	0.61502000	2.21583100
H	-3.67741200	1.20382400	3.68956900
H	-6.40712000	0.17597600	0.52135900
H	-5.82288900	0.17694200	2.94301700
C	-2.00968500	4.22158100	-0.45379800
C	-2.88073000	4.90579100	0.41324400
C	-0.95369200	4.95183200	-1.03516000
C	-2.69310100	6.26236900	0.69763200
H	-3.71319800	4.38155700	0.87185100
C	-0.76760300	6.30496100	-0.75220300
H	-0.26439300	4.45588400	-1.71550100
C	-1.63651100	6.97007400	0.12015700
H	-3.37973600	6.76490800	1.37429700
H	0.06103800	6.83899100	-1.20974500
H	-1.49060400	8.02270300	0.34493600

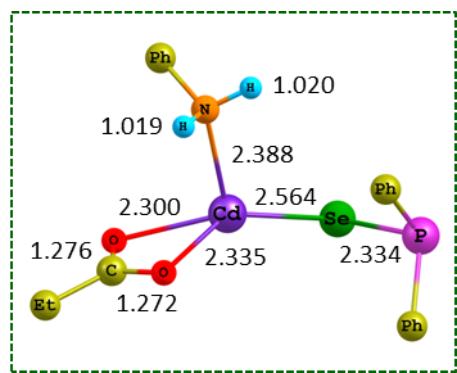
E-i/G-IM2



P	3.28410800	-0.55797600	0.27507000
Se	2.51204900	1.64794700	0.31859000
P	-2.20089000	-2.04540200	-0.38076700
Se	-0.02096700	-1.79122200	-0.10592000
H	-2.80309200	-0.81656200	-0.73377300
Cd	0.03727000	1.09530500	-0.12577200
C	4.56612200	-0.56980900	-1.07005500
C	4.72553100	0.44055900	-2.02849300
C	5.35011000	-1.73448400	-1.18579500
C	5.65345600	0.29852200	-3.06701400
H	4.12779400	1.34407900	-1.95761300
C	6.27924500	-1.87303300	-2.21745700
H	5.23834900	-2.53742100	-0.46069900
C	6.43457300	-0.85451700	-3.16483700
H	5.76564000	1.09651400	-3.79643100
H	6.87987700	-2.77643600	-2.28294400
H	7.15572700	-0.96203100	-3.97037800
C	4.35900000	-0.59955400	1.78365000
C	3.87031900	-1.29660600	2.90079600
C	5.61114100	0.03143000	1.87519700
C	4.61294300	-1.36166300	4.08381800
H	2.90412400	-1.79169400	2.84174000
C	6.35416400	-0.03498800	3.05504000
H	6.00541200	0.57523900	1.02185000
C	5.85699600	-0.73085900	4.16301600
H	4.22125300	-1.90671600	4.93850500
H	7.32071300	0.45872200	3.11146100
H	6.43771800	-0.78168200	5.08000600
C	-3.12610900	-2.52648700	1.11082200
C	-3.03716200	-3.83417900	1.61454600
C	-3.87926900	-1.56168500	1.79752900
C	-3.70960600	-4.17492500	2.78803200
H	-2.44713400	-4.58248800	1.09283900
C	-4.54844700	-1.90950100	2.97418100
H	-3.94369700	-0.54249600	1.42636800

C	-4.46537700	-3.21337400	3.46869200
H	-3.64117100	-5.18803600	3.17316100
H	-5.12953100	-1.15893800	3.50140100
H	-4.98550000	-3.48102100	4.38386800
C	-2.64525000	-3.22674100	-1.70565400
C	-1.66652900	-3.70679300	-2.58539700
C	-3.98566700	-3.61691500	-1.86920300
C	-2.02573800	-4.57417700	-3.62114800
H	-0.63180700	-3.40377400	-2.45568200
C	-4.33808400	-4.47944300	-2.90782200
H	-4.75085800	-3.25593500	-1.18780200
C	-3.35828300	-4.95945700	-3.78401900
H	-1.26235200	-4.94575800	-4.29824100
H	-5.37504500	-4.77776600	-3.03095800
H	-3.63503000	-5.63274100	-4.59021400
P	-2.32213800	1.87176000	-0.63139100
C	-2.98155700	2.47222200	0.99800400
C	-2.20113300	2.72655100	2.14062600
C	-4.37755100	2.63546200	1.10829000
C	-2.78904800	3.12415100	3.34631500
H	-1.12026200	2.62499400	2.09214700
C	-4.96750700	3.04605700	2.30668100
H	-5.00488600	2.44156500	0.24175300
C	-4.17383700	3.28756500	3.43277900
H	-2.16119700	3.31183000	4.21307400
H	-6.04554100	3.17332700	2.36093700
H	-4.63034300	3.60086300	4.36755100
C	-2.03604600	3.43335300	-1.58611800
C	-2.09271100	4.72448400	-1.03308300
C	-1.77813600	3.31257900	-2.96576200
C	-1.89491500	5.85411200	-1.83267900
H	-2.29074800	4.85173400	0.02663000
C	-1.56609500	4.44024700	-3.76015700
H	-1.74920300	2.32571600	-3.42323200
C	-1.62550200	5.71971500	-3.19729900
H	-1.94496900	6.84229400	-1.38258400
H	-1.36325400	4.31971600	-4.82111600
H	-1.46718100	6.59894700	-3.81518500

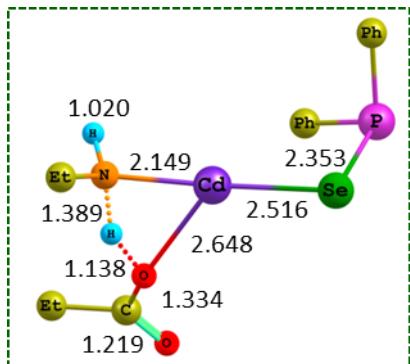
C/H-IM1



Cd	1.17217600	0.17403400	-0.67126800
Se	-0.65338200	-0.82507200	-2.16845300
P	-2.37583600	-1.24245700	-0.64922900
C	-3.10567700	0.41218600	-0.22533800
C	-4.12336300	0.42085700	0.74882900
C	-2.80744800	1.60874600	-0.89107700
C	-4.79746300	1.59979700	1.06901600
H	-4.39041500	-0.49919900	1.26415300
C	-3.48968500	2.78953700	-0.57570400
H	-2.04309900	1.61684100	-1.66193000
C	-4.48176900	2.79142600	0.40624800
H	-5.57279800	1.58688200	1.83028900
H	-3.24104500	3.70745400	-1.10157000
H	-5.01018100	3.70880800	0.64993400
C	-1.46566300	-1.64253500	0.92319600
C	-1.05701600	-0.68807600	1.87180700
C	-1.18664000	-2.99880800	1.17342100
C	-0.38462800	-1.07926900	3.03441600
H	-1.26905700	0.36458100	1.71038600
C	-0.50817500	-3.39053400	2.33140500
H	-1.50850100	-3.75100900	0.45735100
C	-0.10736200	-2.43044700	3.26831500
H	-0.08270100	-0.32529800	3.75635600
H	-0.31046600	-4.44405400	2.51092200
H	0.40434600	-2.73431000	4.17745600
C	3.71584600	-1.84673200	0.15722400
H	4.31839200	-0.96924300	-0.09660800
H	4.25481500	-2.40647300	0.93420400
C	3.51589700	-2.72666000	-1.07300400
H	2.90771400	-3.60792500	-0.83845700
H	3.01682000	-2.17992800	-1.87968700
H	4.48284600	-3.07673900	-1.44737700
N	2.41560200	-1.35261400	0.67979800
H	2.55596800	-0.81615800	1.53473900
H	1.81236900	-2.13549700	0.93282900
O	2.89459500	1.68374900	-0.88487800

O	1.58595500	1.85117000	0.90022800
C	2.56145800	2.26933300	0.19925100
C	3.34902800	3.49784500	0.62667800
H	4.41233800	3.26410600	0.49999000
H	3.13178200	4.27376600	-0.11920100
C	3.04763300	4.00455800	2.03790300
H	3.63130400	4.90635100	2.25164000
H	1.98677500	4.24258900	2.15208100
H	3.29738500	3.25172200	2.79231800

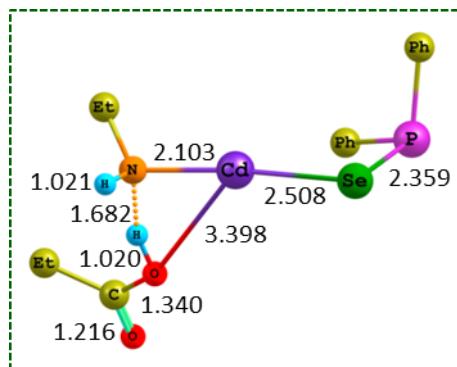
C/H-TS1



Cd	-0.51921900	-1.06459600	-0.39429600
C	-2.32716900	-3.03501000	1.28156400
H	-2.63097100	-3.43327300	0.30562000
H	-1.46288100	-3.63076600	1.60952800
C	-3.47233500	-3.21233900	2.28243700
H	-3.18918700	-2.83803400	3.27382200
H	-4.36540300	-2.66872000	1.95706700
H	-3.73379100	-4.27141500	2.38835800
O	-3.96468900	1.69146000	-1.39854200
C	-3.95577000	0.78167800	-0.58736600
C	-5.04789600	0.59961800	0.46780800
H	-5.51550100	-0.37788100	0.28810400
H	-4.56258000	0.51905500	1.45007700
C	-6.09944300	1.70886900	0.46807600
H	-6.86003000	1.51652700	1.23239400
H	-5.64449000	2.68285000	0.67062200
H	-6.59363500	1.77829700	-0.50462100
N	-1.96748900	-1.61449300	1.09541200
H	-1.72487000	-1.20400600	1.99717000
O	-2.99700300	-0.14520400	-0.56457700
H	-2.81252600	-0.81313200	0.33839000
P	2.36237100	1.07721800	-1.11986100
Se	1.30712400	-0.78299900	-2.10203500
C	1.03386300	1.71188600	0.01792300
C	1.03239000	1.53275200	1.41473000
C	-0.00165300	2.47010600	-0.56492300

C	0.02005400	2.09557200	2.20073400
H	1.82819600	0.96903200	1.89132200
C	-1.01816400	3.01683300	0.21931800
H	-0.02104200	2.61950800	-1.64119400
C	-1.00584300	2.83647800	1.60685800
H	0.04086200	1.95847000	3.27887300
H	-1.82157500	3.57001700	-0.25655800
C	3.58566100	0.38090400	0.09103500
C	4.49458300	1.30874400	0.63454600
C	3.71882400	-0.97041800	0.43891600
C	5.48366300	0.90023100	1.53134600
H	4.42961900	2.35803800	0.35473000
C	4.71736100	-1.38200200	1.32844300
H	3.05227600	-1.70581600	-0.00108400
C	5.59770600	-0.44925800	1.88171600
H	6.17105700	1.63252400	1.94570400
H	4.80808800	-2.43457100	1.58316100
H	6.37404200	-0.77081800	2.57019900

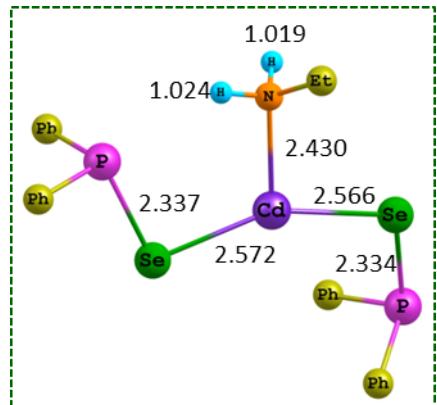
C/H-IM2



Cd	-0.39826300	-1.43887600	-0.21761200
P	2.33926300	0.78504700	-1.41335300
Se	1.57532000	-1.41907200	-1.76565000
C	0.87972500	1.58775300	-0.59092800
C	0.77313300	1.80526000	0.79567200
C	-0.15302800	2.05412100	-1.42864600
C	-0.33891500	2.47048900	1.32435400
H	1.56492700	1.47388400	1.46021500
C	-1.27090800	2.69803000	-0.89647100
H	-0.08548400	1.90055900	-2.50268100
C	-1.36204200	2.91481900	0.48239300
H	-0.39920400	2.64429900	2.39567700
H	-2.07358100	3.01879700	-1.55288800
H	-2.22683400	3.42655100	0.89468900
C	3.54133400	0.66676600	-0.00370500
C	4.29202900	1.83120300	0.24785800

C	3.80955200	-0.48092000	0.75469400	C	2.04138500	2.78298500	-2.08272100
C	5.25665000	1.85617800	1.25664800	H	2.24846600	0.65472600	-1.87921700
H	4.12165800	2.72517700	-0.34821500	C	3.48446100	4.13551000	-0.69086300
C	4.78541800	-0.45974600	1.75734900	H	4.82651600	3.05369000	0.60158300
H	3.26583700	-1.39805500	0.55050800	C	2.48248600	4.04180000	-1.66097400
C	5.50664000	0.70807200	2.01581400	H	1.26354300	2.70019100	-2.83691400
H	5.82049600	2.76654200	1.44028100	H	3.83682900	5.10939600	-0.36207300
H	4.98281700	-1.36042800	2.33250400	H	2.05130300	4.94251300	-2.08920600
H	6.26526900	0.72196700	2.79319600	C	4.20369300	-1.06541700	-1.04180800
C	-2.07020500	-1.20803600	2.36067300	C	4.78449800	-0.82247100	-2.30260100
H	-1.80688900	-0.14462900	2.40563600	C	3.65615000	-2.33281900	-0.79446800
H	-3.07714900	-1.29606500	2.79675600	C	4.78948100	-1.80786500	-3.29050700
C	-1.09118600	-2.01547300	3.21983100	H	5.22980800	0.14548500	-2.51879500
H	-1.33528000	-3.08418100	3.19689100	C	3.66525200	-3.32198900	-1.78425000
H	-0.06005700	-1.89820200	2.86166200	H	3.22130300	-2.54816600	0.17670200
H	-1.12055800	-1.68611500	4.26552100	C	4.22738900	-3.06373500	-3.03558800
O	-3.43136900	-0.02172300	-0.79714700	H	5.23307900	-1.59457200	-4.25933100
O	-4.99536500	1.45564800	-1.36818800	H	3.22850900	-4.29442100	-1.57298100
C	-4.58689100	0.62152700	-0.58283900	H	4.23142600	-3.83122100	-3.80433500
C	-5.33644200	0.23355300	0.69129000	Cd	0.57327900	-0.35147000	0.97274400
H	-5.49622200	-0.85280900	0.66960100	Se	-1.12143100	-0.50556400	-0.95640400
H	-4.66870500	0.41842500	1.54348000	N	-0.77261400	-0.30249600	2.99504300
C	-6.66172900	0.97387100	0.86998700	H	-0.67246900	0.61819300	3.42122000
H	-7.15385500	0.65933100	1.79636100	H	-1.73590300	-0.36584100	2.65416400
H	-6.50479300	2.05529000	0.90964000	C	-0.49838400	-1.35656900	4.00158400
H	-7.33677200	0.77461300	0.03330800	H	0.56099600	-1.29011600	4.26940400
H	-3.11388400	-0.62364100	-0.03742900	H	-0.64078600	-2.32353800	3.50761200
N	-2.14791500	-1.59452200	0.93856600	C	-1.37430900	-1.26621400	5.25252800
H	-2.48448400	-2.55704100	0.88193400	H	-2.43727000	-1.35326500	5.00070100

E/H-IM1

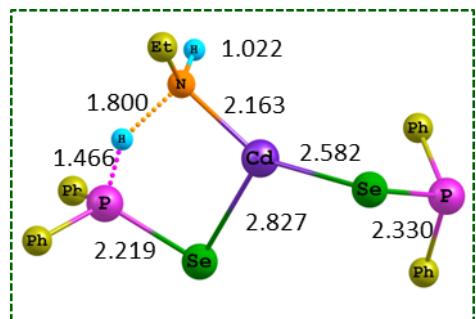


Se	2.93205500	-0.30686900	1.98071800
P	4.40556600	0.24448700	0.25657500
C	3.60276700	1.70436400	-0.55726200
C	2.59645300	1.62396800	-1.53503600
C	4.04286100	2.97505400	-0.14787800

C	2.04138500	2.78298500	-2.08272100
H	2.24846600	0.65472600	-1.87921700
C	3.48446100	4.13551000	-0.69086300
H	4.82651600	3.05369000	0.60158300
C	2.48248600	4.04180000	-1.66097400
H	1.26354300	2.70019100	-2.83691400
H	3.83682900	5.10939600	-0.36207300
H	2.05130300	4.94251300	-2.08920600
C	4.20369300	-1.06541700	-1.04180800
C	4.78449800	-0.82247100	-2.30260100
C	3.65615000	-2.33281900	-0.79446800
C	4.78948100	-1.80786500	-3.29050700
H	5.22980800	0.14548500	-2.51879500
C	3.66525200	-3.32198900	-1.78425000
H	3.22130300	-2.54816600	0.17670200
C	4.22738900	-3.06373500	-3.03558800
H	5.23307900	-1.59457200	-4.25933100
H	3.22850900	-4.29442100	-1.57298100
H	4.23142600	-3.83122100	-3.80433500
Cd	0.57327900	-0.35147000	0.97274400
Se	-1.12143100	-0.50556400	-0.95640400
N	-0.77261400	-0.30249600	2.99504300
H	-0.67246900	0.61819300	3.42122000
H	-1.73590300	-0.36584100	2.65416400
C	-0.49838400	-1.35656900	4.00158400
H	0.56099600	-1.29011600	4.26940400
H	-0.64078600	-2.32353800	3.50761200
C	-1.37430900	-1.26621400	5.25252800
H	-2.43727000	-1.35326500	5.00070100
H	-1.12623400	-2.07118100	5.95312200
H	-1.22382000	-0.31302100	5.77281000
P	-3.06323900	-0.23132000	0.31419300
C	-4.27147800	-1.19588800	-0.69959800
C	-4.81489500	-0.73077100	-1.90890200
C	-4.64568900	-2.46686300	-0.23324700
C	-5.71210900	-1.51943900	-2.63125400
H	-4.53786800	0.24973400	-2.28430400
C	-5.54176800	-3.25790600	-0.95774300
H	-4.23372300	-2.83878300	0.70165500
C	-6.07685900	-2.78492400	-2.15872100
H	-6.12456900	-1.14754700	-3.56520900
H	-5.82226200	-4.23851100	-0.58325900
H	-6.77487700	-3.39680200	-2.72321200
C	-3.61745000	1.51224300	-0.01003400
C	-4.87866700	1.88037400	0.49817400
C	-2.82723500	2.49652600	-0.61910800

C	-5.34213800	3.19116200	0.38067400
H	-5.50733600	1.13599400	0.98178200
C	-3.28935300	3.81348100	-0.72896900
H	-1.85315100	2.22981800	-1.01777500
C	-4.54606900	4.16521500	-0.23318700
H	-6.32211100	3.45269200	0.77065200
H	-2.66365300	4.56173700	-1.20818400
H	-4.90384100	5.18718000	-0.32126700

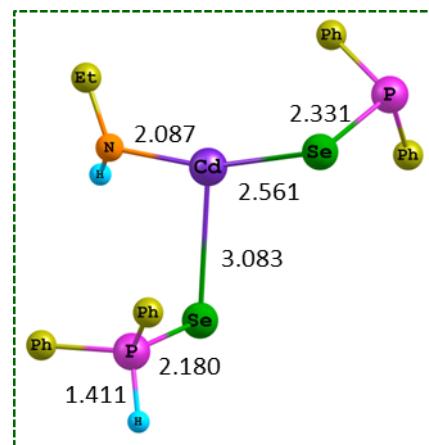
E/H-TS1



Se	2.93876000	-2.23020500	0.14772400
P	3.90267000	-0.84536500	-1.45958100
C	3.47586100	0.85353000	-0.83840000
C	2.27744200	1.53248300	-1.12359800
C	4.42184100	1.48255900	-0.01063100
C	2.02928500	2.79821400	-0.58330900
H	1.53852100	1.07837900	-1.77709100
C	4.17213800	2.74502800	0.53405700
H	5.35721300	0.97529000	0.21216900
C	2.97380800	3.40693300	0.24981100
H	1.09911600	3.30900700	-0.81887900
H	4.91509400	3.21290200	1.17424400
H	2.78038400	4.39131600	0.66702500
C	2.82562400	-0.96819100	-2.96813100
C	3.08568200	-0.06925600	-4.02110100
C	1.88477500	-1.98663900	-3.17750600
C	2.40232500	-0.16939000	-5.23380700
H	3.82388800	0.71904700	-3.89238000
C	1.20483700	-2.09126900	-4.39642800
H	1.68431200	-2.69993500	-2.38376300
C	1.45674800	-1.18314400	-5.42631800
H	2.61175600	0.54072200	-6.02947100
H	0.47487800	-2.88432000	-4.53485100
H	0.92700500	-1.26476000	-6.37135400
Cd	0.78121300	-0.94716800	0.75376000
Se	-1.28587500	-0.97065400	-1.17416600
N	-0.30810700	-0.01834100	2.37522500
H	-0.05225500	0.97004900	2.40902000

H	-1.90774400	-0.06388100	1.55129700
C	-0.15702400	-0.58023300	3.72551200
H	0.89256900	-0.60214200	4.06515300
H	-0.48335000	-1.62998300	3.69755500
C	-0.98995000	0.17468300	4.76932000
H	-2.05408900	0.16551900	4.50600600
H	-0.87587000	-0.27122900	5.76516000
H	-0.67202500	1.22262000	4.83485800
P	-2.73821700	-0.31202000	0.36904500
C	-3.96142100	-1.58091400	0.82953000
C	-4.99277200	-1.95339200	-0.04766000
C	-3.83837000	-2.22447900	2.07076400
C	-5.89415100	-2.95268300	0.31908500
H	-5.08937700	-1.46626900	-1.01384000
C	-4.74344400	-3.22615200	2.43308900
H	-3.03939300	-1.94701800	2.75258800
C	-5.77064100	-3.59011600	1.55912300
H	-6.69008600	-3.23687000	-0.36303700
H	-4.64415800	-3.71970700	3.39545500
H	-6.47279300	-4.36944300	1.84071800
C	-3.68248400	1.17830800	-0.11857800
C	-4.71184100	1.64095800	0.72045400
C	-3.35873600	1.89550700	-1.27788800
C	-5.40421400	2.80910300	0.39957600
H	-4.97756200	1.08986300	1.61850500
C	-4.05867000	3.06313200	-1.59638500
H	-2.56650800	1.53518200	-1.92748700
C	-5.07859200	3.52209400	-0.75966000
H	-6.19747700	3.16094500	1.05276100
H	-3.80570000	3.61017900	-2.50001200
H	-5.62009600	4.43019100	-1.00862000

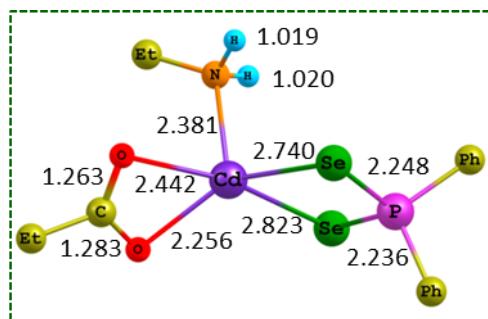
E/H-IM2



Se	1.63153800	-1.00526100	1.72187700
P	3.84339900	-0.71492900	1.04423500
C	3.94013500	1.09668000	0.65584000

C	3.66534600	1.66004700	-0.60259200	H	-5.04432300	-0.34426200	1.53797900
C	4.32610400	1.95084800	1.70390600	C	-2.07182600	-2.17367900	3.24341300
C	3.76861000	3.03957700	-0.80329300	H	-1.31119100	-2.49433300	1.25354800
H	3.38507800	1.01966500	-1.43395100	C	-3.09440700	-1.61971000	4.01830400
C	4.42254700	3.33031000	1.50569100	H	-4.95700600	-0.52743900	3.99971600
H	4.54991800	1.53016500	2.68109500	H	-1.22996600	-2.66937700	3.71673400
C	4.14522900	3.87883100	0.24988500	H	-3.05317100	-1.68908900	5.10145900
H	3.55636500	3.45718900	-1.78392500	H	-4.00633000	-2.48572900	-0.97797300
H	4.72184300	3.97404700	2.32834300	N	-0.74650600	2.24879200	-0.43657000
H	4.22569600	4.95061900	0.09163100	H	-0.86525300	2.20713400	-1.44935300
C	3.96910400	-1.45590500	-0.65461300				
C	5.22002100	-1.34788800	-1.29385100				
C	2.96373500	-2.20755100	-1.27877900				
C	5.44542200	-1.94692100	-2.53375900				
H	6.02397900	-0.78790700	-0.82125300				
C	3.19239400	-2.81531000	-2.51922700				
H	2.00066400	-2.32582300	-0.79175800				
C	4.42953000	-2.68455800	-3.15266900				
H	6.41513900	-1.84345200	-3.01326600				
H	2.39794400	-3.39106100	-2.98653300				
H	4.60525400	-3.15650400	-4.11533200				
Cd	0.27329600	0.54325700	0.20072900				
Se	-1.32363000	-1.38554900	-1.59694700				
C	-0.26756800	3.58424500	-0.05805100				
H	0.70144800	3.84763100	-0.51561000				
H	-0.10250100	3.59584600	1.02706100				
C	-1.28509900	4.67709600	-0.41321600				
H	-2.24122700	4.49423800	0.09009200				
H	-0.91981900	5.66807400	-0.11495000				
H	-1.46991100	4.70166600	-1.49479900				
P	-3.26270000	-1.34731500	-0.60104500				
C	-4.41132000	-0.01221200	-1.05941700				
C	-4.04027400	1.33286400	-0.89733000				
C	-5.66707100	-0.33921200	-1.59511400				
C	-4.93923900	2.33797000	-1.25879100				
H	-3.05569200	1.60288400	-0.51166400				
C	-6.55773200	0.67523100	-1.95566200				
H	-5.95330900	-1.37866600	-1.73401000				
C	-6.19451000	2.01388000	-1.78513800				
H	-4.65162000	3.37787900	-1.13407700				
H	-7.52789700	0.41886800	-2.37104100				
H	-6.88569100	2.80300400	-2.06741800				
C	-3.19084800	-1.42369200	1.22790100				
C	-4.21624900	-0.86485300	2.00823300				
C	-2.11694100	-2.07782600	1.85061100				
C	-4.16516600	-0.96691800	3.40018900				

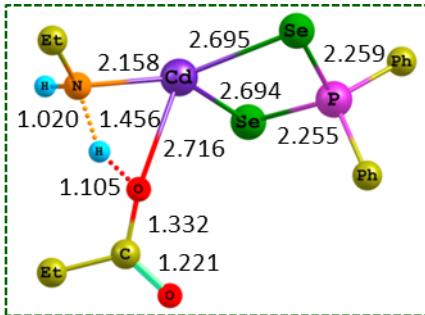
F/I-i-IM1



Cd	-1.70361600	-0.10714500	0.01708000
P	1.65373400	0.05911000	-0.00176600
Se	0.44442700	-0.35861000	1.83181800
Se	0.32008500	0.17187100	-1.80839800
C	2.95458900	-1.21924800	-0.22783300
C	3.93924600	-1.36063200	0.76505900
C	2.97235600	-2.06224800	-1.34555800
C	4.93105200	-2.33188200	0.63317600
H	3.93057700	-0.71624000	1.63940100
C	3.96909500	-3.03558500	-1.47273400
H	2.21153300	-1.95463800	-2.11266900
C	4.94771200	-3.17209500	-0.48632500
H	5.68865700	-2.43485200	1.40468700
H	3.97823500	-3.68272100	-2.34517100
H	5.72112900	-3.92827400	-0.58662700
C	2.59224900	1.62881100	0.17592100
C	3.59174900	1.93502600	-0.76315400
C	2.29588400	2.54088500	1.19609900
C	4.28950400	3.13924900	-0.67372000
H	3.82609600	1.23757700	-1.56215400
C	2.99704100	3.74778300	1.27950100
H	1.52399400	2.30438500	1.92181900
C	3.99262500	4.04867800	0.34779600
H	5.06189000	3.36846200	-1.40219900
H	2.76235100	4.44935000	2.07478800
H	4.53606300	4.98688900	0.41476700

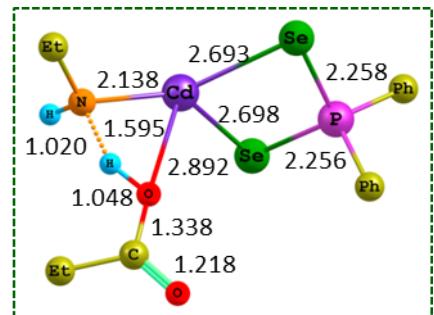
C	-3.67935000	-2.80025100	0.31089900	H	-5.61710000	3.75928300	0.46826900
H	-4.29883900	-2.26829600	-0.41611100	N	-3.36251200	-1.73921400	0.12016900
H	-3.82275600	-3.87890500	0.15782300	H	-3.67040000	-2.07422600	1.03297700
C	-4.08100400	-2.41626600	1.73192500	O	-3.01872600	0.69401100	-0.24896100
H	-3.45904200	-2.92920600	2.47549400	H	-3.46681600	-0.29836600	-0.05936900
H	-3.98975800	-1.33733100	1.89338000	P	1.69821800	0.00339100	-0.00821800
H	-5.12175500	-2.69997300	1.91763000	Se	0.53594800	-0.36451100	1.88900200
O	-3.26483500	1.31681100	0.80709900	Se	0.79996000	-1.27053300	-1.64332600
O	-3.83954300	0.31201600	-1.08898700	C	3.46199600	-0.40178800	0.26270000
C	-4.08613400	1.13240300	-0.16079700	C	4.08882400	-1.44387700	-0.43179700
C	-5.37185300	1.94724300	-0.15175700	C	4.18004200	0.32463900	1.22887700
H	-5.84159500	1.79713000	0.82798200	C	5.42872900	-1.74828900	-0.17232300
H	-5.07209900	3.00269400	-0.16942200	H	3.53191900	-2.01693400	-1.16651100
C	-6.34437500	1.63496400	-1.28960300	C	5.51531400	0.01449600	1.48442000
H	-7.23131300	2.27434300	-1.22034100	H	3.69983300	1.12761100	1.78065300
H	-5.87553600	1.79821300	-2.26400800	C	6.14217500	-1.02203700	0.78334300
H	-6.67163100	0.59125500	-1.25661800	H	5.90977800	-2.55532400	-0.71709500
N	-2.26912200	-2.41957800	0.03548300	H	6.06436800	0.57953600	2.23189600
H	-1.98910900	-2.74424300	-0.88898100	H	7.18200700	-1.26253200	0.98516800
H	-1.63636700	-2.86477400	0.70027700	C	1.63223200	1.76816900	-0.48639600

F/I-i-TS1



Cd	-1.24420800	-1.32960100	0.11215600
C	-3.94962500	-2.59341600	-0.93058800
H	-3.63998100	-2.18811800	-1.90181400
H	-3.56293200	-3.62262700	-0.88333500
C	-5.47936800	-2.62988100	-0.85904100
H	-5.81795200	-3.04632000	0.09778400
H	-5.90089400	-1.62385000	-0.95815800
H	-5.89173700	-3.25566200	-1.65921200
O	-2.99259600	2.88178100	0.17776000
C	-3.58938100	1.81670200	0.18489000
C	-5.03148500	1.67519300	0.66823600
H	-5.62552500	1.30434700	-0.17787800
H	-5.05987100	0.87586200	1.42092200
C	-5.62671600	2.96883300	1.22357100
H	-6.66112200	2.80716500	1.54502500
H	-5.05033200	3.32997600	2.08007500

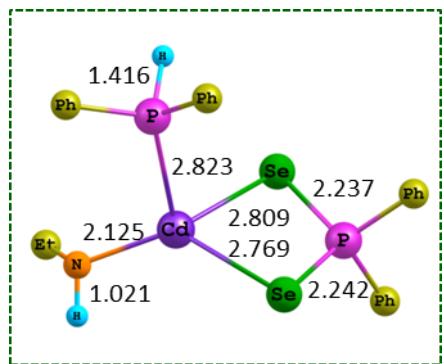
F/I-i-IM2



Cd	-1.17620600	-1.43181400	0.15374600
C	-3.89413200	-2.64251500	-0.82545200
H	-3.58727000	-2.27855700	-1.81402200
H	-3.52849900	-3.67835800	-0.74718400
C	-5.42399900	-2.65158500	-0.74194300
H	-5.76140500	-3.02255800	0.23387400

H	-5.83039300	-1.64378400	-0.87887200
H	-5.85276400	-3.30295100	-1.51269300
O	-3.26291600	2.96569900	-0.08244200
C	-3.73117300	1.84906600	0.05131200
C	-5.14573700	1.58651500	0.55915700
H	-5.68473800	1.04578500	-0.23032600
H	-5.07837100	0.88638700	1.40240200
C	-5.89882700	2.85474700	0.95966100
H	-6.90690000	2.60581800	1.30735700
H	-5.37679100	3.38436600	1.76149800
H	-5.98284600	3.54334100	0.11460400
N	-3.28876400	-1.75779600	0.18949000
H	-3.58254200	-2.07154600	1.11482900
O	-3.01415500	0.76226500	-0.25747500
H	-3.41053900	-0.18456700	-0.04482100
P	1.71577600	0.01956900	-0.00670500
Se	0.63534300	-0.47781400	1.91030600
Se	0.78808600	-1.18992400	-1.67195900
C	3.49942600	-0.35572400	0.16544800
C	4.19991200	-1.02035800	-0.85029100
C	4.17136700	0.03275500	1.33670700
C	5.56557200	-1.27957200	-0.70208600
H	3.68145100	-1.34309400	-1.74757100
C	5.53419900	-0.22968400	1.47890300
H	3.63281600	0.52991700	2.13806300
C	6.23322600	-0.88529500	0.45962200
H	6.10196300	-1.79558500	-1.49292100
H	6.04704200	0.07144500	2.38760000
H	7.29323000	-1.09256500	0.57482000
C	1.57843400	1.80782800	-0.37084200
C	2.71282900	2.58438500	-0.65379300
C	0.30443300	2.40036900	-0.38954300
C	2.56864900	3.94371600	-0.94734600
H	3.70240100	2.14042800	-0.64681600
C	0.16843800	3.75613700	-0.68302300
H	-0.59055400	1.82319000	-0.18187600
C	1.30071700	4.52997900	-0.96108200
H	3.45044600	4.54010000	-1.16364800
H	-0.82727200	4.18861400	-0.68889100
H	1.19410200	5.58706100	-1.18799300

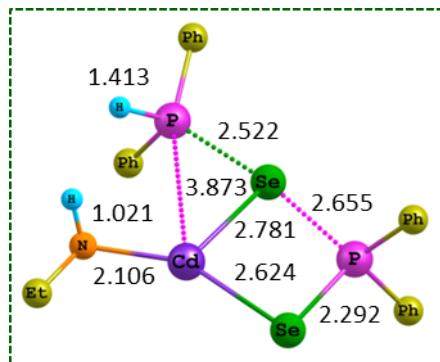
I-i/H-IM1



Cd	-0.74582000	-1.41983100	0.15680400
C	-2.18966200	-4.07173000	-0.55040600
H	-2.56261700	-3.54602000	-1.44159000
H	-1.25215800	-4.56736000	-0.86330800
C	-3.19967500	-5.16108700	-0.16458200
H	-2.84987300	-5.72086800	0.71220700
H	-4.16987700	-4.71858200	0.08685900
H	-3.34290500	-5.87789600	-0.98345200
N	-2.01320400	-3.08615800	0.52345600
H	-1.68346500	-3.57710500	1.35530100
P	2.33212900	-0.07439800	-0.03590300
Se	1.07828300	-0.16569200	1.82020000
Se	1.19333700	-0.85684800	-1.79543500
C	3.88812000	-1.02214500	0.21078600
C	4.13506100	-2.21385100	-0.48088300
C	4.82705100	-0.55277600	1.14516700
C	5.31423800	-2.92795900	-0.24498100
H	3.40909500	-2.57628200	-1.20213300
C	6.00200300	-1.26766700	1.37547900
H	4.64249800	0.36752300	1.69179000
C	6.24757900	-2.45789700	0.68099500
H	5.49950600	-3.85062600	-0.78746700
H	6.72365700	-0.89778000	2.09816200
H	7.16273000	-3.01419100	0.86302800
C	2.90706400	1.64173600	-0.35610300
C	3.81462800	1.86449500	-1.40595600
C	2.44297000	2.72419900	0.40021300
C	4.25475800	3.15718000	-1.68770800
H	4.17580500	1.03205900	-2.00310200
C	2.88800200	4.01903900	0.11361900
H	1.73914900	2.55300200	1.20872600
C	3.79194100	4.23788400	-0.92756200
H	4.95663800	3.32126500	-2.50031400
H	2.52520300	4.85309300	0.70740600
H	4.13601300	5.24439900	-1.14845300
P	-2.55634700	0.60906400	-0.59999400

H	-2.51111600	0.83836700	-1.99634800	H	3.16126800	-6.12905400	-1.76104500
C	-4.34552900	0.25287300	-0.33954100	C	-3.55245400	1.08588900	-0.96992500
C	-4.70297800	-1.00329600	0.17677600	C	-4.03433500	0.50850200	-2.15376600
C	-5.34681600	1.18908800	-0.65289500	C	-3.86768400	2.42881600	-0.68931600
C	-6.05494900	-1.31395500	0.37017100	C	-4.82375100	1.25464800	-3.03419800
H	-3.93352000	-1.73773200	0.42555200	H	-3.79988900	-0.52734300	-2.37867100
C	-6.69074400	0.87077900	-0.45645800	C	-4.65703900	3.16958800	-1.56974400
H	-5.07687800	2.16704900	-1.04199300	H	-3.50261200	2.89652100	0.22095600
C	-7.04649100	-0.38317000	0.05595100	C	-5.13783900	2.58482600	-2.74640300
H	-6.32619000	-2.28659100	0.77115000	H	-5.19579600	0.79061400	-3.94351400
H	-7.45949900	1.59846600	-0.70146400	H	-4.89675400	4.20328600	-1.33609100
H	-8.09376400	-0.62871200	0.20967500	H	-5.75238000	3.16243500	-3.43113500
C	-2.31789200	2.34066800	-0.03457200	C	-3.10658200	0.49846300	1.82874200
C	-1.91333500	3.35044000	-0.92178900	C	-2.23267700	0.77254000	2.89194500
C	-2.48219000	2.65380800	1.32553900	C	-4.48805200	0.42278400	2.07639500
C	-1.68956700	4.65111100	-0.45997100	C	-2.73264900	0.97132500	4.18273100
H	-1.77133900	3.12579900	-1.97533000	H	-1.16364700	0.82914000	2.70699500
C	-2.26886500	3.95492300	1.78241800	C	-4.98371800	0.62329700	3.36509500
H	-2.78149500	1.88236400	2.03023800	H	-5.17452700	0.20751800	1.26299000
C	-1.87214900	4.95742100	0.89063100	C	-4.10692600	0.89773800	4.42113000
H	-1.37895300	5.42290500	-1.15858400	H	-2.04736500	1.18439800	4.99841400
H	-2.40686100	4.18450300	2.83514700	H	-6.05325700	0.56201500	3.54630200
H	-1.70526900	5.96960500	1.24790600	H	-4.49532100	1.05232000	5.42395300
				C	3.71938500	0.04003200	0.96175700
				C	4.32407400	0.87097900	1.91747900
				C	3.80569600	-1.35757300	1.09435400
				C	5.02503200	0.31009800	2.98846800
				H	4.26012100	1.95123400	1.82467600
				C	4.51147000	-1.90699700	2.16706800
				H	3.31631500	-2.01001500	0.36933300
				C	5.12194500	-1.07841100	3.11450300
				H	5.49543100	0.95957300	3.72141500
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				H	5.66870400	-1.51234300	3.94695400

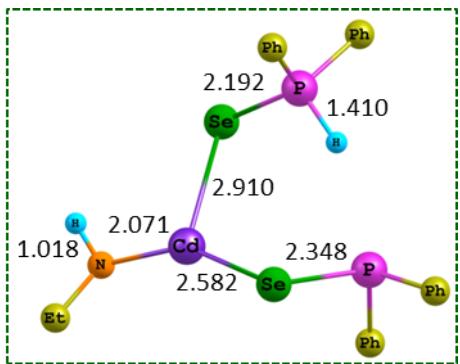
I-i/H-TS1



P	-2.39446600	0.20267900	0.15752400	C	3.39768100	2.38094800	-0.79082200
Se	-2.56873900	-2.04525000	-0.25614200	C	2.61105500	3.52238000	-0.57913500
P	2.70856100	0.72711800	-0.40235400	C	4.69587900	2.52402400	-1.31152200
Se	0.20502200	0.67346000	-0.10354300	C	3.11949400	4.79170600	-0.87320100
H	3.17038600	-0.04380200	-1.49242500	H	1.59934600	3.41535500	-0.19864100
Cd	0.00144800	-2.01571800	-0.78341600	C	5.19727300	3.79160000	-1.61076000
C	1.77001400	-4.47460100	-1.44960400	H	5.31589900	1.64752200	-1.47947300
H	1.35469100	-4.91106500	-0.53149800	C	4.41010700	4.92748700	-1.38914300
H	1.12488100	-4.82724200	-2.27422300	H	2.50286400	5.67002700	-0.70567100
C	3.18080500	-5.03565000	-1.66963500	H	6.20001500	3.89282600	-2.01609800
H	3.62098800	-4.63236400	-2.59063300	H	4.80203200	5.91330600	-1.62285000
H	3.84009400	-4.76626700	-0.83727800	N	1.78447400	-3.01217700	-1.29475000

H 2.16363100 -2.60458000 -2.15091800

I-i/H-IM2



Se -1.52903000 -0.05599800 -1.65984300

P -1.39595000 1.44986200 0.13631300

C -2.97242300 1.16994600 1.06482000

C -4.24962800 1.38631600 0.51957200

C -2.86763400 0.69441100 2.38148100

C -5.39307400 1.13767200 1.27837500

H -4.34570100 1.74263400 -0.50178500

C -4.01491400 0.44156200 3.14212700

H -1.88504700 0.51894200 2.81268500

C -5.27844100 0.66428500 2.59186400

H -6.37515400 1.30813300 0.84553200

H -3.91819100 0.07133200 4.15895900

H -6.17120600 0.46845300 3.17928300

C -1.75149900 3.06649000 -0.70200100

C -2.16820300 4.14522200 0.10245600

C -1.49078400 3.30963100 -2.05938900

C -2.32976400 5.42144200 -0.43862100

H -2.37769000 3.98659500 1.15708400

C -1.65099300 4.59001100 -2.60032300

H -1.17538200 2.49432400 -2.70298500

C -2.07077300 5.65017000 -1.79444500

H -2.66112700 6.23650200 0.19920100

H -1.45286500 4.75285800 -3.65643100

H -2.19798500 6.64315900 -2.21632900

Cd -0.86268700 -2.22101700 -0.42163200

Se 1.52818700 -1.88332800 1.20160600

C -2.31293800 -4.97784000 -0.59622100

H -1.99378200 -5.33688600 -1.59234900

H -3.19053700 -4.34151300 -0.77036800

C -2.74236300 -6.19133700 0.23974100

H -3.12588400 -5.86945600 1.21374000

H -3.52079400 -6.77007300 -0.27446400

H -1.89136900 -6.86088600 0.41840000

P 2.28310100 0.00743300 0.38963300

C 3.25411000 -0.10883200 -1.14653300

C 4.62066100 -0.42739600 -1.10882900

C 2.60689100 0.06653000 -2.37988900

C 5.33661400 -0.55776400 -2.29917300

H 5.12510500 -0.56711800 -0.15698500

C 3.33154000 -0.06552000 -3.56719000

H 1.54374000 0.29253100 -2.41559200

C 4.69327500 -0.37678300 -3.52851100

H 6.39454800 -0.80104800 -2.26738100

H 2.82901400 0.07344200 -4.51985300

H 5.25336800 -0.47927700 -4.45350800

C 3.27835400 0.96072000 1.58985400

C 3.72608000 2.24368600 1.23090200

C 3.57504000 0.44705200 2.85788300

C 4.46833500 3.00100000 2.13736900

H 3.50091400 2.65132000 0.24894600

C 4.32477500 1.20842100 3.75959000

H 3.21533100 -0.53873100 3.13728300

C 4.77029900 2.48275800 3.40172400

H 4.80880600 3.99353000 1.85758300

H 4.55450000 0.80461900 4.74117000

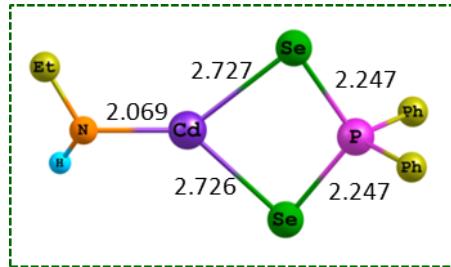
H 5.34915700 3.07388500 4.10550000

H 1.20993200 0.85496200 0.04748400

N -1.29544200 -4.18111300 0.08981200

H -0.45848200 -4.73909100 0.24588500

I-i



Cd -2.27820800 -0.05547700 0.24995000

C -5.22194400 -0.30430200 -0.68947600

H -4.80170300 0.03256300 -1.64623600

H -5.31073700 -1.40332100 -0.76324400

C -6.62901400 0.28677100 -0.53347800

H -7.08822800 -0.04435400 0.40647100

H -6.58671000 1.38081000 -0.51954300

H -7.28295700 -0.03247100 -1.35507700

N -4.33321600 0.14238800 0.38744700

H -4.69081900 -0.17671800 1.28579900

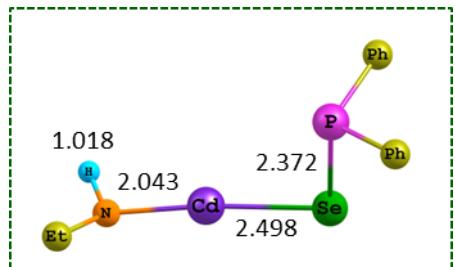
P 1.03920100 -0.00168200 0.00432600

Se -0.39495200 -0.11156800 -1.72215400

Se -0.12879000 0.03027100 1.92387400

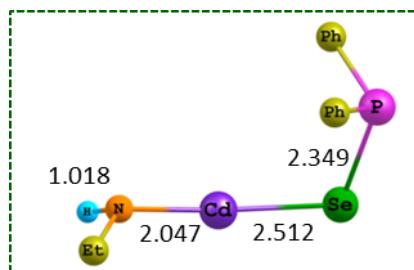
C	2.10443100	1.48351700	-0.14494900	C	1.84984900	2.51251400	1.29151700
C	1.97755900	2.56632000	0.73398100	C	3.53682800	2.83603300	-0.90776900
C	3.03596300	1.54385500	-1.19599700	H	2.94601400	0.84668400	-1.46888100
C	2.78152600	3.69830900	0.56774700	C	2.55548800	3.70977200	1.12414100
H	1.25648000	2.52183300	1.54416100	H	1.19283900	2.39002000	2.14923600
C	3.83604000	2.67461900	-1.35536600	C	3.39909800	3.87282800	0.02402000
H	3.13800500	0.71272400	-1.88782700	H	4.19018700	2.96001500	-1.76707500
C	3.70972600	3.75439400	-0.47377400	H	2.44367500	4.50936000	1.85116600
H	2.67980000	4.53302900	1.25510700	H	3.94668400	4.80144800	-0.11060700
H	4.55474000	2.71424600	-2.16866600	Se	-0.21316200	-0.27600200	-1.35690300
H	4.33306100	4.63481100	-0.60093600	C	-5.05927100	-0.55817800	1.19997300
C	2.20483400	-1.41676900	-0.01385400	H	-4.84769800	-1.57767400	0.85255700
C	3.34719900	-1.36780000	0.80330300	H	-4.70314600	-0.50701900	2.24336800
C	1.94863000	-2.55976700	-0.78194700	C	-6.57585500	-0.33454900	1.18670000
C	4.22399800	-2.45175000	0.84341100	H	-6.82403400	0.67266700	1.54387900
H	3.55526400	-0.48728400	1.40398400	H	-6.97181400	-0.43901700	0.17144500
C	2.83043900	-3.64344400	-0.73636800	H	-7.08284500	-1.05475700	1.84069600
H	1.06733000	-2.59797700	-1.41462400	N	-4.37765000	0.38594700	0.30502500
C	3.96681200	-3.59174400	0.07399600	H	-4.54960500	1.34185600	0.61061000
H	5.10609400	-2.40622800	1.47539000				
H	2.62773900	-4.52478600	-1.33780900				
H	4.65112600	-4.43465500	0.10657200				

H-ii



Cd	-2.44981600	0.09900400	-0.30868200
P	0.99014200	-0.06478400	0.67647200
C	2.27203800	-1.38895500	0.46971300
C	1.94607900	-2.65428500	-0.04794900
C	3.56108200	-1.19507000	1.00100300
C	2.88436600	-3.68952500	-0.04776100
H	0.96112800	-2.82660700	-0.47048600
C	4.49679300	-2.23237800	1.00173000
H	3.84267400	-0.22935900	1.40987700
C	4.16349300	-3.48377500	0.47611900
H	2.61405300	-4.65662800	-0.46299800
H	5.48870400	-2.05784000	1.40970200
H	4.89289300	-4.28874300	0.47370100
C	1.98336500	1.46562200	0.36590100
C	2.83504000	1.64288100	-0.73850600

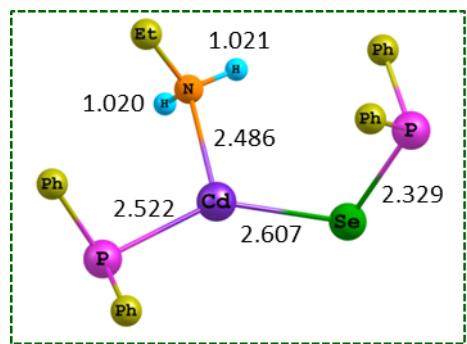
H



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

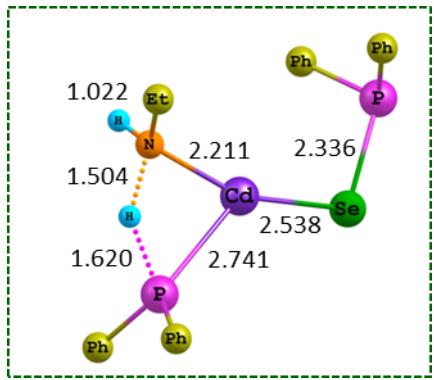
C	-3.29454400	-2.13112700	1.58418100	H	3.86794800	-0.02298400	-1.99342000
H	-2.12796600	-2.20260100	-0.22487000	C	5.51748000	1.96074200	0.23431600
C	-3.92987300	-1.32013200	2.52646200	H	5.50818600	1.67033600	2.37363200
H	-4.38110200	0.71267800	3.10101800	H	5.34126400	1.96362600	-1.91744500
H	-3.32561800	-3.21262400	1.68581100	H	6.16567900	2.83174200	0.26907400
H	-4.45632200	-1.76409000	3.36649000	P	-2.71238100	0.60660800	-1.39155500
Cd	1.41773900	-1.09104300	-0.35384600	C	-3.60334800	-0.84486200	-0.65960400
N	2.79481200	-1.20200600	1.15699900	C	-3.18891400	-2.16145400	-0.93542800
H	2.96806000	-2.15858000	1.46029500	C	-4.80865900	-0.67087700	0.04788700
C	4.05828600	-0.45592900	1.10287300	C	-3.94279400	-3.26000800	-0.51598400
H	4.78033800	-0.86843400	0.37688100	H	-2.26182900	-2.33830000	-1.47545900
H	3.83961800	0.56756700	0.77194400	C	-5.55723300	-1.76974000	0.47685100
C	4.72799000	-0.39988000	2.48096700	H	-5.16845500	0.33047900	0.26577800
H	4.97660900	-1.40807500	2.83515500	C	-5.13006000	-3.07119800	0.19731000
H	5.65944800	0.17834800	2.44023600	H	-3.59248500	-4.26437800	-0.73846200
H	4.05906400	0.05897800	3.21633600	H	-6.48068400	-1.60519600	1.02626900

G/H-IM1



Se	1.52751500	-1.82019700	-1.76473600	H	-3.18063900	4.86277100	2.48093800
P	2.94809000	-1.94438800	0.07620100	Cd	-0.27788300	-0.02370200	-1.20624900
C	1.80775400	-1.84361000	1.53630600	N	1.05687100	2.06239900	-0.99289300
C	1.18220400	-0.67152000	1.99540700	H	2.02753200	1.74698400	-0.95310900
C	1.53381200	-3.04966900	2.20159200	H	0.95178500	2.52047600	-1.89829400
C	0.30462200	-0.70429600	3.08062900	C	0.79523700	3.04594600	0.08828500
H	1.39449900	0.27738400	1.51103800	H	0.93749800	2.52815200	1.04199500
C	0.64941300	-3.08785500	3.28475200	H	-0.26050200	3.32385200	0.03498300
H	2.01220800	-3.96546200	1.86406400	C	1.68515100	4.28869500	0.02802400
C	0.03249500	-1.91574600	3.72683100	H	1.44365500	4.97130800	0.85040700
H	-0.16634400	0.21361200	3.42230300	H	2.74501500	4.02291900	0.10802900
H	0.44596700	-4.03213700	3.78187800	H	1.53838100	4.83493700	-0.91156100
H	-0.65410900	-1.94271700	4.56812500				
C	3.83264800	-0.31104500	0.14489000				
C	4.32331000	0.18046200	1.37034000				
C	4.22031000	0.35021500	-1.03550500				
C	5.14884400	1.30722400	1.41438400				
H	4.05983000	-0.31656700	2.29948600				
C	5.05231200	1.47385500	-0.99098300				

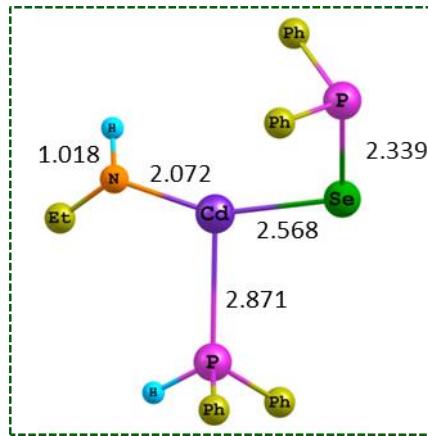
G/H-TS1



Se	1.43393200	-2.14649400	1.79342800
P	3.70325400	-2.06786500	1.24622700
C	4.14162400	-0.27507700	1.42242600
C	3.97547800	0.69957500	0.42358800
C	4.67586100	0.11826600	2.66168700
C	4.33178900	2.02952500	0.66034300
H	3.57753000	0.41870100	-0.54713900
C	5.02163600	1.45048500	2.90359000
H	4.81798900	-0.62499200	3.44221100
C	4.85170200	2.41014500	1.90201000
H	4.20402200	2.76946000	-0.12539100
H	5.43000900	1.73534800	3.86927200
H	5.12730900	3.44515100	2.08376700
C	3.80608200	-2.31334300	-0.59001900
C	5.01627600	-1.98688000	-1.23431400
C	2.81121900	-2.96370800	-1.33684600
C	5.20901600	-2.27408700	-2.58644000
H	5.81356800	-1.49925100	-0.67948300
C	3.00749400	-3.25691800	-2.69103300
H	1.88118800	-3.25021400	-0.85530200
C	4.20312600	-2.90946400	-3.32283500
H	6.14708600	-2.00377200	-3.06376700
H	2.22225400	-3.76080100	-3.24850000
H	4.35470900	-3.13667000	-4.37423700
Cd	0.27289300	-0.43504300	0.32229900
P	-2.38241500	0.21312200	0.11519200
H	-1.41878400	0.96456700	-0.94885100
C	-3.36304300	1.29184300	1.22935500
C	-2.78683900	1.74040900	2.43157400
C	-4.66068500	1.72790500	0.90301600
C	-3.47738200	2.61617300	3.27328900
H	-1.79818600	1.39151200	2.71933600
C	-5.35461200	2.59146500	1.75288900
H	-5.12921800	1.39094700	-0.01689600
C	-4.76517100	3.04365300	2.93833600
H	-3.01403300	2.95017900	4.19765100

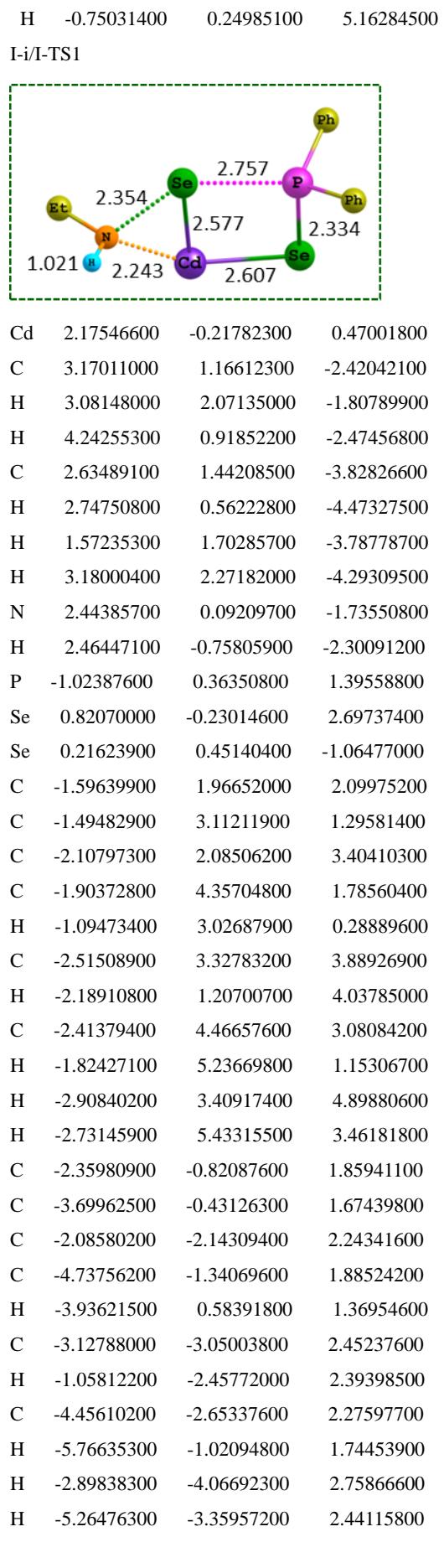
H	-6.35706000	2.91506700	1.48558100
H	-5.30731400	3.71601800	3.59702200
C	-3.58055200	-0.82871500	-0.80530400
C	-3.68437300	-0.73178800	-2.20426400
C	-4.37462100	-1.77899400	-0.13604600
C	-4.55755200	-1.56168200	-2.91529600
H	-3.08686400	0.00217700	-2.73788900
C	-5.25806800	-2.59490800	-0.84438200
H	-4.29890000	-1.87810200	0.94336400
C	-5.34935100	-2.49156500	-2.23718400
H	-4.62505000	-1.47259100	-3.99618800
H	-5.86804600	-3.31876500	-0.31091300
H	-6.03227100	-3.13225200	-2.78785400
N	0.04290100	1.05844100	-1.29177600
H	0.32426500	0.70413800	-2.20779000
C	0.55322800	2.42851800	-1.12485700
H	0.14112700	2.82690600	-0.18692600
H	1.64742500	2.44858500	-1.01032000
C	0.14827000	3.34779200	-2.28237700
H	-0.94130100	3.38768300	-2.38535200
H	0.51662300	4.36775600	-2.12015900
H	0.56580600	2.98863600	-3.23132400

G/H-IM2

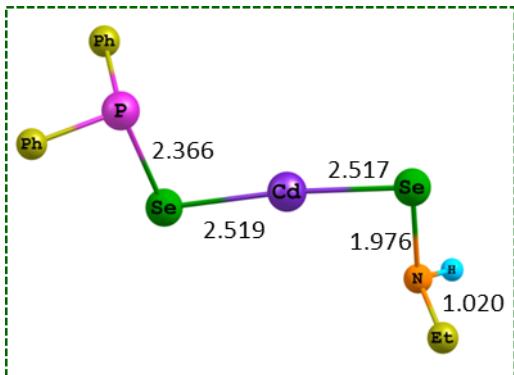


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P	-2.70668400	0.24344400	-1.97525000
C	-2.67939900	1.80934300	-0.98124900
C	-2.65424000	1.87284600	0.42303600
C	-2.65418600	3.01129100	-1.70843000
C	-2.59804700	3.10371400	1.07919600
H	-2.68041100	0.96225700	1.01486700
C	-2.59732700	4.24565300	-1.05277300
H	-2.67911400	2.97853400	-2.79494400
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H	-2.57466700	3.13101600	2.16512300

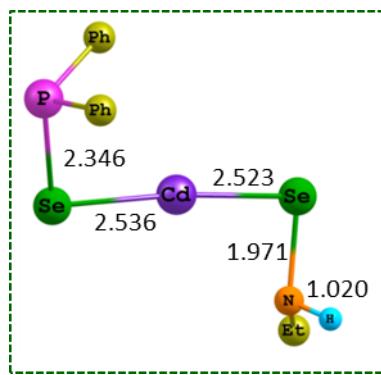
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C	-3.73803400	-0.86912100	-0.90691100
C	-4.96001600	-0.38730100	-0.39793900
C	-3.43943400	-2.23166200	-0.73863400
C	-5.83909300	-1.23575900	0.27807400
H	-5.22624700	0.65866700	-0.52096700
C	-4.32255500	-3.08122800	-0.06482800
H	-2.50990200	-2.62895700	-1.13522000
C	-5.52385900	-2.58745600	0.44936600
H	-6.77076100	-0.83841000	0.67190900
H	-4.06720800	-4.13053000	0.05753200
H	-6.20815400	-3.24711300	0.97542300
Cd	-0.13427500	-0.82075700	0.73699100
P	2.68979100	-0.30918000	0.80013100
H	3.37770600	-0.55231200	2.01138700
C	3.15572800	1.45071400	0.53010000
C	2.36651200	2.23933000	-0.32281800
C	4.26888800	2.02688300	1.16550000
C	2.69602500	3.57926100	-0.54609800
H	1.49497200	1.81268200	-0.81287400
C	4.58878300	3.36829000	0.94718600
H	4.88774200	1.43016600	1.83003700
C	3.80434900	4.14540100	0.08841800
H	2.07879000	4.17906000	-1.20843500
H	5.44918600	3.80532000	1.44606800
H	4.05449800	5.18886700	-0.08067400
C	3.75581700	-1.29546600	-0.32984900
C	4.89381900	-1.97211800	0.13898100
C	3.40369200	-1.40628800	-1.68560800
C	5.66980800	-2.73911700	-0.73448500
H	5.17868200	-1.90292200	1.18533800
C	4.18754200	-2.16460800	-2.55745600
H	2.51598300	-0.90673200	-2.06488400
C	5.32061300	-2.83341400	-2.08428100
H	6.54695800	-3.25893400	-0.35952300
H	3.90551600	-2.23949200	-3.60360200
H	5.92515900	-3.42828700	-2.76280300
N	-0.77959900	-0.94865200	2.70209300
H	-1.64986900	-1.46979300	2.78723900
C	0.09456100	-1.25142300	3.83346800
H	0.36733400	-2.32103200	3.90570000
H	1.03893300	-0.70661200	3.69890700
C	-0.52892000	-0.82266700	5.16915100
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H	0.14448900	-1.04068900	6.00834800



I-ii



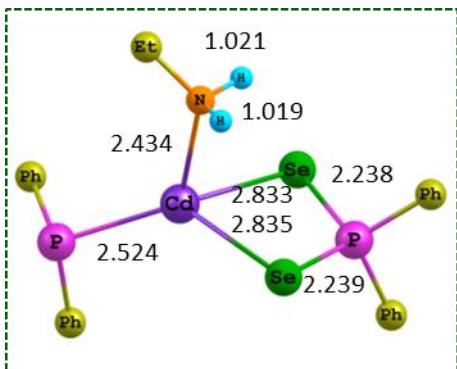
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H	-5.69227800	-1.66078200	1.64575200
C	-6.83009300	-0.96427400	-0.06089700
H	-7.39844300	-0.20488300	0.48990500
H	-6.66582900	-0.59752300	-1.07967500
H	-7.44886000	-1.86714500	-0.12309900
N	-4.57633400	-0.14126300	0.81920900
H	-5.05743900	0.61896700	1.29869000
P	1.82925500	-0.09377500	-0.70986900
Se	0.49866500	-0.55793800	1.19125300
Se	-3.92738800	0.65379100	-0.86962600
C	3.15672700	-1.35639100	-0.44602500
C	3.04753500	-2.55677400	-1.16933500
C	4.25159000	-1.18292500	0.41686600
C	4.00543500	-3.56370600	-1.02906100
H	2.20938500	-2.70177800	-1.84645500
C	5.21169100	-2.18813500	0.55324100
H	4.35781900	-0.26040700	0.97924700
C	5.09029700	-3.38100500	-0.16658100
H	3.90689200	-4.48570600	-1.59528400
H	6.05395900	-2.03997500	1.22358600
H	5.83875800	-4.16105900	-0.05895900
C	2.71826900	1.47680800	-0.27144000
C	3.50043800	2.03648200	-1.29956200
C	2.62930500	2.15768300	0.95059900
C	4.19471200	3.23112600	-1.10042900
H	3.56855200	1.53517500	-2.26266700
C	3.31742600	3.36023300	1.14664700
H	2.01852200	1.74977200	1.75006700
C	4.10358800	3.89864900	0.12554600
H	4.79717900	3.64444400	-1.90463600
H	3.23702100	3.87380200	2.10098800
H	4.63587200	4.83306600	0.27949700

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
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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
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H	-5.94930100	0.32942900	-1.10040300

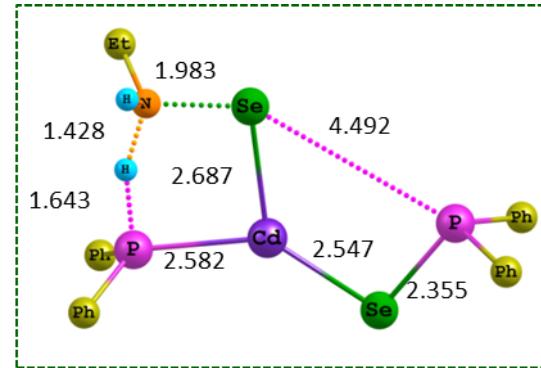
E-i/I-IM1



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C	-3.84642600	-0.20515500	1.63186400
C	-5.27961100	-1.31821200	0.04278200
C	-4.58130300	-0.75724600	2.68239800
H	-3.00569700	0.44652900	1.85366900
C	-6.01214000	-1.88233200	1.09428200
H	-5.56670000	-1.52641100	-0.98499400
C	-5.66606300	-1.60264500	2.41777800
H	-4.30367300	-0.53296600	3.70911100
H	-6.85743200	-2.52985600	0.87609000
H	-6.23561000	-2.03383700	3.23642700
C	-3.08714500	1.98972500	-0.81103800
C	-4.07396400	2.69710900	-0.09886900
C	-2.03219800	2.72925700	-1.38101000
C	-4.00080600	4.08553000	0.04682000
H	-4.90728500	2.16247300	0.34683000
C	-1.96231700	4.11634200	-1.24004200
H	-1.24778500	2.21736400	-1.93356600
C	-2.94608100	4.80454200	-0.52219700
H	-4.77552600	4.60501300	0.60532100
H	-1.13161600	4.65739500	-1.68572900
H	-2.89039300	5.88345000	-0.40779000
P	2.31236700	0.04444200	0.12265600
Se	0.76466900	-0.64391600	1.58556200
Se	1.49809600	0.05548800	-1.96298100
C	3.80663000	-1.02309800	0.23546000
C	4.41557800	-1.20517400	1.48892800
C	4.34181900	-1.65687900	-0.89249300
C	5.55189700	-2.00535800	1.60495600
H	4.00007600	-0.72849800	2.37208700
C	5.48146600	-2.45940500	-0.77079800
H	3.86772500	-1.52188400	-1.85997200
C	6.08710000	-2.63483100	0.47484600
H	6.01636200	-2.14137400	2.57736700

H	5.89208400	-2.94490000	-1.65158900
H	6.97093200	-3.25948400	0.56830300
C	2.91893000	1.72150000	0.56581500
C	4.14496900	2.17055800	0.04734100
C	2.14549800	2.57921600	1.35878900
C	4.59024100	3.46329800	0.32577200
H	4.75241300	1.51580300	-0.57033400
C	2.59492300	3.87405000	1.63152500
H	1.20009500	2.23303200	1.76430700
C	3.81555700	4.31784400	1.11741500
H	5.54068000	3.80252600	-0.07606200
H	1.98888600	4.53231900	2.24720600
H	4.16362000	5.32424800	1.33207600
C	-1.42798200	-4.08798900	-1.20702400
H	-2.05047800	-3.80654600	-2.06276700
H	-0.95156900	-5.04810900	-1.45115200
C	-2.28706200	-4.23969600	0.04469800
H	-1.67694200	-4.52222800	0.91078100
H	-2.81382800	-3.31105800	0.28480500
H	-3.03625000	-5.02357100	-0.10443900
N	-0.40640700	-3.02714300	-1.03022300
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H	0.17827900	-3.22292500	-0.21688200

E-i/I-TS1

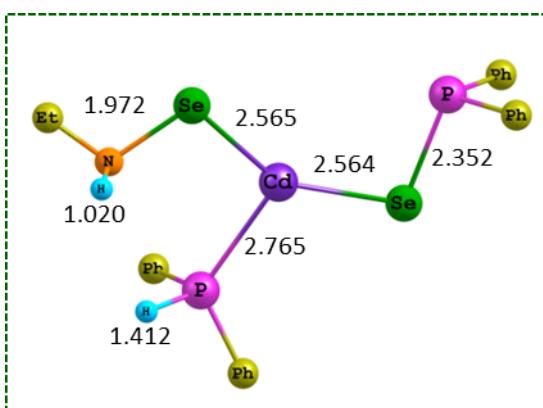


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P	-3.23933300	-0.08125000	0.40022500
C	-4.30703200	-1.40965800	-0.32782300
C	-4.24401100	-2.68033400	0.26620900
C	-5.14858100	-1.22348500	-1.43825900
C	-5.00423100	-3.74275900	-0.23440800
H	-3.59788400	-2.83752500	1.12640900
C	-5.90781700	-2.28196100	-1.93808600
H	-5.20979300	-0.24773500	-1.91143000
C	-5.83722500	-3.54502000	-1.33768900

H	-4.94600600	-4.71933200	0.23858100
H	-6.55365000	-2.12365800	-2.79767800
H	-6.42978100	-4.36757300	-1.72874500
C	-4.38075000	1.38111300	0.29552000
C	-4.00042400	2.62587000	-0.22757700
C	-5.64211400	1.27182200	0.91322500
C	-4.85932500	3.72750500	-0.14728500
H	-3.03473600	2.72988900	-0.71228400
C	-6.49939000	2.37041400	0.99014800
H	-5.96205300	0.32069600	1.33103200
C	-6.11089700	3.60547300	0.45967800
H	-4.54730200	4.68069400	-0.56613800
H	-7.47115200	2.26093800	1.46426700
H	-6.77778800	4.46106200	0.51956500
H	3.01858300	-0.17611500	1.42813000
N	2.58193400	-0.45709800	2.75824300
H	2.80873500	0.32800000	3.36921300
C	3.20653900	-1.69134500	3.28323600
H	2.99288900	-2.48888300	2.56424900
H	2.74022900	-1.98160400	4.23257500
C	4.71552900	-1.50837300	3.45673300
H	5.16308000	-2.43353400	3.83454700
H	5.19986900	-1.26145000	2.506664500
H	4.94104400	-0.71281300	4.17703700
P	2.93368600	0.13700000	-0.18249600
C	3.79327300	-1.13811900	-1.17828600
C	4.75387900	-0.82244300	-2.15369000
C	3.46656000	-2.49128000	-0.96661900
C	5.37488700	-1.83531300	-2.89072400
H	5.01890000	0.21334600	-2.34142600
C	4.08751300	-3.49851700	-1.70558800
H	2.71827600	-2.76186700	-0.22462700
C	5.04686700	-3.17533100	-2.67149000
H	6.11494200	-1.57131000	-3.64133700
H	3.81927400	-4.53636100	-1.52839400
H	5.52910400	-3.95929800	-3.24785900
C	3.70090100	1.76082700	-0.55196400
C	4.92873100	2.12053600	0.03452300
C	3.06129500	2.68361800	-1.39750500
C	5.50377600	3.36666900	-0.22462400
H	5.43746000	1.42145700	0.69252800
C	3.63485600	3.93280000	-1.65273300
H	2.11261700	2.42368600	-1.85837800
C	4.85644800	4.27587900	-1.06766300
H	6.45285500	3.62899000	0.23452500
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H	5.30149300	5.24698200	-1.26486600
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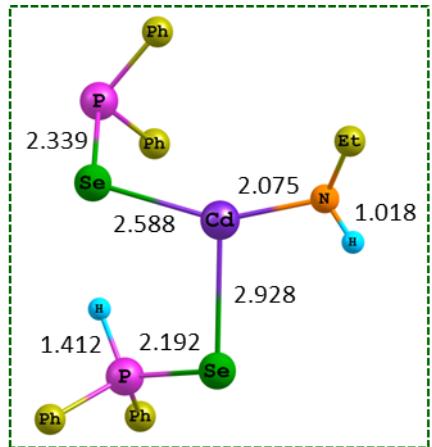
E-i/I-IM2



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Se	1.46947800	0.86608400	-0.16092600
P	3.11544600	-0.71966200	0.39434900
C	3.95868700	0.15526100	1.79410000
C	3.71609100	-0.32917600	3.09007100
C	4.80476000	1.26614000	1.63566000
C	4.30161500	0.28152500	4.20332500
H	3.06682700	-1.19054000	3.22694100
C	5.39197100	1.87488500	2.74613800
H	5.00681600	1.65331000	0.64127500
C	5.14120900	1.38512200	4.03308100
H	4.10512300	-0.10720700	5.19884100
H	6.04455500	2.73289600	2.60802000
H	5.60032900	1.85992500	4.89585800
C	4.38650100	-0.52462500	-0.94845600
C	4.17044900	0.13576400	-2.16567400
C	5.60865100	-1.19902200	-0.75848900
C	5.15383600	0.13543600	-3.16203200
H	3.23361700	0.65830000	-2.33215000
C	6.59115500	-1.19353100	-1.74906900
H	5.79709000	-1.72880800	0.17246000
C	6.36649300	-0.52528800	-2.95815500
H	4.96793600	0.65727400	-4.09718700
H	7.52984200	-1.71388900	-1.57862400
H	7.12893500	-0.52398800	-3.73214800
H	-3.76154700	0.20311900	-1.47519300
N	-3.19366200	-2.82498100	-0.75431100
H	-3.37333900	-2.91572500	-1.75449600
C	-4.00129500	-3.84482100	-0.06163800
H	-3.79753600	-3.75695000	1.01210100
H	-3.72681300	-4.87233900	-0.35013500
C	-5.48864200	-3.61368200	-0.34130600

H	-6.09585100	-4.35146300	0.19492000	C	-0.08182600	4.06169300	-0.81645800
H	-5.79922100	-2.61306600	-0.02388600	H	-0.31970300	2.99628100	-2.67540500
H	-5.71137800	-3.71655400	-1.41046600	C	-0.45857800	4.14542300	0.52638800
P	-2.79234800	0.74005400	-0.60051100	H	-1.66406700	3.27428100	2.09480100
C	-3.73320100	0.84565400	0.98171200	H	0.61635600	4.78213200	-1.23399700
C	-4.15413800	2.06402800	1.53306500	H	-0.05176400	4.92889400	1.15971700
C	-3.98398400	-0.35215600	1.67275000	C	-3.82671900	0.48805700	-1.65329800
C	-4.82714300	2.08262100	2.75874100	C	-4.69692100	1.58803300	-1.52174800
H	-3.96028400	2.99678500	1.01323600	C	-4.35060800	-0.80134000	-1.47224000
C	-4.66430400	-0.32668100	2.89175100	C	-6.04141900	1.40186800	-1.19627600
H	-3.65633300	-1.29536400	1.24403100	H	-4.32293900	2.59840000	-1.66516500
C	-5.08539500	0.88987400	3.43845600	C	-5.69950100	-0.98691900	-1.15163700
H	-5.14843900	3.03131600	3.17931100	H	-3.69961200	-1.66360900	-1.57999000
H	-4.85826500	-1.25711700	3.41785700	C	-6.54928600	0.11189900	-1.00900200
H	-5.60715000	0.90761000	4.39101500	H	-6.69191000	2.26569500	-1.08841000
C	-2.67972400	2.44854200	-1.25181600	H	-6.08206900	-1.99427400	-1.01041100
C	-3.66056200	2.96785300	-2.11443800	H	-7.59569300	-0.03297300	-0.75576000
C	-1.57979400	3.25071700	-0.90369600	Cd	-1.09931100	-1.23110800	0.90545500
C	-3.54515400	4.26704300	-2.61464900	Se	1.66840500	-1.20141300	1.85969700
H	-4.51652100	2.35992500	-2.39458300	C	-3.53072400	-1.78729600	2.78437500
C	-1.47242700	4.55287700	-1.39795200	H	-3.49262100	-2.88976600	2.86045100
H	-0.80069400	2.86157500	-0.25361400	H	-4.10744100	-1.56403700	1.87768600
C	-2.45259800	5.06189700	-2.25471200	C	-4.29520500	-1.24703800	4.00088100
H	-4.30754000	4.65651000	-3.28324500	H	-4.41167000	-0.16031900	3.92975900
H	-0.61703800	5.16202400	-1.12137500	H	-5.29016900	-1.70454200	4.07717300
H	-2.36317300	6.07167900	-2.64480900	H	-3.75408100	-1.46708600	4.93000000

H/I-IM1

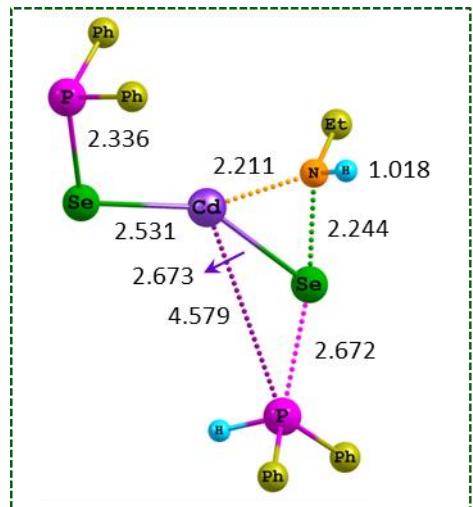


Se	-0.86685400	-1.08617200	-1.66781600
P	-2.10886400	0.79808300	-2.28169900
C	-1.51571200	2.11125100	-1.11196000
C	-1.89061500	2.21034400	0.23968400
C	-0.60974300	3.05300800	-1.62885700
C	-1.36557400	3.21791100	1.05163900
H	-2.59849800	1.50476600	0.66587000

C	-0.08182600	4.06169300	-0.81645800
H	-0.31970300	2.99628100	-2.67540500
C	-0.45857800	4.14542300	0.52638800
H	-1.66406700	3.27428100	2.09480100
H	0.61635600	4.78213200	-1.23399700
H	-0.05176400	4.92889400	1.15971700
C	-3.82671900	0.48805700	-1.65329800
C	-4.69692100	1.58803300	-1.52174800
C	-4.35060800	-0.80134000	-1.47224000
C	-6.04141900	1.40186800	-1.19627600
H	-4.32293900	2.59840000	-1.66516500
C	-5.69950100	-0.98691900	-1.15163700
H	-3.69961200	-1.66360900	-1.57999000
C	-6.54928600	0.11189900	-1.00900200
H	-6.69191000	2.26569500	-1.08841000
H	-6.08206900	-1.99427400	-1.01041100
H	-7.59569300	-0.03297300	-0.75576000
Cd	-1.09931100	-1.23110800	0.90545500
Se	1.66840500	-1.20141300	1.85969700
C	-3.53072400	-1.78729600	2.78437500
H	-3.49262100	-2.88976600	2.86045100
H	-4.10744100	-1.56403700	1.87768600
C	-4.29520500	-1.24703800	4.00088100
H	-4.41167000	-0.16031900	3.92975900
H	-5.29016900	-1.70454200	4.07717300
H	-3.75408100	-1.46708600	4.93000000
P	2.57537700	-0.20995100	0.12789800
C	3.71907000	-1.23380500	-0.84733600
C	4.99663700	-1.55040600	-0.35895100
C	3.28607100	-1.75870300	-2.07500500
C	5.84051800	-2.37368300	-1.10414500
H	5.33112300	-1.15556100	0.59629600
C	4.13688700	-2.58486200	-2.81467300
H	2.29012100	-1.53333300	-2.44736900
C	5.41161200	-2.89123300	-2.33194100
H	6.82984500	-2.61435000	-0.72636900
H	3.79994700	-2.98855200	-3.76482000
H	6.07009500	-3.53450700	-2.90844800
C	3.44284000	1.35058800	0.52967300
C	3.28548000	1.94997700	1.78559000
C	4.23854000	1.97190300	-0.44821800
C	3.92271200	3.16244200	2.06354700
H	2.67029200	1.46625600	2.53827600
C	4.86773700	3.18508100	-0.16587500
H	4.37298700	1.51144800	-1.42280300
C	4.71190600	3.78034200	1.09071200

H	3.80092900	3.62064900	3.04059400
H	5.48180200	3.66187500	-0.92424600
H	5.20681700	4.72225000	1.30942900
H	1.57195800	0.10054700	-0.81610600
N	-2.21161400	-1.16525800	2.65612600
H	-1.64771400	-1.37183800	3.47836800

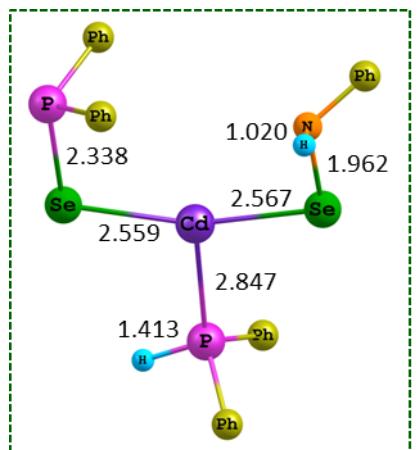
H/I-TS1



Se	2.11296800	1.10392700	-1.92445600
P	4.32527400	1.06859000	-1.17401400
C	4.68532100	-0.73088200	-0.91623300
C	4.38469300	-1.45452600	0.25050700
C	5.30446000	-1.40387300	-1.98383500
C	4.69265600	-2.81400500	0.34337500
H	3.92029100	-0.95391100	1.09489900
C	5.60396800	-2.76583800	-1.89545900
H	5.55008300	-0.85617300	-2.89022200
C	5.29965800	-3.47451100	-0.72998300
H	4.45953100	-3.35778000	1.25496900
H	6.08034500	-3.26930300	-2.73212700
H	5.53762900	-4.53190500	-0.65536600
C	4.29002600	1.70773400	0.56763000
C	5.43140600	1.50277300	1.36856700
C	3.26557700	2.52619900	1.06837700
C	5.52694000	2.07226700	2.63911800
H	6.25002300	0.88881800	1.00204900
C	3.36427700	3.10074900	2.34049900
H	2.38850600	2.72129100	0.45886500
C	4.49108900	2.87313900	3.13272400
H	6.41246600	1.89169800	3.24256900
H	2.55634200	3.72794800	2.70786500
H	4.56679600	3.31843300	4.12067300
Cd	0.79080900	-0.25979300	-0.25106700

Se	-1.62655700	-1.00138800	0.61646800
C	0.62921800	-3.05662700	1.49239900
H	1.69469500	-3.23252700	1.70927900
H	0.44120900	-3.46335500	0.49179600
C	-0.23160200	-3.79651400	2.51987800
H	-1.29561800	-3.65409700	2.30609600
H	-0.01523500	-4.87130200	2.50529000
H	-0.03466000	-3.42902600	3.53470000
P	-3.76514200	-0.00292200	-0.63689200
C	-4.17912600	1.75602600	-0.32507200
C	-4.22075400	2.21891700	1.00151500
C	-4.40003200	2.66614300	-1.37168300
C	-4.50371600	3.55814100	1.27397800
H	-4.02218400	1.53152400	1.81949900
C	-4.66948800	4.01052200	-1.09689600
H	-4.36125500	2.32848300	-2.40393900
C	-4.72676200	4.45743900	0.22554800
H	-4.53813200	3.90250500	2.30371800
H	-4.83548000	4.70457000	-1.91599600
H	-4.93785700	5.50137100	0.43898500
C	-5.33158100	-0.93663600	-0.34240900
C	-5.23160500	-2.27037300	0.08281700
C	-6.60304900	-0.37212800	-0.53672800
C	-6.38459800	-3.03297200	0.29359200
H	-4.25145600	-2.70586200	0.25622500
C	-7.75287300	-1.13459100	-0.32005300
H	-6.69715100	0.66330900	-0.85050600
C	-7.64576000	-2.46716400	0.09235400
H	-6.29479700	-4.06485100	0.62125900
H	-8.73155800	-0.68806200	-0.47267300
H	-8.54170500	-3.05804700	0.26089300
H	-3.73234300	0.02810000	-2.05363800
N	0.36702300	-1.61419200	1.44395000
H	0.43356000	-1.21022700	2.37641000

H/I-IM2



Se	-0.98558400	-0.17092700	-2.58084300
P	-3.28433400	-0.18956300	-2.15459400
C	-3.57397800	1.38438200	-1.22146400
C	-3.21136100	1.60198900	0.11982300
C	-4.17260400	2.43198400	-1.94118800
C	-3.44501000	2.84288900	0.71711800
H	-2.75797000	0.81174700	0.71741000
C	-4.40219800	3.67440300	-1.34160400
H	-4.45892200	2.27314700	-2.97796500
C	-4.03717100	3.88234500	-0.00956700
H	-3.16023700	2.99801900	1.75432700
H	-4.86582300	4.47357400	-1.91354400
H	-4.21442800	4.84546400	0.46146500
C	-3.54377600	-1.47244500	-0.83981400
C	-4.69212100	-1.39106700	-0.02840400
C	-2.73880200	-2.61871600	-0.73814100
C	-5.00816500	-2.41131700	0.87070300
H	-5.34017100	-0.52134500	-0.08960700
C	-3.05627700	-3.64094000	0.16182400
H	-1.85668800	-2.71050200	-1.36471900
C	-4.18971900	-3.54119100	0.97260000
H	-5.89491800	-2.32177700	1.49274000
H	-2.41460000	-4.51582800	0.22641100
H	-4.43679900	-4.33581700	1.67118400

Cd	0.12380300	-0.01185800	-0.28051400
Se	0.28185500	-0.17923600	2.27598100
C	-2.06799100	0.45993700	3.81038100
H	-3.16748200	0.41835700	3.81479900
H	-1.78938900	1.51168400	3.67614900
C	-1.53505000	-0.05542700	5.15302700
H	-0.44281500	0.00877400	5.19693700
H	-1.94322300	0.53587000	5.98158900
H	-1.82172300	-1.10193900	5.31333200
P	2.87995300	0.17741100	-0.96749600
C	3.89002600	-1.33359500	-0.68256000
C	3.72936100	-2.04495900	0.51808600
C	4.80137700	-1.80577000	-1.64173100
C	4.48502500	-3.19374800	0.76363600
H	3.00835300	-1.71242800	1.26090400
C	5.54783500	-2.96105100	-1.39742700
H	4.92946200	-1.27610600	-2.58167900
C	5.39466900	-3.65362500	-0.19281300
H	4.35339800	-3.73334800	1.69696300
H	6.24690700	-3.31892300	-2.14793000
H	5.97571900	-4.55168200	-0.00420600
C	3.85695500	1.58178400	-0.28854300
C	3.49789200	2.12233200	0.95653300
C	4.94895800	2.12797200	-0.98459000
C	4.23050400	3.17987600	1.50362300
H	2.64173100	1.72984300	1.49943900
C	5.67267700	3.18992800	-0.43961500
H	5.23633700	1.72586600	-1.95211100
C	5.31685500	3.71462700	0.80752400
H	3.94388700	3.58845100	2.46822200
H	6.51230600	3.60749200	-0.98795500
H	5.88090000	4.54112400	1.23009500
H	3.11998000	0.35739700	-2.34854100
N	-1.65153000	-0.26270800	2.60149200
H	-1.86062900	-1.25473000	2.71266200

Figure S8. Arrhenius plots of calculated rate constants for the crucial reaction step.

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^{1,2}:

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

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

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

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}), ΔG^* is the activation Gibbs free energy barrier, and ω^* is the imaginary frequency of TS.

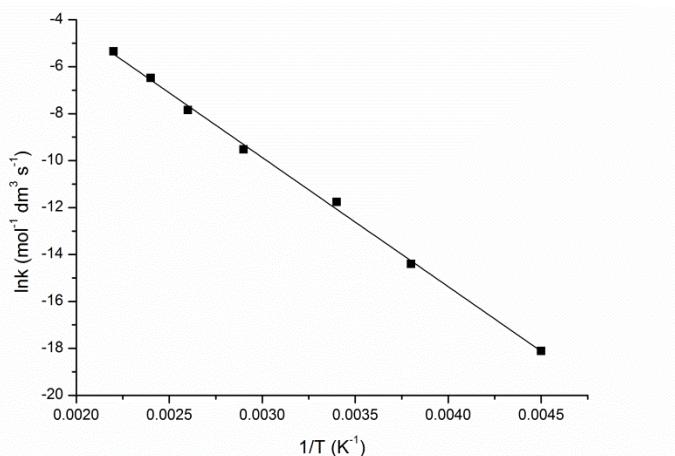
1. Eyring, H. The Activated Complex in Chemical Reactions. *J. Chem. Phys.* **1935**, *3*, 107–115.

2. Wigner, E. Calculation of the Rate of Elementary Association Reactions. *J. Chem. Phys.* **1937**, *5*, 720–725.

For reaction pathway **RP-CFE-iG**, the TDI and TDTS are **E-i** + HPPh_2 and **E-i/G-TS1**, respectively.

the rate constant of **E-i** + $\text{HPPh}_2 \rightarrow \text{E-i/G-TS1}$ (k_G) (in $\text{s}^{-1} \text{ mol}^{-1} \text{ dm}^3$):

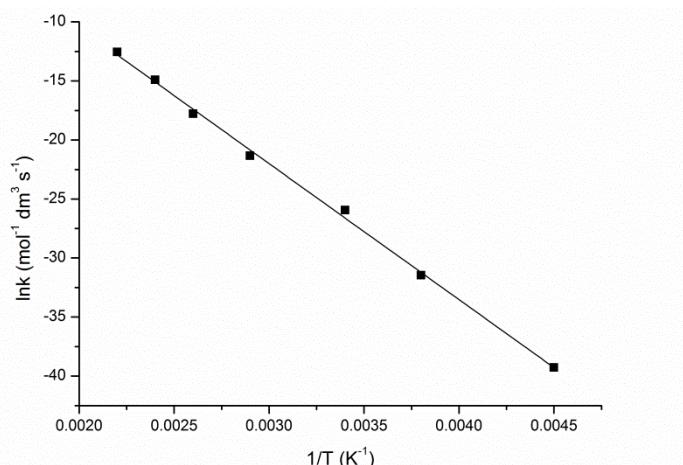
$$k_G = 5.554 \times 10^2 \exp(-44,741 / RT)$$



For reaction pathway **RP-CEH** and **RP-CFEH**, the TDI and TDTS are **E** + RNH_2 and **E/H-TS1**, respectively.

the rate constant of **E** + $\text{RNH}_2 \rightarrow \text{E/H-TS1}$ (k_H) (in $\text{s}^{-1} \text{ mol}^{-1} \text{ dm}^3$):

$$k_H = 1.459 \times 10^5 \exp(-93,682 / RT)$$



For reaction pathway **RP-CFE-iI**, the TDI and TDTs are **E-i** + RNH₂ and **E-i/I-TS1**, respectively.

the rate constant of **E-i** + RNH₂ → **E-i/I-TS1** (k_i) (in s⁻¹ mol⁻¹ dm³):

$$k_i = 5.334 \times 10^5 \exp(-125,250 / RT)$$

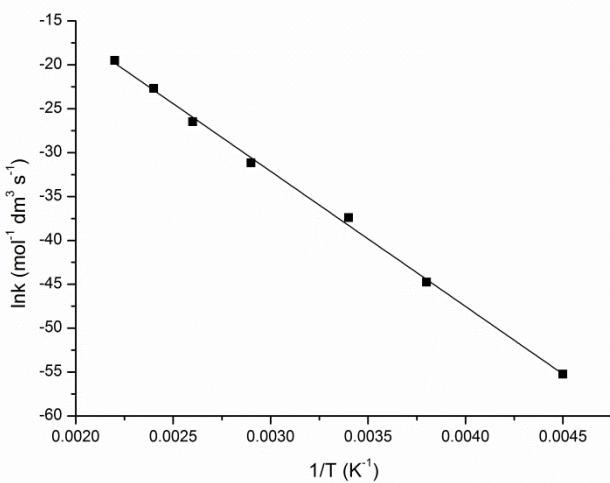


Table S9. Snapshot and standard orientation of all the species in the ODE solution calculated at the M06/6-31++G(d, p), SDD level.

s-Cd(OA) ₂							
Cd	0.00049800	-0.12373700	-0.01956500	H	-2.40082000	-3.72402000	-0.84916900
O	-2.04601100	0.69732600	-0.62321600	H	-4.29886800	-2.93987700	0.55138100
O	-1.90458400	-0.85243800	0.93978600	Se	-0.21787400	2.61544100	-0.05514300
C	-2.60082600	-0.06725700	0.21946300	H	0.07954600	0.45614200	-2.14158100
C	-4.09431900	-0.07478500	0.39784900	s-C-IM1			
H	-4.42058100	-1.11552900	0.25065700	Cd	1.96190100	-0.08068700	-0.04780600
H	-4.28241800	0.13493600	1.46199500	O	0.73371500	1.36770100	-1.53430600
C	-4.85953300	0.87850400	-0.49841100	O	1.98287200	2.21884300	0.08196700
H	-5.93638900	0.79941100	-0.31135100	C	1.21252100	2.36342000	-0.91092700
H	-4.56398600	1.91903000	-0.32333200	C	0.84889400	3.74833400	-1.39132700
H	-4.68404400	0.66131200	-1.55786500	H	1.14544500	3.79812400	-2.45023000
O	2.04180600	0.69705500	0.60289400	H	-0.25116700	3.80176500	-1.39961400
O	1.91165500	-0.83641300	-0.97702500	C	1.44394800	4.89432500	-0.59721300
C	2.60267100	-0.05820300	-0.24399900	H	1.11670200	5.85815700	-1.00634000
C	4.09728200	-0.06225800	-0.41291000	H	1.13873700	4.85288100	0.45505300
H	4.29171800	0.17401500	-1.47044400	H	2.53969200	4.87270100	-0.62028100
H	4.42282100	-1.10625500	-0.29007900	O	3.93528000	-0.99219000	0.79069200
C	4.85724500	0.86891600	0.51071700	O	3.35042800	-1.45680000	-1.29031100
H	4.67577300	0.62595500	1.56362700	C	4.15561900	-1.56637400	-0.31466800
H	5.93515900	0.79425100	0.32800000	C	5.39656100	-2.40279600	-0.51014200
H	4.56263800	1.91345400	0.35977800	H	5.93039000	-1.97074400	-1.37052800
				H	5.05900000	-3.39332100	-0.85092900
s- SePPh ₂ H							
P	-0.01865800	0.59348300	-0.73348700	C	6.30178500	-2.51227600	0.70088700
C	1.48260400	-0.27495100	-0.20052600	H	5.78153400	-2.97247500	1.54935500
C	1.72354300	-0.46702000	1.16323600	H	7.18223100	-3.12503200	0.47129500
C	2.39733500	-0.74002400	-1.14708600	H	6.65159800	-1.52637300	1.02889400
C	2.86931100	-1.13848600	1.57343300	P	-1.59501800	-0.67873500	-0.36504500
H	1.01282200	-0.08741300	1.90064600	C	-2.84018900	-1.95460600	-0.70774500
C	3.54693300	-1.40900100	-0.73087600	C	-2.68289500	-3.26607200	-0.25865600
H	2.21369800	-0.58174400	-2.21139700	C	-3.96326400	-1.59790200	-1.46480800
C	3.78107400	-1.60839100	0.62710800	C	-3.65159300	-4.21990800	-0.56221400
H	3.05638500	-1.29219900	2.63549400	H	-1.80685200	-3.53946900	0.33072100
H	4.26059300	-1.77261200	-1.46915400	C	-4.92219200	-2.55696800	-1.76942100
H	4.67948400	-2.13174200	0.95245600	H	-4.09286700	-0.57132000	-1.81262800
C	-1.39971900	-0.51801900	-0.30624700	C	-4.76691500	-3.86688100	-1.31665500
C	-2.46628000	-0.07612600	0.47382000	H	-3.53064900	-5.24226800	-0.20697600
C	-1.37647900	-1.83342400	-0.78388800	H	-5.79520000	-2.28089200	-2.35913900
C	-3.50616700	-0.95047800	0.78477700	H	-5.52246500	-4.61548700	-1.55210300
H	-2.47919500	0.95493300	0.83206000	C	-2.49271900	0.82690500	0.05986800
C	-2.41863600	-2.70068000	-0.47636900	C	-2.43913400	1.93162800	-0.79297800
H	-0.54121900	-2.18394700	-1.39440500	C	-3.26013500	0.86475100	1.22844900
C	-3.48341700	-2.25896800	0.30979200	C	-3.16951000	3.07578400	-0.47716300
H	-4.33833400	-0.60426000	1.39647900	H	-1.81654100	1.89902100	-1.68899100
				C	-3.98467100	2.00981100	1.53550400

H	-3.28887100	-0.00055300	1.89432800	H	2.32153000	1.71742500	-3.19376100
C	-3.93907400	3.11371900	0.68243200	C	5.41663200	1.60038900	-0.85624500
H	-3.13289200	3.94067400	-1.13864200	H	4.11838900	0.67782500	0.59005000
H	-4.58433700	2.04409200	2.44398000	C	5.52684200	2.14128600	-2.13635500
H	-4.50768900	4.01007700	0.92742300	H	4.49625800	2.60378700	-3.97383000
Se	-0.14553300	-1.34149000	1.14554500	H	6.28431700	1.56681500	-0.19871500
H	-0.96991100	-0.36169800	-1.59117900	H	6.48355000	2.53015000	-2.48304900
				Se	0.12805700	0.07200000	-2.32758700
s-C-TS1				H	0.74681500	1.58256500	0.34806900
Cd	-1.88938800	0.13481700	-0.66938100				
O	0.15755300	2.50021000	1.19430400	s-C-IM2			
O	-1.95372200	1.85425000	0.75305000	Cd	-1.61532600	-0.47196800	-0.67822300
C	-1.09878300	2.57969700	1.33509800	O	0.07555000	2.34652400	1.71130400
C	-1.64867600	3.62909600	2.27465300	O	-1.70156800	1.58153800	0.57717800
H	-2.31974500	4.25936500	1.67059300	C	-1.20144200	2.36734200	1.37327700
H	-2.31075100	3.10228600	2.97844000	C	-1.96905500	3.45737900	2.05486500
C	-0.61815500	4.46618900	3.00570000	H	-1.73081400	3.40178500	3.12781700
H	-1.11122800	5.20172800	3.65280100	H	-1.53249800	4.40907100	1.71141600
H	0.03015300	3.84603900	3.63618200	C	-3.46211200	3.40397200	1.80124100
H	0.02729700	5.01075100	2.30665300	H	-3.96700100	4.22703500	2.31908800
O	-4.07242800	-0.53904900	-0.76009100	H	-3.69150300	3.48267200	0.73221600
O	-2.74133600	-1.56291000	0.67888900	H	-3.89237300	2.46217900	2.16310900
C	-3.88312700	-1.39851200	0.15399000	O	-3.84306200	-0.22315500	-1.16428200
C	-5.02265400	-2.26393200	0.62942200	O	-3.27675800	-1.26858300	0.69663700
H	-4.99024000	-2.25932600	1.72863800	C	-4.16271100	-0.80261700	-0.08481400
H	-4.76672300	-3.29495900	0.33801800	C	-5.60958200	-0.94868400	0.31064700
C	-6.39319300	-1.87490600	0.11020700	H	-5.71027700	-0.46956500	1.29672600
H	-6.43157900	-1.91000300	-0.98456800	H	-5.78163500	-2.02007800	0.49408800
H	-7.16025100	-2.55553700	0.49938500	C	-6.61227900	-0.38761100	-0.67824000
H	-6.66056200	-0.85553000	0.41395700	H	-6.53325400	-0.88146500	-1.65324400
P	1.48257600	0.55905800	-0.59901000	H	-7.63565400	-0.52684300	-0.31115100
C	1.80827900	-0.95451800	0.34131700	H	-6.45512100	0.68438300	-0.84279300
C	2.62070000	-1.97890000	-0.15752800	P	1.83946500	0.09778800	0.05054500
C	1.16857800	-1.10473800	1.57558500	C	2.63223600	-1.32035100	0.92044100
C	2.80245900	-3.13869600	0.58559800	C	2.27179200	-2.65696000	0.74607800
H	3.10669300	-1.86766600	-1.12878800	C	3.60045700	-0.99657900	1.88267800
C	1.34719000	-2.27354400	2.31227200	C	2.88069300	-3.65550600	1.50700400
H	0.52380900	-0.31113600	1.95955100	H	1.52045600	-2.92245200	0.00160000
C	2.16599900	-3.28567300	1.81967700	C	4.21127300	-1.99335500	2.63543700
H	3.43778000	-3.93510700	0.19998300	H	3.88797400	0.04606000	2.03839000
H	0.84315900	-2.39206400	3.27039400	C	3.85091000	-3.32836800	2.44920700
H	2.30771600	-4.19936700	2.39581100	H	2.59408700	-4.69601200	1.35614600
C	3.07803900	1.13425200	-1.25507400	H	4.96906800	-1.72713200	3.37172400
C	3.18990400	1.68323500	-2.53452800	H	4.32731400	-4.11057600	3.03907600
C	4.19732500	1.09965800	-0.41299200	C	3.27203800	0.81942600	-0.84405700
C	4.41423700	2.18224000	-2.97282500	C	3.34087400	2.21218200	-0.94701400

C	4.26526500	0.03682900	-1.44521900	H	-8.51168300	2.49618500	0.06581700
C	4.39079700	2.81779000	-1.63551200	Se	-2.87647700	-0.04672500	-2.83564300
H	2.56804200	2.82875400	-0.48320600				
C	5.31246400	0.64186100	-2.13179400	s-C			
H	4.21686500	-1.05149600	-1.37403400	Cd	0.23387700	0.08410300	-1.29488600
C	5.37643700	2.03278700	-2.22751700	Se	0.72241500	0.94277100	-3.62330400
H	4.43856600	3.90384300	-1.70695000	P	-0.24128400	3.04859900	-3.48985100
H	6.08200900	0.02662300	-2.59716500	C	0.43843700	3.68167100	-1.89401600
H	6.19919200	2.50418900	-2.76417000	C	1.68363000	4.32121500	-1.95469000
Se	0.68359900	-0.83579900	-1.71605800	C	-0.20293000	3.56656100	-0.65452500
H	0.55647200	1.62368600	1.22630800	C	2.28061500	4.82378400	-0.80192800
				H	2.18932300	4.42115200	-2.91768500
s-C-i				C	0.39400900	4.07126900	0.49873100
Cd	-1.16561600	1.47767000	-1.79960700	H	-1.17971000	3.08549200	-0.58340000
O	-0.18062800	2.51678200	-0.04712800	C	1.63601000	4.69957300	0.42814700
O	0.64184000	2.85990500	-2.06426700	H	3.24911100	5.31906800	-0.86516300
C	0.66672200	3.07236500	-0.81639000	H	-0.11727100	3.97227300	1.45621300
C	1.69065800	3.99075900	-0.20725200	H	2.09870900	5.09724600	1.33082100
H	2.18151100	3.42595100	0.59962300	C	-2.00642500	2.77599700	-3.02945300
H	1.12803200	4.78720900	0.30407400	C	-2.75538400	3.93861200	-2.78908300
C	2.70235300	4.56541300	-1.17877300	C	-2.65644700	1.54113300	-2.99108000
H	2.21508100	5.15277800	-1.96484000	C	-4.10702700	3.86118600	-2.47418800
H	3.40791400	5.22058100	-0.65555100	H	-2.27075600	4.91686700	-2.83620400
H	3.27896700	3.77445100	-1.67141100	C	-4.01581200	1.46344800	-2.68493300
P	-3.80759300	-0.67365500	-0.78032800	H	-2.09968100	0.62835900	-3.20943100
C	-4.54697500	-2.26830700	-1.33395300	C	-4.74183200	2.61975400	-2.41871600
C	-3.82869100	-3.43262200	-1.03666700	H	-4.66916200	4.77328000	-2.27584500
C	-5.74885700	-2.37094900	-2.04388300	H	-4.50548600	0.49035400	-2.65522600
C	-4.29989500	-4.67849200	-1.44336200	H	-5.80169100	2.55752100	-2.17483000
H	-2.89067300	-3.35909500	-0.48245300	O	0.44501200	-1.34399300	0.42846900
C	-6.22262600	-3.61700600	-2.44437300	O	-1.06907100	0.24852500	0.61851600
H	-6.31811300	-1.47180900	-2.28544800	C	-0.46725600	-0.75437400	1.09562200
C	-5.49953300	-4.77153400	-2.14553500	C	-0.80396500	-1.28862600	2.46186900
H	-3.73214100	-5.57773400	-1.20656400	H	-1.10100500	-2.33943000	2.32228900
H	-7.16015300	-3.68761300	-2.99536400	H	0.14105100	-1.33208900	3.02408300
H	-5.87275800	-5.74504900	-2.46191100	C	-1.86382200	-0.50904700	3.21461000
C	-5.32222700	0.37443300	-0.63746700	H	-2.05227200	-0.96247300	4.19427300
C	-5.68458700	1.41388300	-1.49574600	H	-1.55626700	0.53009500	3.37839500
C	-6.11929400	0.11781600	0.48816100	H	-2.81124100	-0.48627300	2.66481200
C	-6.82698100	2.17412000	-1.24189600				
H	-5.07786600	1.62654100	-2.37704700	s-RCOOH			
C	-7.26378100	0.86801900	0.73509800	C	0.63286900	-0.13411400	0.14700800
H	-5.84222000	-0.68422300	1.17704300	O	1.58148600	-0.87998800	0.28086700
C	-7.61940800	1.90264800	-0.13046000	O	0.77075800	1.12112000	-0.30268500
H	-7.09954000	2.98085600	-1.92211300	H	1.73009100	1.27079200	-0.47278100
H	-7.87496700	0.64874600	1.61011500	C	-0.78330600	-0.48852900	0.49193100

C	-1.85759500	0.20400400	-0.32868800
H	-0.85858500	-1.58134500	0.42445100
H	-0.89989400	-0.24075100	1.55993200
H	-1.74489100	-0.00697800	-1.39932900
H	-2.85023000	-0.14697400	-0.02376400
H	-1.83250000	1.29124200	-0.19772400