Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Uncovering the Mechanism Governing the Nucleation of Lead Sulfide Quantum Dots through a Hines Synthesis: Electronic Supplementary Information

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1 Lead Acetate Monomer Structures

Two closely related structures are possible for lead ethanoate, with the minimum energy configuration depending on the level of theory applied (Table 1). The Stuttgart-Dresden-Bonn (SDB) core potential is more accurate than the LANL2DZ core potential,[1] and the triple-zeta cc-pVTZ basis set is more accurate than the double-zeta basis set included in LANL2DZ.[2]

Table 1 Lead ethanoate isomer bond distances. SDB is both more costly and more accurate than LANL2DZ because it allows a greater number of explicit electrons.

Level of theory	r_{Pb-H_2O} (Å)	r_{Pb-COO} (Å)
Zherebetskyy *et al.* (Reference)[3]	2.69	2.10
HSE06/LANL2DZ	2.23	2.18
PBE/plane wave	2.77	2.36
HSE06/SDB+TZ	2.35	2.27

2 DFT Calculation Details

To reproduce the calculations of Zherebetskyy *et al.*, we used scalar-relativistic pseudopotentials with the Perdew-Burke-Ernzerhof (PBE) functional,[4] a more recent functional in the family of the Perdew-Wang-1991 (PW91) functional used by Zherebetskyy *et al.*.[5] Our kinetic energy cutoff was 30.0 Ry. For geometry optimization, we used a force convergence threshold of 0.01 eV/Å like Zherebetskyy, and we added an energy convergence threshold of 0.0001 Har (0.0027 eV).

For the initial calculations in Gaussian 09, we used the Correlation-Consistent Polarizable Valence (*) Zeta (cc-pV*Z) family, where (*) describes the level of multiple basis functions used, which correspond to different valence atomic orbitals and are denoted as double-zeta, triple-zeta, *etc.*[6] For this system of atoms, we found it necessary to select the (expensive) triple-zeta cc-pVTZ basis set, as described in our tests of alternate basis sets in the Supporting Information. For the functional, we selected the Heyd-Scuseria-Ernzerhof method (HSE06), a range-separated DFT hybrid.[7] The popular HSE06 functional, based on the Perdew-Burke-Ernzerhof (PBE) family,[4] is a good choice for metal-containing systems.[8] It has the advantage of a long-range correction which makes it more accurate for systems with longer- ranged non-bonded interactions.[9] To compare directly with the calculations in Zherebetskyy *et al.*'s paper, we also performed some calculations in Gaussian 09 with the PW91 non-hybrid functional. For these calculations, we compared two isomers of lead ethanoate hydrate, one with the carboxylate ion hydrogen-bonded to the water molecule, and one with no hydrogen bonding. Both functionals show a preference for the hydrogen-bonded form, with the preference substantially stronger for HSE06 than for PW91 (Table 2). These calculations may not be converged with respect to the basis set since they were performed at the double-zeta level[2] (D95, the default basis set of core potential SDD in Gaussian09).[10]

Table 2 PW91 vs. HSE06 isomerization energies for Pb ethanoate hydrate

Level of theory	Isomerization energy (k_BT)
HSE06/SDB+DZ	12.5
PW91/SDB+DZ	3.4

For atomic orbital calculations with heavy elements, such as Pb, it is also helpful to replace the inner electrons with an Effective Core Potential (ECP). The principal core potentials belong to three families: the Compact Effective Potentials,[11]

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the Los Alamos National Laboratory Double-Zeta (LANL2DZ) ECP,[12] and the Stuttgart-Dresden-Bonn (SDB) ECP.[13] All of these core potentials have been benchmarked and proven to be effective for organic molecules containing a metal atom,[14] while LANL2DZ and SDB are preferred for a system like ours with polar lead-oxygen bonds.[1] Although LANL2DZ and SDB are parameterized differently - LANL2DZ with quantum calculations on isolated atoms, whereas SDB is semi-empirical - they give similar results for the Pb systems we studied. The SDB potentials are generally acknowledged to be more reliable because they include more of the core electrons.[1] For the atoms with core potentials, we used each core potential's Gaussian 09 default basis for the valence atoms. To represent the solvent, toluene, we used the Polarizable Continuum Method (PCM) with the integral equation formalism variant (IEFPCM).[15]

For binding energies and geometries with small basis sets, significant error can be introduced by the overlap of basis sets on adjacent atoms, which produces spurious energies due to better fitting of the wavefunction at locations where more basis functions are present.[16] In the Gaussian 09 single-point calculations with LANL2DZ basis sets (a small basis set), we corrected for the basis set superposition error (BSSE),[16] using the equations:

$$E_{binding} = E_{interact} + E_{deform} \tag{1}$$

$$E_{interact} = E(AB)^{AB}_{AB} - E(A)^{AB}_{AB} - E(B)^{AB}_{AB} \tag{2}$$

$$E_{deform} = E(A)^{A}_{AB} - E(A)^{A}_{A} + E(B)^{B}_{AB} - E(B)^{B}_{B} \tag{3}$$

where the superscript indicates the basis set, the subscript indicates the conditions under which the geometry was optimized, and the symbol in brackets represents the chemical system considered. $E_{interact}$ accounts for the interaction energy between the two monomers in a dimer. However, this assumes the monomers do not change geometry as they approach each other. Therefore, a correction term, E_{deform}, accounts for the difference in energy between an isolated monomer and one in a dimer complex. For the final Orca calculations, whenever we used double-zeta basis sets, we also used the Gaussian Counterpoise Correction (GCP) method, which removes BSSE using a fast approximate correction which could be applied even during energy optimizations. This reduces the problems associated with use of smaller basis sets.[17] We performed the final optimizations with the triple-zeta def2-TZVP basis set, which is large and accurate enough not to benefit from the GCP correction, particularly for our system since Pb is not yet included in the GCP parameter set.[17]

3 Comparison of Methods for Finding the Minimum Energy Pathway

Selecting which method to use to determine the Minimum Energy Pathway (MEP) is not always straightforward, since each method has its own strengths and weaknesses. That being said, the Nudged Elastic Band (NEB) method[18] is a more popular choice for this application. NEB has the convenient property of being variational; that is, given a sufficient discretization of the path, it will never find an energy path lower than reality.[18] This property is shared by other path-based algorithms such as Steered Molecular Dynamics and Forward Flux Sampling, but not by higher-order optimization algorithms such as Synchronous-Transition Quasi-Newton method, which can converge to the wrong saddle point in the energy surface.[19,20] Similarly, the variational property is not shared by reaction coordinate-based methods such as Thermodynamic Integration and Adaptive Biasing Force, which can overlook certain energy barriers.

The trade-off is that the NEB algorithm does not exhaustively explore configuration space because the harmonic constraints weight it toward the geometrically shortest path between the given start and end points. The start and end geometries are completely fixed and, therefore, must be correct for NEB to have meaning. This is not true for methods such as Thermodynamic Integration, which restrain a given reaction coordinate. However, the choice of this reaction coordinate for complicated systems is even more fraught than the choice of start and end states for NEB: if the reaction coordinate is chosen incorrectly, the true barrier may be missed entirely, and the resulting E_a can be either higher or lower than the true value. Therefore, NEB is a good choice for metal organic-complex reactions such as this one. The pitfalls of both approaches are presented below (Figure 1).

4 NEB Method

As explained in the "Methods" section of the main text, all NEB simulations were performed at the B97-D3 level of DFT theory with Ahlrichs' def2-TZVP ("triple zeta") basis set[21–23] for optimization. However, our group's NEB algorithm[24] also requires specification of several arguments. A spring constant, k, was specified to be 0.1837 Ha/A. Additionally, a Climbing Image algorithm was used to ensure convergence of the highest energy frame to the transition state.[25] We employed the

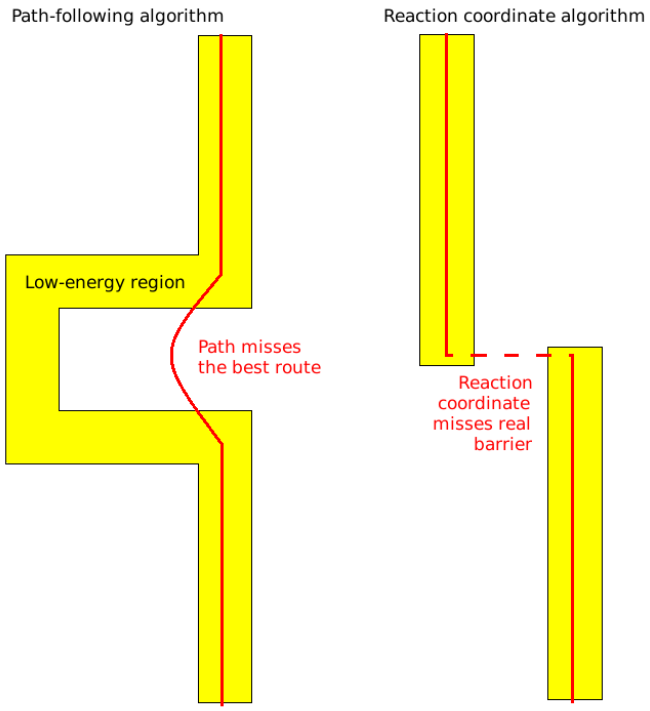

Fig. 1 Types of energy pathways which cause problems for NEB (left) and reaction-coordinate-based methods (right). Yellow indicates the low-energy region and red indicates the path found by each method. NEB fails to find the optimum path when it is far from the geometric minimum distance. Reaction-coordinate-based methods skip the real barrier entirely when it is orthogonal to the chosen reaction coordinate.

LBFGS optimizer,[26] based on the recommendation of Herbol *et al.* who found this optimizer to converge with the least amount of iterations, as compared to other popular optimizers.[24] We instated an accelerated backtrack linesearch method that improved convergence. The step size (dimensionless), step size adjustment (dimensionless), and maximum step size were set to 1.0, 0.5, and 0.04 Å, respectively. Our convergence criterion was determined by either the root mean squared force or the maximum force, set to 1.0 x 10^{-3} Ha/Åand 1.0 x 10^{-3} Ha/Å, respectively. An example of results using our NEB method with these criteria is shown in Figure 2.

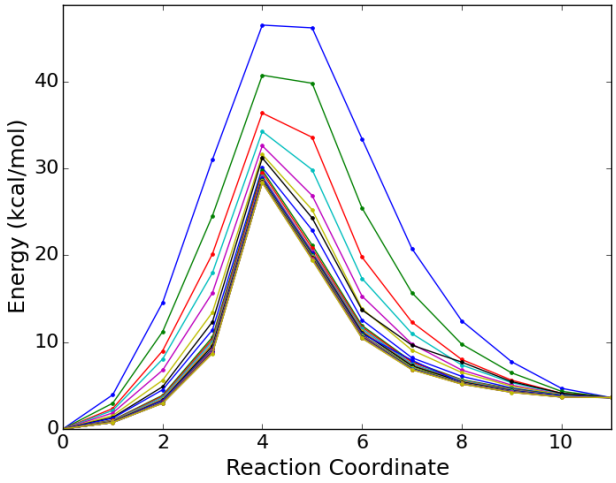

Fig. 2 Results for the energy barrier obtained from our custom Nudged Elastic Band method using one of the TMS transfers in our alternative reaction mechanism at the B97-D3/TZVP level of DFT in an implicit toluene solvent. The colors allow the different paths to be seen as successive steps converge, in this case downward, to a final barrier of around 28 kcal/mol.

5 Comparison of Results between Levels of *Ab Initio* Theory

As concerns all computational studies, we evaluated the trade-off between cost and accuracy for our final reaction energies. While functionals under the umbrella of double-hybrid provide results with small errors,[27] the time required to perform these calculations is not justified. Instead, we desired a computationally inexpensive method for finding physically accurate results. As part of our analysis of the NEB paths, we compared final energies using both the pure B97-D3 functional and the computationally more costly double-hybrid PWPB95-D3 functional, as shown in Figure 3. As expected, the two energy curves have the same shape, but differ in magnitude. More importantly, Figure 3 highlights that the minima and maxima will coincide at these different levels of theory. This is because the thermodynamics of the system are mostly attributable to the pure DFT functional, while a second-order MÃ¿llerâĹŠPlesset correlation energy term fine-tunes the calculation to account for weak interactions that were previously poorly estimated.[28] So, while accurate geometries can be obtained with a lower level of DFT theory because of coincident minima/maxima, the binding energies of these complexes are systematically underpredicted due to negligence of important close-range interactions. The solution is to use a cheaper pure DFT functional for geometry optimization, but a more accurate, albeit more expensive level of theory for the final energy evaluation, as per our procedure here.

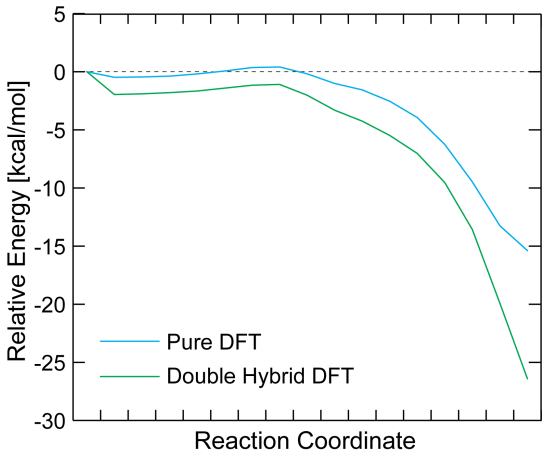

Fig. 3 Binding energy of the lead precursor to the sulfur precursor using our custom NEB method,[24] comparing results from pure and hybrid DFT. Color key as given in the legend.

For a more practical example, we also compared the final energies of the important stationary points for each mechanism at both levels of *ab initio* theory. In both Zherebetskyy *et al.*'s mechanism and the alternative mechanism, the B97-D3 underpredicts the energies, with the final heats of reaction being significantly underpredicted.

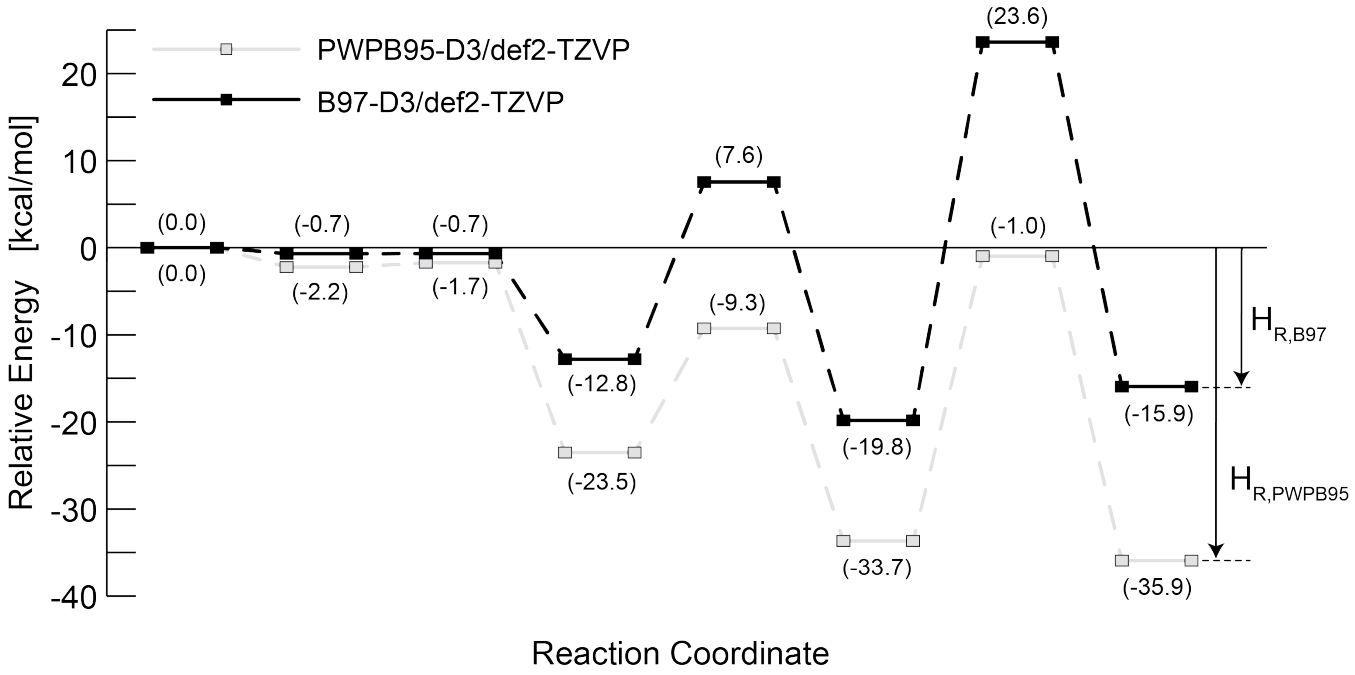

Fig. 4 Comparison of the relative energies of Zherebetskyy *et al.*'s mechanism for the different levels of DFT theory used in our study. Color key as given in the legend.

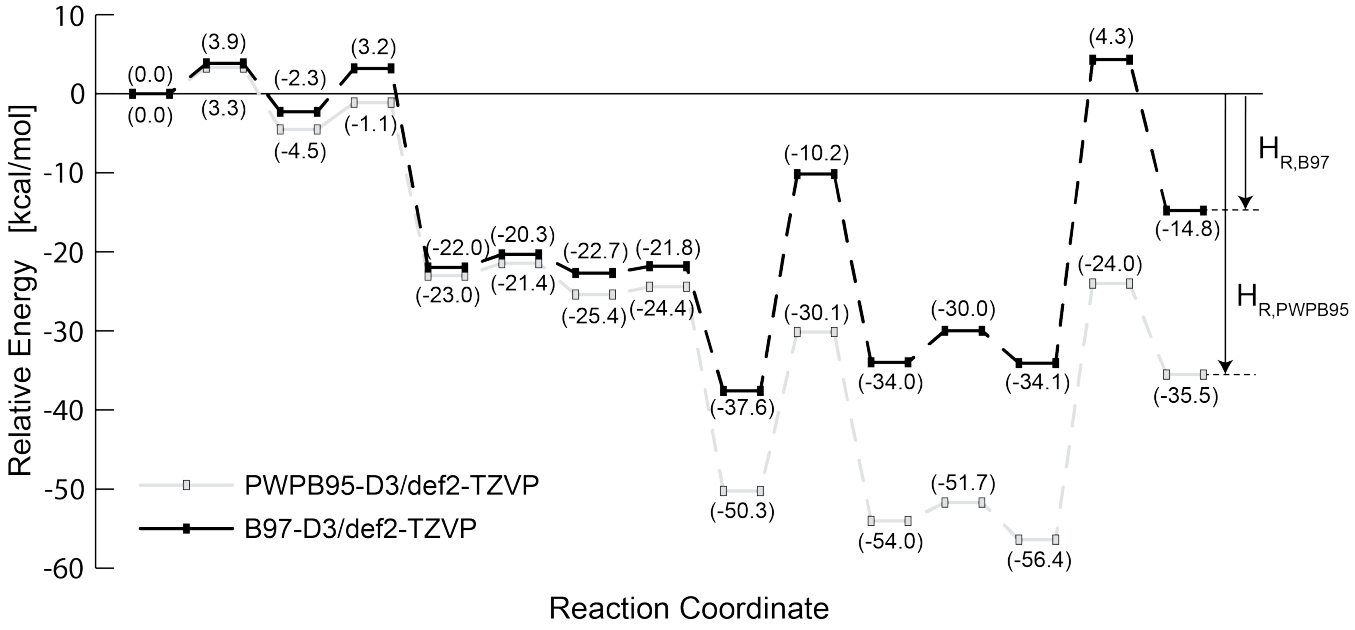

Fig. 5 Comparison of the relative energies of our alternative mechanism for the different levels of DFT theory used in our study. Color key as given in the legend.

6 Geometry of Stationary Points

For both Zherebetskyy *et al.*'s mechanism and our alternative mechanism, important geometries (minima, transition states) had to be calculated along the reaction coordinate. The final Cartesian coordinates, as well as the absolute energy (calculated at the B97-D3/def2-TZVP level) are provided below, allowing other researchers to recreate our reaction mechanism.

6.1 Zherebetskyy *et al.* Mechanism

Table 3 Cartesian Coordinates in Angstroms (Å) for the starting geometry, corresponding to two lead oleate monomers and a TMS_2S molecule, all non-interacting.

Element	X	Y	Z	Element	X	Y	Z
S	0.3551	-0.45395	-2.07138	C	-18.57596	17.11955	15.55379
Si	2.29386	-1.41518	-1.77955	C	-18.6421	17.13934	20.06442
Si	0.60785	1.38473	-3.23624	C	-19.43572	17.99053	21.03683
C	1.39287	0.94987	-4.88961	C	-19.325	17.89845	14.4904
C	-1.15628	1.98928	-3.44944	H	-19.5947	17.22109	13.67272
C	1.64729	2.67291	-2.3561	H	-20.25644	18.29361	14.90692
C	2.75696	-2.34229	-3.34778	H	-20.13252	18.61751	20.46967
C	1.99864	-2.62713	-0.37475	H	-18.77039	18.62425	21.62489
C	3.62392	-0.16672	-1.33468	H	-18.70848	18.71102	14.10324
H	2.70346	2.39306	-2.31984	H	-20.03247	17.35127	21.69494
H	1.30436	2.84064	-1.33308	O	-16.5426	15.99303	17.84194
H	1.56616	3.61873	-2.90797	H	-16.72359	16.55855	18.66211
H	3.94066	0.40601	-2.21238	H	-16.72804	16.59366	17.04447
H	3.27776	0.5373	-0.57333	Pb	2.0118	-10.47213	22.50942
H	4.50296	-0.69673	-0.94645	O	2.66174	-12.49378	23.32576
H	1.75663	-2.10627	0.55695	O	2.08272	-11.23211	20.36536
H	2.90128	-3.22896	-0.21026	H	3.38943	-14.46415	24.88752
H	1.17641	-3.31131	-0.61394	C	1.87698	-13.44251	23.74718
H	3.69946	-2.88426	-3.19637	C	2.59633	-14.70729	24.17379
H	1.98171	-3.06964	-3.61233	H	1.99651	-11.42371	17.7594
H	2.8885	-1.66206	-4.19499	C	1.07883	-11.70648	19.68669
H	0.84935	0.14294	-5.39189	O	-0.21809	-11.20114	22.6386
H	2.436	0.63921	-4.76685	C	1.4356	-12.19483	18.29599
H	1.38267	1.83223	-5.54243	H	3.07527	-15.15731	23.29712
H	-1.78141	1.23775	-3.94364	O	0.63446	-13.37266	23.81013
H	-1.16515	2.90037	-4.06066	H	2.08864	-13.07064	18.38437
H	-1.5931	2.22686	-2.47372	H	-0.03898	-12.07306	23.12568
Pb	-18.5834	14.83054	17.82119	H	-0.32544	-11.44974	21.66082
O	-19.28417	16.20571	16.15079	H	1.89658	-15.41914	24.61362
O	-19.34966	16.2562	19.42122	O	-0.09515	-11.78462	20.09796
O	-17.37723	17.36783	15.78852	H	0.53613	-12.46439	17.74097
O	-17.41671	17.31866	19.92541				

Single Point Energy: -2670.19001584 Ha

Table 4 Cartesian Coordinates in Angstroms (Å) for the start of the first exchange of oxygen with the central sulfur atom in TMS_2S. This state corresponds to one lead oleate monomer, and a TMS_2S molecule and lead oleate monomer complex. At this point, no reaction has occurred.

Element	X	Y	Z	Element	X	Y	Z
S	0.3551	-0.45395	-2.07138	C	-2.67755	1.84028	2.93291
Si	2.29386	-1.41518	-1.77955	C	1.59581	0.79664	1.75855
Si	0.60785	1.38473	-3.23624	C	2.88912	0.50264	2.49693
C	1.39287	0.94987	-4.88961	C	-3.35969	2.03729	4.27522
C	-1.15628	1.98928	-3.44944	H	-3.63985	3.08207	4.41962
C	1.64729	2.67291	-2.3561	H	-4.24454	1.39626	4.34092
C	2.75696	-2.34229	-3.34778	H	2.67279	0.32927	3.55626
C	1.99864	-2.62713	-0.37475	H	3.59091	1.3314	2.39192
C	3.62392	-0.16672	-1.33468	H	-2.67373	1.7282	5.07195
H	2.70346	2.39306	-2.31984	H	3.33544	-0.41611	2.10206
H	1.30436	2.84064	-1.33308	O	-1.00254	2.08403	0.20481
H	1.56616	3.61873	-2.90797	H	-0.04374	2.14832	0.50976
H	3.94066	0.40601	-2.21238	H	-1.56063	2.49142	0.9645
H	3.27776	0.5373	-0.57333	Pb	2.0118	-10.4721	22.5094
H	4.50296	-0.69673	-0.94645	O	2.6617	-12.4938	23.3258
H	1.75663	-2.10627	0.55695	O	2.0827	-11.2321	20.3654
H	2.90128	-3.22896	-0.21026	H	3.3894	-14.4642	24.8875
H	1.17641	-3.31131	-0.61394	C	1.877	-13.4425	23.7472
H	3.69946	-2.88426	-3.19637	C	2.5963	-14.7073	24.1738
H	1.98171	-3.06964	-3.61233	H	1.9965	-11.4237	17.7594
H	2.8885	-1.66206	-4.19499	C	1.0788	-11.7065	19.6867
H	0.84935	0.14294	-5.39189	O	-0.2181	-11.2011	22.6386
H	2.436	0.63921	-4.76685	C	1.4356	-12.1948	18.296
H	1.38267	1.83223	-5.54243	H	3.0753	-15.1573	23.2971
H	-1.78141	1.23775	-3.94364	O	0.6345	-13.3727	23.8101
H	-1.16515	2.90037	-4.06066	H	2.0886	-13.0706	18.3844
H	-1.5931	2.22686	-2.47372	H	-0.039	-12.0731	23.1257
Pb	-1.29684	-0.19194	0.71887	H	-0.3254	-11.4497	21.6608
O	-2.40993	0.61544	2.62669	H	1.8966	-15.4191	24.6136
O	0.71315	-0.15143	1.82591	O	-0.0951	-11.7846	20.098
O	-2.4151	2.83853	2.22181	H	0.5361	-12.4644	17.741
O	1.45353	1.87525	1.14927				

Single Point Energy: -2670.21042213 Ha

Table 5 Cartesian Coordinates in Angstroms (Å) for the transition state of the first exchange of oxygen with the central sulfur atom in TMS_2S. This state corresponds to one lead oleate monomer, and a TMS_2S molecule and lead oleate monomer complex.

Element	X	Y	Z	Element	X	Y	Z
S	-0.48188	-1.41472	-1.22965	C	-3.2856	1.55901	2.55485
Si	1.59398	-2.07943	-1.22239	C	1.08054	-0.35038	2.5968
Si	-0.66051	0.94544	-1.6684	C	2.31378	-0.64468	3.43076
C	-0.00703	0.60376	-3.45025	C	-4.22991	2.30824	3.46154
C	-2.48092	1.34834	-1.99736	H	-5.00066	2.80744	2.86682
C	0.53202	2.34618	-1.18762	H	-4.6858	1.63156	4.18506
C	1.96445	-2.79553	-2.92117	H	2.02425	-1.01454	4.41864
C	1.71252	-3.4275	0.0832	H	2.93584	0.24684	3.52671
C	2.77042	-0.66866	-0.83974	H	-3.66975	3.08719	3.99107
H	0.9764	2.80226	-2.07856	H	2.88805	-1.43933	2.93972
H	1.34651	1.96878	-0.5597	O	-1.15212	0.91771	0.32109
H	0.01418	3.11696	-0.60673	H	-0.32774	0.96917	0.87499
H	2.76478	0.08185	-1.63647	H	-2.09544	1.69951	0.98365
H	2.51983	-0.16911	0.10051	Pb	2.0118	-10.4721	22.5094
H	3.79082	-1.06543	-0.75847	O	2.6617	-12.4938	23.3258
H	1.5154	-3.0314	1.08446	O	2.0827	-11.2321	20.3654
H	2.71924	-3.86472	0.07769	H	3.3894	-14.4642	24.8875
H	0.99392	-4.2308	-0.11624	C	1.877	-13.4425	23.7472
H	2.9981	-3.16354	-2.95585	C	2.5963	-14.7073	24.1738
H	1.29357	-3.6322	-3.14412	H	1.9965	-11.4237	17.7594
H	1.84229	-2.04148	-3.70543	C	1.0788	-11.7065	19.6867
H	-0.56171	-0.19129	-3.96006	O	-0.2181	-11.2011	22.6386
H	1.05662	0.33845	-3.45662	C	1.4356	-12.1948	18.296
H	-0.11634	1.53078	-4.03265	H	3.0753	-15.1573	23.2971
H	-3.11974	0.49774	-1.72768	O	0.6345	-13.3727	23.8101
H	-2.65027	1.56626	-3.0569	H	2.0886	-13.0706	18.3844
H	-2.81164	2.20469	-1.40038	H	-0.039	-12.0731	23.1257
Pb	-1.68027	-1.39389	1.31483	H	-0.3254	-11.4497	21.6608
O	-2.99005	0.36947	2.7763	H	1.8966	-15.4191	24.6136
O	0.21622	-1.3247	2.56562	O	-0.0951	-11.7846	20.098
O	-2.82033	2.26434	1.55958	H	0.5361	-12.4644	17.741
O	0.96398	0.7313	1.99855				

Single Point Energy: -2670.17798814 Ha

Table 6 Cartesian Coordinates in Angstroms (Å) for the end of the first exchange of oxygen with the central sulfur atom in TMS_2S, and the start of the second exchange. This state corresponds to one lead oleate monomer, and a TMS_2S molecule and lead oleate monomer complex.

Element	X	Y	Z	Element	X	Y	Z
S	-0.21008	-1.93642	-1.84967	C	-2.13663	3.03448	1.82352
Si	1.84535	-1.76333	-2.46753	C	1.47089	1.17091	1.2182
Si	-0.55061	2.48864	-2.6643	C	2.5353	1.223	2.29155
C	1.24667	2.63488	-3.17177	C	-2.66554	3.9592	2.88741
C	-1.50378	1.2632	-3.70847	H	-1.91935	4.73398	3.09543
C	-1.37368	4.17487	-2.71088	H	-3.56937	4.46398	2.53198
C	1.87387	-1.19345	-4.2673	H	2.04313	1.32636	3.26562
C	2.6128	-3.48283	-2.36339	H	3.20495	2.07003	2.13467
C	2.85603	-0.58846	-1.39929	H	-2.87815	3.39833	3.79752
H	-1.36024	4.57304	-3.73305	H	3.09918	0.28622	2.30611
H	-0.85477	4.89112	-2.0634	O	-0.61351	1.93725	-1.0536
H	-2.41926	4.12041	-2.38601	H	0.26795	2.06583	-0.44436
H	2.43599	0.42011	-1.37011	H	-1.54984	3.01856	0.00216
H	2.91385	-0.95967	-0.37141	Pb	2.0118	-10.4721	22.5094
H	3.87585	-0.52054	-1.79993	O	2.6617	-12.4938	23.3258
H	2.61961	-3.8431	-1.32851	O	2.0827	-11.2321	20.3654
H	3.64826	-3.46249	-2.72801	H	3.3894	-14.4642	24.8875
H	2.04992	-4.20139	-2.96962	C	1.877	-13.4425	23.7472
H	2.90762	-1.10143	-4.62514	C	2.5963	-14.7073	24.1738
H	1.35469	-1.91957	-4.90336	H	1.9965	-11.4237	17.7594
H	1.38056	-0.22508	-4.39593	C	1.0788	-11.7065	19.6867
H	1.7556	1.6672	-3.16979	O	-0.2181	-11.2011	22.6386
H	1.7885	3.30405	-2.49353	C	1.4356	-12.1948	18.296
H	1.31787	3.04974	-4.1847	H	3.0753	-15.1573	23.2971
H	-1.07079	0.25921	-3.64517	O	0.6345	-13.3727	23.8101
H	-1.50312	1.57746	-4.75934	H	2.0886	-13.0706	18.3844
H	-2.54955	1.20185	-3.38154	H	-0.039	-12.0731	23.1257
Pb	-1.16439	-0.28544	-0.04575	H	-0.3254	-11.4497	21.6608
O	-1.88189	1.8524	2.00186	H	1.8966	-15.4191	24.6136
O	0.78621	0.09159	1.15556	O	-0.0951	-11.7846	20.098
O	-1.96566	3.65499	0.64621	H	0.5361	-12.4644	17.741
O	1.32001	2.17335	0.46481				

Single Point Energy: -2670.22160612 Ha

Table 7 Cartesian Coordinates in Angstroms (Å) for the transition state of the second exchange of oxygen with the central sulfur atom in TMS_2S. This state corresponds to one lead oleate monomer, and a TMS_2S molecule and lead oleate monomer complex.

Element	X	Y	Z	Element	X	Y	Z
S	-0.84273	-1.50439	-0.97108	C	-1.82653	1.89947	1.27967
Si	1.27633	-0.70135	-1.92151	C	1.82042	1.27514	1.30646
Si	0.06839	2.29382	-2.75235	C	2.26528	1.77417	2.6524
C	1.27629	2.29921	-4.20019	C	-2.95697	2.7527	1.78861
C	-1.67325	1.94383	-3.37118	H	-2.76285	3.80769	1.57586
C	0.15388	4.03392	-2.02802	H	-3.87312	2.47311	1.25518
C	0.74173	-1.06189	-3.70159	H	1.37799	1.83592	3.29455
C	2.06609	-2.34578	-1.28308	H	2.72391	2.76171	2.58517
C	2.95271	0.23994	-1.93909	H	-3.09754	2.59493	2.85787
H	-0.05272	4.76303	-2.82209	H	2.95351	1.05587	3.10449
H	1.15529	4.24643	-1.63539	O	0.43794	1.19205	-1.52494
H	-0.56945	4.19386	-1.22376	H	1.25966	1.7292	-0.51217
H	2.92693	1.27736	-2.27347	H	-0.7166	1.66082	-0.3572
H	3.41917	0.20957	-0.94853	Pb	2.0118	-10.4721	22.5094
H	3.61055	-0.32152	-2.61638	O	2.6617	-12.4938	23.3258
H	2.31675	-2.26317	-0.21739	O	2.0827	-11.2321	20.3654
H	3.00575	-2.52916	-1.82332	H	3.3894	-14.4642	24.8875
H	1.40255	-3.20449	-1.41217	C	1.877	-13.4425	23.7472
H	1.60342	-0.98285	-4.37592	C	2.5963	-14.7073	24.1738
H	0.36617	-2.0898	-3.74237	H	1.9965	-11.4237	17.7594
H	-0.04829	-0.41008	-4.07823	C	1.0788	-11.7065	19.6867
H	1.41476	1.32681	-4.676	O	-0.2181	-11.2011	22.6386
H	2.25993	2.67509	-3.89834	C	1.4356	-12.1948	18.296
H	0.8796	2.99009	-4.95622	H	3.0753	-15.1573	23.2971
H	-1.77538	0.92089	-3.74789	O	0.6345	-13.3727	23.8101
H	-1.93703	2.63363	-4.1827	H	-0.039	-12.0731	23.1257
H	-2.40151	2.07237	-2.56328	H	2.0886	-13.0706	18.3844
Pb	-0.40603	-1.37306	1.44821	H	-0.3254	-11.4497	21.6608
O	-1.30461	1.0172	1.96983	H	1.8966	-15.4191	24.6136
O	1.54735	0.07274	1.11292	O	-0.0951	-11.7846	20.098
O	-1.48125	2.19401	0.04569	H	0.5361	-12.4644	17.741
O	1.73079	2.16729	0.36595				

Single Point Energy: -2670.15236988 Ha

Table 8 Cartesian Coordinates in Angstroms (Å) for the end of the second exchange of oxygen with the central sulfur atom in TMS_2S. This state corresponds to one lead oleate monomer, one TMS_2O molecule, and a PbS quantum dot.

Element	X	Y	Z	Element	X	Y	Z
S	-1.86007	-1.20943	-0.60021	C	-2.14661	1.83557	1.54513
Si	1.94674	-0.40129	-2.58823	C	1.46523	1.12541	1.62633
Si	0.20432	2.10723	-2.86799	C	1.64322	1.93759	2.87985
C	1.22372	2.72521	-4.32471	C	-2.30442	3.26262	1.99659
C	-1.41755	1.3903	-3.47099	H	-1.43869	3.8329	1.6378
C	-0.1108	3.53515	-1.69452	H	-3.20101	3.71076	1.56218
C	1.0313	-1.1981	-4.02066	H	0.65025	2.07339	3.32494
C	2.11816	-1.64326	-1.20157	H	2.0791	2.91682	2.67577
C	3.64838	0.18999	-3.129	H	-2.33216	3.31294	3.08585
H	-0.66254	4.31928	-2.22799	H	2.25462	1.38022	3.59253
H	0.82277	3.96928	-1.32118	O	1.08695	0.93819	-2.03078
H	-0.71453	3.22403	-0.83774	H	1.28577	1.32788	-0.30531
H	3.59049	0.87448	-3.98191	H	-2.30669	0.65243	0.00714
H	4.15589	0.71294	-2.30917	Pb	2.0118	-10.4721	22.5094
H	4.27409	-0.66238	-3.42165	O	2.6617	-12.4938	23.3258
H	2.60817	-1.22504	-0.31781	O	2.0827	-11.2321	20.3654
H	2.71392	-2.49415	-1.55613	H	3.3894	-14.4642	24.8875
H	1.13068	-2.0105	-0.90377	C	1.877	-13.4425	23.7472
H	1.58033	-2.08671	-4.35661	C	2.5963	-14.7073	24.1738
H	0.03204	-1.51666	-3.70377	H	1.9965	-11.4237	17.7594
H	0.9248	-0.52873	-4.88097	C	1.0788	-11.7065	19.6867
H	1.43152	1.93187	-5.05115	O	-0.2181	-11.2011	22.6386
H	2.18109	3.14339	-3.99316	C	1.4356	-12.1948	18.296
H	0.6739	3.5171	-4.849	H	3.0753	-15.1573	23.2971
H	-1.26827	0.67767	-4.28845	O	0.6345	-13.3727	23.8101
H	-2.0674	2.1946	-3.83845	H	-0.039	-12.0731	23.1257
H	-1.93553	0.86708	-2.66052	H	-0.3254	-11.4497	21.6608
Pb	-1.04663	-1.49431	1.65169	H	2.0886	-13.0706	18.3844
O	-1.68234	0.96491	2.29719	H	1.8966	-15.4191	24.6136
O	1.32519	-0.09383	1.62983	O	-0.0951	-11.7846	20.098
O	-2.51083	1.62689	0.2993	H	0.5361	-12.4644	17.741
O	1.44753	1.86715	0.52075				

Single Point Energy: -2670.2154172 Ha

6.2 Alternative Mechanism

Table 9 Cartesian Coordinates in Angstroms (Å) for the starting geometry, corresponding to two lead oleate monomers and a TMS_2S molecule, all non-interacting. This geometry has the same absolute energy as the start of Zherebetskyy *et al.*'s mechanism.

Element	X	Y	Z	Element	X	Y	Z
Pb	-14.401687	13.500881	7.665458	H	6.078293	-16.748799	14.457888
O	-15.102457	14.876051	5.995058	O	3.963623	-12.530799	12.482868
O	-15.167947	14.926541	9.265488	H	4.142733	-13.402719	12.969948
O	-13.195517	16.038171	5.632788	H	3.856273	-12.779399	11.505088
O	-13.234997	15.989001	9.769678	S	4.536813	-1.783609	-12.227112
C	-14.394247	15.789891	5.398058	Si	6.475573	-2.744839	-11.935282
C	-14.460387	15.809681	9.908688	Si	4.789563	0.055071	-13.391972
C	-15.254007	16.660871	10.881098	C	5.574583	-0.379789	-15.045342
C	-15.143287	16.568791	4.334668	C	3.025433	0.659621	-13.605172
H	-15.412987	15.891431	3.516988	C	5.829003	1.343251	-12.511832
H	-16.074727	16.963951	4.751188	C	6.938673	-3.671949	-13.503512
H	-15.950807	17.287851	10.313938	C	6.180353	-3.956789	-10.530482
H	-14.588677	17.294591	11.469158	C	7.805633	-1.496379	-11.490412
H	-14.526767	17.381361	3.947508	H	6.885173	1.063401	-12.475572
H	-15.850757	16.021611	11.539208	H	5.486073	1.510981	-11.488812
O	-12.360887	14.663371	7.686208	H	5.747873	2.289071	-13.063702
H	-12.541877	15.228891	8.506378	H	8.122373	-0.923649	-12.368112
H	-12.546327	15.264001	6.888738	H	7.459473	-0.792359	-10.729062
Pb	6.193513	-11.801789	12.353688	H	8.684673	-2.026389	-11.102182
O	6.264433	-12.561769	10.209628	H	5.938343	-3.435929	-9.598782
O	6.843453	-13.823439	13.170028	H	7.082993	-4.558619	-10.365992
O	4.086563	-13.114279	9.942228	H	5.358123	-4.640969	-10.769672
O	4.816173	-14.702319	13.654398	H	7.881173	-4.213919	-13.352102
C	5.260543	-13.036139	9.530958	H	6.163423	-4.399299	-13.768062
C	6.058693	-14.772169	13.591448	H	7.070213	-2.991719	-14.350722
C	6.778043	-16.036949	14.018058	H	5.031063	-1.186719	-15.547622
C	5.617313	-13.524489	8.140258	H	6.617713	-0.690449	-14.922582
H	6.178223	-12.753369	7.603668	H	5.564383	0.502571	-15.698162
H	6.270353	-14.400299	8.228638	H	2.400303	-0.091909	-14.099372
H	7.571143	-15.793809	14.731788	H	3.016563	1.570711	-14.216392
H	7.256983	-16.486969	13.141388	H	2.588613	0.897201	-12.629452
H	4.717843	-13.794049	7.585238				

Single Point Energy: -2670.19005227 Ha

Table 10 Cartesian Coordinates in Angstroms (Å) for the transition state of the first hydrogen bond cleaving within the lead oleate hydrate. This state corresponds to two lead oleate monomers and a TMS_2S molecule, all non-interacting.

Element	X	Y	Z	Element	X	Y	Z
Pb	-13.879656	14.509482	2.395408	H	10.27935	-15.941697	7.414179
O	-12.801501	13.301974	4.079585	O	6.447489	-14.441734	10.419304
O	-12.007305	14.237055	1.128117	H	7.196195	-14.523242	9.73132
O	-12.367279	15.418448	4.660836	H	6.886056	-14.433276	11.28902
O	-11.483795	16.392291	0.681914	S	3.788708	0.731623	-9.374149
C	-12.251837	14.185149	4.847483	Si	2.351821	-0.514137	-8.284986
C	-11.31579	15.163774	0.538043	Si	2.911107	2.721385	-9.653516
C	-10.244076	14.655581	-0.406911	C	1.97667	3.298976	-8.132785
C	-11.41344	13.655357	5.993485	C	4.385935	3.833936	-9.986484
H	-11.844209	12.735529	6.396452	C	1.780202	2.65004	-11.152226
H	-10.416484	13.414896	5.604786	C	2.248641	-0.014194	-6.481846
H	-10.718611	14.410316	-1.364956	C	3.04344	-2.249454	-8.437989
H	-9.785812	13.742045	-0.020317	C	0.671513	-0.377096	-9.117429
H	-11.310007	14.409553	6.775694	H	1.371818	3.648023	-11.35783
H	-9.487981	15.424702	-0.574422	H	0.941615	1.965492	-10.992759
O	-13.319835	16.92467	2.430698	H	2.331951	2.314747	-12.036807
H	-12.571129	16.843162	1.742714	H	0.237125	0.620618	-8.996851
H	-12.881268	16.933128	3.300414	H	0.741508	-0.596625	-10.18805
Pb	5.887673	-16.85691	10.384016	H	-0.016585	-1.099955	-8.660624
O	6.965822	-18.064431	12.068191	H	3.188548	-2.531599	-9.486028
O	7.760026	-17.129345	9.116718	H	2.352387	-2.966315	-7.977601
O	7.400052	-15.947951	12.649437	H	4.005295	-2.31454	-7.92213
O	8.283536	-14.974109	8.670515	H	1.621852	-0.73368	-5.939789
C	7.515494	-17.181251	12.836085	H	3.242755	-0.009266	-6.027924
C	8.45154	-16.202617	8.52665	H	1.807641	0.979327	-6.360636
C	9.523255	-16.710819	7.58169	H	2.62893	3.293333	-7.25432
C	8.35389	-17.711035	13.982092	H	1.093246	2.686016	-7.92819
H	7.92312	-18.630863	14.38506	H	1.637762	4.329972	-8.297229
H	9.350847	-17.951504	13.593387	H	4.976678	3.972818	-9.075223
H	9.048713	-16.956089	6.62365	H	4.038127	4.82062	-10.31843
H	9.981519	-17.624355	7.968284	H	5.029418	3.420898	-10.771085
H	8.457324	-16.956847	14.764296				

Single Point Energy: -2670.18392329 Ha

Table 11 Cartesian Coordinates in Angstroms (Å) for the end of the first hydrogen bond-cleaving and the start of the second cleaving within the lead oleate hydrate. This state corresponds to two lead oleate monomers and a TMS_2S molecule, all non-interacting.

Element	X	Y	Z	Element	X	Y	Z
Pb	-14.594465	15.35231	3.167726	H	10.234455	-15.492109	6.62445
O	-13.698397	13.714271	4.938078	O	6.313017	-13.496558	9.186514
O	-12.672201	14.868279	2.020521	H	7.139618	-13.713896	8.623539
O	-13.449556	15.913381	5.167587	H	6.657332	-13.196024	10.040858
O	-11.933597	16.935041	1.467952	S	4.475359	-0.240143	-9.241393
C	-13.27268	14.707604	5.58732	Si	2.916342	-1.411652	-8.241458
C	-11.835503	15.688961	1.469464	Si	3.649471	1.727183	-9.746289
C	-10.653013	15.023181	0.791572	C	2.555132	2.403301	-8.38075
C	-12.510724	14.516321	6.878274	C	5.160594	2.8153	-9.983488
H	-12.642678	13.502394	7.259172	C	2.692824	1.557992	-11.354508
H	-11.446015	14.686834	6.679576	C	2.615843	-0.794647	-6.497638
H	-11.008108	14.267934	0.083457	C	3.607699	-3.153373	-8.202695
H	-10.054352	14.503639	1.547951	C	1.340784	-1.329172	-9.264195
H	-12.830218	15.252143	7.621193	H	2.317503	2.540428	-11.669112
H	-10.03538	15.761401	0.277823	H	1.83655	0.885494	-11.245863
O	-13.956823	17.756939	2.839886	H	3.337538	1.165386	-12.147942
H	-13.130216	17.539613	2.276913	H	0.90313	-0.325633	-9.258267
H	-13.6125	18.057477	3.694226	H	1.528463	-1.618374	-10.303647
Pb	5.675376	-15.901186	9.514354	H	0.600499	-2.020446	-8.841354
O	6.571443	-17.539225	11.284706	H	3.867021	-3.503589	-9.207259
O	7.597648	-16.385229	8.367151	H	2.864122	-3.838427	-7.777024
O	6.820285	-15.340116	11.514215	H	4.505292	-3.184678	-7.579108
O	8.336243	-14.318455	7.81458	H	1.926969	-1.47698	-5.983611
C	6.997152	-16.545897	11.933952	H	3.552945	-0.760151	-5.936405
C	8.434337	-15.564535	7.816092	H	2.171517	0.20475	-6.491553
C	9.61682	-16.23032	7.138204	H	3.104962	2.455113	-7.436198
C	7.759117	-16.737175	13.224902	H	1.649793	1.805199	-8.237044
H	7.627162	-17.751102	13.6058	H	2.244492	3.421363	-8.6489
H	8.82382	-16.566675	13.026202	H	5.64671	3.013485	-9.022719
H	9.261724	-16.985567	6.430089	H	4.859516	3.778174	-10.415839
H	10.215488	-16.749857	7.894579	H	5.884696	2.351651	-10.662439
H	7.439622	-16.001353	13.967821				

Single Point Energy: -2670.19368753 Ha

Table 12 Cartesian Coordinates in Angstroms (Å) for the transition state of the second hydrogen bond cleaving within the lead oleate hydrate. This state corresponds to two lead oleate monomers and a TMS_2S molecule, all non-interacting.

Element	X	Y	Z	Element	X	Y	Z
Pb	-9.01515	12.175106	5.907893	H	6.373089	-11.822437	5.1606
O	-10.296696	14.012008	7.170416	O	6.481435	-14.890599	9.885201
O	-9.769473	13.039389	3.893339	H	6.062849	-14.695353	9.017741
O	-11.18244	11.995273	6.8657	H	5.742128	-14.892363	10.511794
O	-10.479798	10.923636	3.666869	S	2.763095	0.381471	-10.730258
C	-11.247694	13.195384	7.324464	Si	3.553411	1.670501	-9.143866
C	-10.297953	12.074563	3.21235	Si	3.626876	-1.619868	-10.493814
C	-10.68048	12.404295	1.783893	C	3.732558	-2.13317	-8.692492
C	-12.492645	13.603775	8.079492	C	2.453543	-2.743293	-11.434538
H	-12.719563	14.656325	7.894079	C	5.327031	-1.614747	-11.293576
H	-13.341075	12.97229	7.810091	C	2.793872	1.248244	-7.483534
H	-11.330928	13.284883	1.768382	C	3.050129	3.39877	-9.666229
H	-11.17987	11.558284	1.310899	C	5.424668	1.495134	-9.090794
H	-12.298869	13.487379	9.153052	H	5.762661	-2.621296	-11.247684
H	-9.774539	12.661483	1.224362	H	6.009213	-0.925346	-10.787002
O	-9.666195	9.59332	5.948964	H	5.258286	-1.316837	-12.345173
H	-10.08477	9.788562	5.081501	H	5.73134	0.502811	-8.744506
H	-10.4055	9.591556	6.575557	H	5.866266	1.668621	-10.077817
Pb	7.132478	-12.308814	9.844131	H	5.836024	2.235816	-8.393046
O	5.850929	-10.471916	11.106645	H	3.416105	3.635907	-10.670658
O	6.378156	-11.444531	7.829577	H	3.4623	4.133609	-8.963715
O	4.965176	-12.488648	10.801933	H	1.960351	3.487495	-9.661339
O	5.66782	-13.560287	7.603115	H	3.111203	1.989316	-6.738911
C	4.899935	-11.288536	11.260701	H	1.702913	1.264415	-7.545823
C	5.849676	-12.409356	7.148587	H	3.106187	0.260127	-7.13376
C	5.467149	-12.079624	5.720129	H	2.746426	-2.08877	-8.220528
C	3.654985	-10.880145	12.015729	H	4.431841	-1.513425	-8.122459
H	3.428052	-9.827595	11.830311	H	4.086847	-3.170821	-8.641398
H	2.80654	-11.51163	11.746323	H	1.50345	-2.841978	-10.89952
H	4.8167	-11.199043	5.704626	H	2.894696	-3.743877	-11.528978
H	4.967744	-12.925636	5.247132	H	2.258741	-2.363269	-12.44345
H	3.84876	-10.99654	13.089289				

Single Point Energy: -2670.18494744 Ha

Table 13 Cartesian Coordinates in Angstroms (Å) for the end of the second hydrogen bond cleaving within the lead oleate hydrate. This state corresponds to two lead oleate monomers and a TMS_2S molecule, all non-interacting.

Element	X	Y	Z	Element	X	Y	Z
Pb	-8.273339	11.873553	4.245611	H	5.641202	-10.55572	3.819044
O	-9.327425	13.548265	5.925398	O	6.815555	-14.611204	8.198867
O	-9.427908	13.153296	2.572652	H	6.458937	-14.579569	7.29545
O	-10.350981	11.649912	5.375379	H	6.047349	-14.425334	8.761706
O	-9.489618	10.969838	2.147665	S	2.033692	0.34451	-8.674885
C	-10.309047	12.76606	6.021343	Si	3.013383	1.482596	-7.078701
C	-9.799066	12.162215	1.851756	Si	2.917321	-1.661042	-8.740807
C	-10.642702	12.451587	0.630605	C	3.241432	-2.344773	-7.024161
C	-11.49998	13.123884	6.880638	C	1.636501	-2.700729	-9.636523
H	-11.241606	13.909628	7.592461	C	4.507146	-1.560682	-9.737078
H	-12.298958	13.489953	6.22486	C	2.461652	0.893927	-5.387263
H	-11.631224	12.790495	0.960951	C	2.45231	3.247806	-7.365585
H	-10.754991	11.560312	0.011325	C	4.876902	1.322766	-7.270876
H	-11.876643	12.239643	7.401532	H	4.943835	-2.562284	-9.842513
H	-10.194791	13.26467	0.052009	H	5.24694	-0.916241	-9.252659
O	-9.020438	9.209186	4.431832	H	4.310933	-1.163343	-10.738554
H	-9.377055	9.24082	3.528415	H	5.222281	0.304943	-7.062512
H	-9.788635	9.395051	4.994667	H	5.194938	1.595443	-8.282717
Pb	7.562654	-11.946837	8.012646	H	5.371295	1.996913	-6.559697
O	6.508567	-10.272124	9.692433	H	2.693247	3.584711	-8.379238
O	6.408086	-10.667085	6.339681	H	2.948087	3.915686	-6.650362
O	5.485003	-12.170475	9.142417	H	1.371391	3.32409	-7.219607
O	6.346376	-12.850552	5.914699	H	2.868447	1.562938	-4.618308
C	5.526947	-11.05433	9.788378	H	1.37127	0.904475	-5.314552
C	6.036928	-11.658166	5.618785	H	2.813065	-0.119987	-5.175734
C	5.193283	-11.368792	4.397638	H	2.320342	-2.356619	-6.433713
C	4.336012	-10.696497	10.647666	H	4.005857	-1.775606	-6.485904
H	4.594387	-9.910761	11.359495	H	3.597985	-3.378694	-7.117587
H	3.537027	-10.330425	9.991894	H	0.758693	-2.860689	-9.002074
H	4.20477	-11.029887	4.72798	H	2.06155	-3.682781	-9.880673
H	5.081001	-12.260078	3.77836	H	1.320489	-2.227123	-10.572527
H	3.959341	-11.580742	11.168571				

Single Point Energy: -2670.1899906 Ha

Table 14 Cartesian Coordinates in Angstroms (Å) for the beginning of the two lead oleate monomers dimerizing. This state corresponds to two interacting lead oleate monomers and a non-interacting TMS_2S molecule.

Element	X	Y	Z	Element	X	Y	Z
Pb	-5.797174	-3.343113	18.950272	H	-4.896742	-1.900807	22.912405
O	-5.581181	-5.758131	17.622966	O	-5.761676	-4.942088	20.833819
O	-4.483551	-1.02719	18.567115	H	-5.298066	-4.613094	21.646265
O	-3.854081	-4.476793	18.20156	H	-5.172367	-5.696069	20.577053
O	-4.125216	-2.266792	20.383827	S	5.839019	7.195312	-28.183289
C	-4.352048	-5.574381	17.700125	Si	3.922292	6.208249	-28.577083
C	-3.886247	-1.222721	19.648515	Si	6.783435	6.217119	-26.463243
C	-2.83033	-0.265155	20.152865	C	6.561329	4.354788	-26.50239
C	-3.358056	-6.618936	17.2506	C	8.598838	6.67063	-26.613594
H	-2.970193	-7.114651	18.147868	C	6.041878	6.951233	-24.900697
H	-3.842039	-7.361026	16.613783	C	4.173882	4.515069	-29.33984
H	-2.825188	0.654375	19.566017	C	3.063692	7.346435	-29.793782
H	-1.850376	-0.750217	20.070897	C	2.958337	6.083562	-26.967566
H	-2.517628	-6.153159	16.728884	H	6.538446	6.526942	-24.018492
H	-2.996199	-0.045258	21.211541	H	4.971355	6.738691	-24.823721
O	-2.116368	-4.07856	20.232456	H	6.177034	8.037854	-24.882698
H	-2.707067	-3.326845	20.492182	H	3.426896	5.387039	-26.264748
H	-2.581327	-4.408626	19.42107	H	2.873239	7.060941	-26.480873
Pb	-2.078311	-5.678659	22.113515	H	1.946981	5.71466	-27.181379
O	-3.38703	-8.001872	22.486072	H	2.979392	8.364227	-29.398872
O	-2.293866	-3.261545	23.438522	H	2.054854	6.970794	-30.004868
O	-3.750255	-6.750391	20.67851	H	3.624357	7.38086	-30.73189
O	-4.020836	-4.545394	22.864406	H	3.202259	4.103412	-29.641047
C	-3.984598	-7.801279	21.406015	H	4.810683	4.584444	-30.225378
C	-3.522816	-3.446499	23.363202	H	4.635007	3.81694	-28.635493
C	-4.51729	-2.401378	23.810634	H	6.95308	3.939388	-27.435765
C	-5.032979	-8.761552	20.891053	H	5.514227	4.057104	-26.388318
H	-5.054472	-9.673169	21.489691	H	7.126867	3.914296	-25.67115
H	-6.01308	-8.272751	20.940196	H	9.058909	6.142682	-27.455142
H	-4.03578	-1.66282	24.453473	H	9.130525	6.378489	-25.698883
H	-5.362785	-2.866544	24.324495	H	8.731545	7.749277	-26.751689
H	-4.841141	-8.997349	19.840014				

Single Point Energy: -2670.22502204 Ha

Table 15 Cartesian Coordinates in Angstroms (Å) for the transition state of the two lead oleate monomers dimerizing. This state corresponds to two interacting lead oleate monomers and a non-interacting TMS_2S molecule.

Element	X	Y	Z	Element	X	Y	Z
Pb	-3.917969	-2.176265	10.10005	H	-2.689511	0.959602	12.683249
O	-4.433887	-4.876344	10.498005	O	-4.223532	-2.297132	12.488413
O	-2.688683	0.263452	9.189611	H	-3.59001	-1.714213	12.985147
O	-2.402415	-4.027816	10.155892	H	-3.893374	-3.195017	12.774902
O	-1.870404	-1.128459	10.725031	S	2.373672	4.393427	-14.954212
C	-3.20176	-5.028585	10.392711	Si	3.54519	2.561237	-14.683166
C	-1.773895	-0.075238	9.958402	Si	2.342324	4.888138	-17.090017
C	-0.470905	0.690047	10.043906	C	2.149652	3.361964	-18.163834
C	-2.571678	-6.397695	10.531106	C	0.858722	6.022496	-17.279517
H	-2.780952	-6.788388	11.527951	C	3.933522	5.800982	-17.496187
H	-3.033178	-7.078893	9.809451	C	2.605441	1.057706	-15.289932
H	-0.609785	1.718084	9.706247	C	3.808295	2.45703	-12.830333
H	0.25499	0.202243	9.381649	C	5.18105	2.743021	-15.592063
H	-1.488706	-6.366167	10.369282	H	3.922161	6.118796	-18.546847
H	-0.065252	0.662953	11.059387	H	4.812583	5.168019	-17.341678
O	-0.369075	-3.093262	11.652274	H	4.038856	6.691842	-16.868011
H	-0.696598	-2.195685	11.364601	H	5.044052	2.760782	-16.678149
H	-0.999282	-3.67525	11.151121	H	5.699271	3.660555	-15.293904
Pb	-0.686541	-3.22365	14.040788	H	5.824829	1.887912	-15.349135
O	-1.944829	-5.651927	14.9629	H	4.283981	3.363625	-12.441932
O	-0.137996	-0.535207	13.625047	H	4.450239	1.599358	-12.594306
O	-2.731477	-4.265741	13.40497	H	2.848564	2.321654	-12.324268
O	-2.180358	-1.358147	13.968007	H	3.161373	0.149403	-15.024835
C	-2.849437	-5.306643	14.185845	H	1.618323	1.008671	-14.823538
C	-1.368788	-0.36897	13.716158	H	2.475142	1.071372	-16.375792
C	-2.008636	0.989805	13.540643	H	1.245516	2.809803	-17.890284
C	-4.167804	-6.047386	14.108623	H	3.013282	2.692898	-18.096673
H	-4.040172	-7.084792	14.420631	H	2.051176	3.677108	-19.210657
H	-4.869033	-5.564245	14.799941	H	-0.073237	5.459745	-17.163642
H	-1.251116	1.757838	13.378672	H	0.86117	6.471322	-18.281142
H	-2.606576	1.233275	14.424862	H	0.880199	6.835111	-16.545035
H	-4.596723	-5.990159	13.103612				

Single Point Energy: -2670.22243349 Ha

Table 16 Cartesian Coordinates in Angstroms (Å) for the end of the two lead oleate monomers dimerizing. This state corresponds to two interacting lead oleate monomers and a non-interacting TMS_2S molecule.

Element	X	Y	Z	Element	X	Y	Z
Pb	-2.24685	-0.114759	4.521585	H	-0.780862	2.171572	8.423918
O	-3.712508	-2.438067	4.041974	O	-3.097593	-0.387771	6.741487
O	-0.870478	2.000311	5.706446	H	-2.439296	-0.111648	7.433321
O	-1.536015	-2.41813	4.50713	H	-3.222692	-1.345319	6.978881
O	-0.001904	-0.024294	5.388855	S	1.619812	2.993248	-7.694079
C	-2.626695	-3.039543	4.160949	Si	3.479824	1.932387	-8.053575
C	0.10289	1.222006	5.751056	Si	0.154823	2.255219	-9.118639
C	1.471752	1.676204	6.205247	C	0.227569	0.382795	-9.305539
C	-2.498513	-4.522	3.89132	C	-1.503494	2.753984	-8.381088
H	-2.063651	-5.023431	4.760766	C	0.395188	3.087889	-10.789944
H	-3.470161	-4.957479	3.654725	C	3.389796	0.178554	-7.376882
H	1.437172	2.703203	6.570814	C	4.769812	2.906774	-7.088749
H	2.163545	1.610347	5.358082	C	3.908915	1.905748	-9.887071
H	-1.811372	-4.671578	3.05132	H	-0.383399	2.766366	-11.494354
H	1.84792	1.010203	6.987127	H	1.369002	2.842869	-11.224733
O	0.304312	-2.457519	6.435706	H	0.333864	4.176957	-10.686239
H	0.430909	-1.500408	6.197149	H	3.200657	1.298359	-10.461415
H	-0.356562	-2.733471	5.745843	H	3.905841	2.918998	-10.302577
Pb	-0.542328	-2.729215	8.654592	H	4.908584	1.475924	-10.032077
O	-1.914381	-4.841779	7.455318	H	4.804154	3.952967	-7.410549
O	0.928368	-0.403184	9.103298	H	5.764416	2.466593	-7.236872
O	-2.788186	-2.821684	7.788055	H	4.547958	2.88723	-6.015649
O	-1.256149	-0.427753	8.676165	H	4.377615	-0.297367	-7.43147
C	-2.889495	-4.06534	7.41642	H	3.071828	0.187786	-6.328722
C	-0.160187	0.196341	9.000115	H	2.68351	-0.438667	-7.940248
C	-0.286768	1.679582	9.266606	H	0.128974	-0.110589	-8.332544
C	-4.257352	-4.519312	6.958549	H	1.161451	0.04612	-9.767303
H	-4.221072	-5.543452	6.585336	H	-0.599241	0.048063	-9.944828
H	-4.94909	-4.461226	7.80634	H	-1.709865	2.182094	-7.469422
H	0.691967	2.127698	9.442696	H	-2.312948	2.56392	-9.097493
H	-0.921102	1.825789	10.14827	H	-1.516752	3.819273	-8.125136
H	-4.635463	-3.848388	6.181734				

Single Point Energy: -2670.22621885 Ha

Table 17 Cartesian Coordinates in Angstroms (Å) for the beginning of the main reaction between the lead oleate dimer and the TMS_2S molecule. This state corresponds to an interacting lead oleate dimer and TMS_2S complex.

Element	X	Y	Z	Element	X	Y	Z
Pb	-1.148891	-0.044996	-1.430375	H	2.267485	-3.332398	-1.953222
O	-1.869793	2.684044	-0.806309	O	1.212212	0.337857	-2.289321
O	-0.586489	-2.792125	-1.621758	H	1.819484	-0.385392	-2.00448
O	-0.469287	1.421086	0.377082	H	1.632358	1.108117	-1.831303
O	-0.169398	-1.563034	0.186355	S	-3.753176	-0.823001	0.178616
C	-1.140937	2.518726	0.189348	Si	-3.562838	-0.920115	2.359791
C	-0.20198	-2.702975	-0.440071	Si	-5.255852	0.693628	-0.320516
C	0.212697	-3.923757	0.352298	C	-5.122159	2.206796	0.780201
C	-1.019861	3.577517	1.264462	C	-4.88654	1.139282	-2.106283
H	-1.306073	4.554725	0.871145	C	-6.952008	-0.100702	-0.170541
H	-1.702893	3.31685	2.08131	C	-2.660006	0.578844	3.030597
H	0.421367	-4.760856	-0.315211	C	-2.556416	-2.472152	2.661958
H	-0.615567	-4.198928	1.015036	C	-5.278194	-1.065288	3.115947
H	-0.007998	3.606406	1.674069	H	-7.726263	0.615462	-0.474717
H	1.081634	-3.705643	0.977553	H	-7.16194	-0.412814	0.856905
O	1.306549	0.011609	1.736457	H	-7.024458	-0.981571	-0.817189
H	0.895777	-0.779052	1.292762	H	-5.860703	-0.147706	2.984196
H	0.717018	0.742836	1.403246	H	-5.836865	-1.896234	2.672316
Pb	3.535972	0.388513	0.972877	H	-5.182064	-1.249715	4.193624
O	2.556156	2.990208	1.273016	H	-3.027015	-3.349502	2.206162
O	3.46536	-2.391713	0.808506	H	-2.462177	-2.649162	3.740483
O	2.695281	1.923621	-0.678555	H	-1.55419	-2.354749	2.240829
O	3.137459	-1.033677	-0.927241	H	-2.469137	0.43951	4.102219
C	2.399922	2.968421	0.035838	H	-1.701543	0.708471	2.521617
C	3.272529	-2.218819	-0.41268	H	-3.244943	1.494507	2.905951
C	3.198411	-3.380582	-1.379804	H	-4.117632	2.636879	0.723934
C	1.871734	4.167371	-0.723271	H	-5.359763	1.984671	1.825315
H	1.603059	4.973716	-0.040234	H	-5.835422	2.963333	0.428424
H	2.640995	4.514865	-1.421766	H	-3.955685	1.711384	-2.175486
H	3.261221	-4.332008	-0.850395	H	-5.696988	1.760974	-2.508046
H	4.024847	-3.301796	-2.09504	H	-4.804564	0.244536	-2.733089
H	1.000972	3.879896	-1.321307				

Single Point Energy: -2670.24996444 Ha

Table 18 Cartesian Coordinates in Angstroms (Å) for the transition state of the first TMS group bonding with one of the carboxyl groups in the lead oleate dimer. This state corresponds to a lead oleate dimer and TMS_2S complex.

Element	X	Y	Z	Element	X	Y	Z
Pb	0.06026	-0.810758	-1.834687	H	3.78104	-3.382731	-2.271195
O	-1.246625	1.737937	-0.932301	O	2.451978	-0.004291	-2.814476
O	0.515112	-3.47127	-1.492601	H	3.175979	-0.585118	-2.488773
O	0.721183	1.05464	-0.220868	H	2.724202	0.849798	-2.412584
O	1.451753	-1.917145	-0.21607	S	-2.374934	-0.811985	-0.312775
C	-0.254238	1.850865	-0.128622	Si	-2.308228	-1.313794	1.78774
C	1.255899	-3.160617	-0.536076	Si	-3.235633	1.544784	-0.73588
C	1.926151	-4.209925	0.318544	C	-3.303521	3.384794	-0.244395
C	-0.218925	2.93565	0.914148	C	-3.521029	1.345084	-2.582428
H	-0.493939	3.893364	0.466438	C	-4.821554	0.985252	0.173985
H	-0.957819	2.716096	1.691245	C	-1.804309	0.179953	2.818824
H	2.061936	-5.132782	-0.248152	C	-1.051486	-2.688994	2.030857
H	1.266174	-4.419361	1.168079	C	-4.006158	-1.926131	2.323643
H	0.771631	3.000297	1.364697	H	-5.62132	1.693546	-0.08481
H	2.879119	-3.84989	0.709417	H	-4.698749	1.019964	1.262732
O	2.710724	-0.095755	1.229297	H	-5.132648	-0.024642	-0.103631
H	2.400857	-0.947689	0.816262	H	-4.773173	-1.154103	2.215622
H	2.04957	0.549358	0.880579	H	-4.306956	-2.792282	1.723864
Pb	4.861073	0.552145	0.391053	H	-3.970889	-2.233025	3.37706
O	3.421401	2.929316	0.691344	H	-1.217764	-3.504302	1.318467
O	4.990535	-2.228792	0.398037	H	-1.135678	-3.095304	3.046644
O	3.752557	1.903033	-1.261442	H	-0.034158	-2.311997	1.893656
O	4.609999	-0.998998	-1.421935	H	-1.843559	-0.07159	3.886822
C	3.26615	2.869833	-0.546434	H	-0.778658	0.482105	2.584973
C	4.782716	-2.141351	-0.829969	H	-2.469608	1.034225	2.652694
C	4.724879	-3.367531	-1.716473	H	-2.604086	4.001747	-0.814083
C	2.497921	3.935771	-1.300531	H	-3.110155	3.53975	0.823307
H	2.077322	4.672867	-0.615407	H	-4.324313	3.741543	-0.433305
H	3.169809	4.43328	-2.008497	H	-2.672283	1.706326	-3.17078
H	4.824144	-4.280451	-1.128188	H	-4.404999	1.932831	-2.862636
H	5.532131	-3.315434	-2.45536	H	-3.715693	0.30138	-2.848
H	1.698886	3.470503	-1.886669				

Single Point Energy: -2670.20629315 Ha

Table 19 Cartesian Coordinates in Angstroms (Å) for the end of the first TMS group bonding with one of the carboxyl groups in the lead oleate dimer. This state corresponds to a lead oleate dimer and TMS_2S complex.

Element	X	Y	Z	Element	X	Y	Z
Pb	-1.508947	-1.109847	-1.263215	H	2.554043	-3.227172	-1.672064
O	-2.731854	1.956237	-0.555138	O	0.894405	0.101226	-2.331347
O	-0.558851	-3.545156	-0.987814	H	1.679029	-0.415973	-2.058306
O	-0.956112	1.033181	0.346788	H	1.094704	0.960002	-1.908661
O	0.002152	-1.947798	0.441841	S	-3.792093	-1.418017	0.113349
C	-1.822434	1.909956	0.397136	Si	-3.566207	-1.86864	2.189869
C	0.072101	-3.172881	0.028613	Si	-4.348839	2.564957	-0.676843
C	0.906423	-4.139856	0.833635	C	-4.234397	4.400698	-1.028911
C	-1.84767	2.918348	1.508857	C	-5.021446	1.613779	-2.130775
H	-2.331032	3.849341	1.209757	C	-5.246988	2.172963	0.911373
H	-2.405516	2.487256	2.347324	C	-2.71734	-0.459192	3.119342
H	1.170417	-5.011016	0.232068	C	-2.573529	-3.44269	2.488812
H	0.307143	-4.476399	1.687717	C	-5.308242	-2.083747	2.888335
H	-0.825491	3.110494	1.840526	H	-6.31633	2.385852	0.788945
H	1.803094	-3.651496	1.221401	H	-4.883098	2.759159	1.760043
O	1.175747	0.003648	1.744867	H	-5.134497	1.10599	1.133716
H	0.897823	-0.873395	1.353255	H	-5.909388	-1.180399	2.732608
H	0.466289	0.604731	1.424421	H	-5.822523	-2.919208	2.399688
Pb	3.264795	0.828082	0.911537	H	-5.265377	-2.287064	3.966344
O	1.583887	3.097373	1.210906	H	-2.889277	-4.249681	1.819424
O	3.702499	-1.914204	0.883685	H	-2.697377	-3.780082	3.526268
O	2.079499	2.114771	-0.731929	H	-1.510375	-3.248426	2.322293
O	3.176623	-0.701525	-0.911729	H	-2.623122	-0.707708	4.184391
C	1.497067	3.03684	-0.033888	H	-1.713974	-0.275923	2.723498
C	3.482787	-1.827035	-0.343218	H	-3.297184	0.46723	3.041298
C	3.547561	-3.036038	-1.252177	H	-3.566489	4.595738	-1.875768
C	0.694003	4.054965	-0.82173	H	-3.875876	4.974616	-0.167789
H	0.18027	4.751546	-0.157708	H	-5.22796	4.785819	-1.289277
H	1.368623	4.611739	-1.48126	H	-4.401112	1.764066	-3.02192
H	3.88776	-3.917546	-0.70734	H	-6.040787	1.941676	-2.365003
H	4.218592	-2.830777	-2.091954	H	-5.047873	0.54368	-1.896924
H	-0.029637	3.541939	-1.463615				

Single Point Energy: -2670.24408186 Ha

Table 20 Cartesian Coordinates in Angstroms (Å) for the transition state of the second TMS group rotating in position to react with the second carboxyl group in the lead oleate dimer. This state corresponds to a lead oleate dimer and TMS_2S complex.

Element	X	Y	Z	Element	X	Y	Z
Pb	-0.021317	-1.177504	-1.367556	H	5.482295	-3.058805	-2.321698
O	-1.338785	2.037409	-0.978236	O	2.167919	-0.137747	-2.769461
O	0.881079	-3.569304	-0.630683	H	2.984843	-0.589188	-2.466527
O	0.614907	1.284024	-0.300589	H	2.364684	0.781544	-2.494614
O	1.652322	-1.716487	0.304638	S	-1.939448	-0.688742	0.443522
C	-0.3226	2.070342	-0.139633	Si	-2.443554	-2.310701	1.71259
C	1.619139	-3.003891	0.21166	Si	-3.021723	2.451389	-0.913919
C	2.466552	-3.797646	1.176599	C	-3.127513	4.176024	-1.630542
C	-0.319914	3.071034	0.979546	C	-3.812199	1.176479	-2.023448
H	-0.8888	3.969122	0.73048	C	-3.686732	2.391961	0.833024
H	-0.783109	2.595349	1.852443	C	-1.30344	-2.294317	3.213658
H	2.605993	-4.819048	0.81901	C	-2.284537	-3.9257	0.760124
H	1.943457	-3.830596	2.140185	C	-4.222249	-2.029376	2.291656
H	0.709736	3.332165	1.229676	H	-4.779758	2.484713	0.785621
H	3.430041	-3.307616	1.335623	H	-3.308587	3.203475	1.462991
O	2.794057	0.444206	1.220318	H	-3.446849	1.43201	1.299953
H	2.525644	-0.495737	1.00915	H	-4.309835	-1.062511	2.80281
H	2.049912	0.962569	0.838021	H	-4.920612	-2.026464	1.446967
Pb	4.788727	1.106147	0.070484	H	-4.532813	-2.812985	2.995247
O	3.136709	3.38214	0.197788	H	-2.854251	-3.864313	-0.174254
O	5.212969	-1.615922	0.452426	H	-2.646386	-4.787382	1.333465
O	3.41436	2.115626	-1.619671	H	-1.235542	-4.097625	0.497092
O	4.547616	-0.711397	-1.474155	H	-1.525541	-3.113975	3.908668
C	2.887939	3.124209	-0.998805	H	-0.257647	-2.373086	2.895897
C	4.880741	-1.732738	-0.745867	H	-1.414307	-1.344785	3.751858
C	4.843643	-3.082545	-1.433012	H	-2.655007	4.217213	-2.617864
C	1.949598	3.993267	-1.81317	H	-2.638327	4.911759	-0.982342
H	1.440472	4.71962	-1.177505	H	-4.177592	4.472013	-1.741912
H	2.528689	4.526304	-2.575174	H	-3.328917	1.158516	-3.006791
H	3.824607	-3.29236	-1.774746	H	-4.876405	1.397802	-2.168091
H	5.17272	-3.873381	-0.757811	H	-3.716482	0.185464	-1.567833
H	1.219406	3.369979	-2.337276				

Single Point Energy: -2670.23786908 Ha

Table 21 Cartesian Coordinates in Angstroms (Å) for the start of the second TMS group bonding with the second carboxyl group in the lead oleate dimer. This state corresponds to a lead oleate dimer and TMS_2S complex.

Element	X	Y	Z	Element	X	Y	Z
Pb	-1.149173	-1.346514	-0.54801	H	4.341382	-3.138051	-1.58596
O	-2.595099	1.729544	-0.568661	O	0.879217	-0.426555	-2.315758
O	-0.205015	-3.53152	0.589522	H	1.744052	-0.76034	-1.991841
O	-0.556905	1.238859	0.087694	H	1.017822	0.537053	-2.222738
O	0.812331	-1.580044	0.839721	S	-2.538376	-0.862841	1.705418
C	-1.53543	1.985502	0.172533	Si	-3.717983	-2.631815	1.915542
C	0.659978	-2.822854	1.158697	Si	-4.292711	2.046265	-0.46344
C	1.527165	-3.37443	2.262268	C	-4.59342	3.574087	-1.500905
C	-1.537895	3.170465	1.093457	C	-5.030523	0.505427	-1.212404
H	-2.204834	3.961243	0.745547	C	-4.806883	2.258227	1.318477
H	-1.884829	2.82624	2.074771	C	-2.922969	-3.819113	3.145125
H	1.595757	-4.461611	2.192858	C	-3.931932	-3.545458	0.270361
H	1.054703	-3.113481	3.21761	C	-5.425115	-2.116667	2.539781
H	-0.519941	3.549262	1.199766	H	-5.901954	2.222499	1.378221
H	2.519123	-2.917511	2.241324	H	-4.478438	3.208521	1.750046
O	1.77994	0.762282	1.488436	H	-4.405852	1.432804	1.917475
H	1.573031	-0.212274	1.386852	H	-5.344043	-1.577111	3.490802
H	0.977563	1.187157	1.109742	H	-5.919314	-1.455796	1.817884
Pb	3.638296	1.370925	0.105031	H	-6.063611	-2.995706	2.697123
O	1.855221	3.551881	0.035444	H	-4.355988	-2.900522	-0.508131
O	4.200702	-1.234116	0.876514	H	-4.613551	-4.395617	0.404255
O	2.099008	2.059033	-1.608173	H	-2.978313	-3.951763	-0.087919
O	3.388313	-0.668475	-1.121804	H	-3.55454	-4.703471	3.299773
C	1.562586	3.122969	-1.101284	H	-1.949721	-4.150055	2.767205
C	3.783172	-1.552355	-0.256393	H	-2.766978	-3.333428	4.115045
C	3.713084	-2.998389	-0.699946	H	-4.232256	3.432202	-2.525723
C	0.556382	3.84621	-1.976511	H	-4.092335	4.453474	-1.080539
H	0.020808	4.608423	-1.40796	H	-5.667327	3.792218	-1.548048
H	1.089578	4.329301	-2.803217	H	-4.635221	0.322834	-2.21786
H	2.685802	-3.24336	-0.98813	H	-6.121292	0.590225	-1.282125
H	4.04309	-3.667531	0.095821	H	-4.789421	-0.353579	-0.577568
H	-0.147265	3.134307	-2.418468				

Single Point Energy: -2670.2443262 Ha

Table 22 Cartesian Coordinates in Angstroms (Å) for the transition state of the second TMS group bonding with the second carboxyl group in the lead oleate dimer. This state corresponds to a lead oleate dimer and TMS_2S complex.

Element	X	Y	Z	Element	X	Y	Z
Pb	-0.311934	-0.903983	-1.288699	H	5.516629	-3.188015	-1.346221
O	-1.491471	2.178231	-1.121448	O	2.296863	-0.260821	-2.775909
O	0.104202	-2.991002	0.560184	H	3.031359	-0.697217	-2.30363
O	0.550734	1.567469	-0.604145	H	2.552641	0.676986	-2.681306
O	1.754681	-1.576142	0.235084	S	-1.696178	-0.778563	0.810117
C	-0.381047	2.360827	-0.436405	Si	-1.647962	-3.256218	1.401173
C	1.144117	-2.364365	1.000898	Si	-3.153819	2.631137	-0.918438
C	1.575812	-2.531679	2.428438	C	-3.35683	4.287487	-1.765963
C	-0.269674	3.504597	0.526487	C	-4.037247	1.25043	-1.804897
H	-0.902303	4.346973	0.241994	C	-3.572264	2.674408	0.899807
H	-0.594418	3.141557	1.5091	C	-0.96129	-4.904231	2.113132
H	1.58171	-3.586	2.711108	C	-2.693055	-3.7926	-0.076219
H	0.837567	-2.018	3.058351	C	-2.669081	-2.733793	2.926446
H	0.774822	3.813967	0.59918	H	-4.663303	2.698622	1.013194
H	2.557295	-2.08453	2.590029	H	-3.162956	3.548537	1.415188
O	2.669774	0.84429	0.991357	H	-3.201297	1.763394	1.384201
H	2.482902	-0.117904	0.826992	H	-2.023431	-2.251676	3.671286
H	1.948175	1.302236	0.500418	H	-3.456781	-2.021567	2.665023
Pb	4.783131	1.434239	0.008965	H	-3.111118	-3.623808	3.394747
O	3.09796	3.655688	-0.336107	H	-3.466319	-3.054548	-0.303723
O	5.079369	-1.143887	0.975239	H	-3.166831	-4.761209	0.129046
O	3.557875	2.160736	-1.929853	H	-2.064919	-3.917068	-0.966955
O	4.643799	-0.640836	-1.155555	H	-1.810926	-5.540937	2.395161
C	2.95788	3.224491	-1.50194	H	-0.34514	-5.452255	1.391024
C	4.842907	-1.49729	-0.200285	H	-0.365127	-4.751097	3.021453
C	4.763128	-2.9583	-0.585286	H	-3.026929	4.236346	-2.80969
C	2.070056	3.942611	-2.499584	H	-2.789628	5.079309	-1.264126
H	1.442216	4.681173	-1.997106	H	-4.413869	4.581431	-1.760573
H	2.701676	4.454355	-3.234652	H	-3.685134	1.152433	-2.838033
H	3.78191	-3.157832	-1.026861	H	-5.11866	1.431074	-1.827281
H	4.911812	-3.597431	0.286539	H	-3.852668	0.306829	-1.277725
H	1.450608	3.222938	-3.042742				

Single Point Energy: -2670.18313882 Ha

Table 23 Cartesian Coordinates in Angstroms (Å) for the end of the second TMS group bonding with the second carboxyl group in the lead oleate dimer. This state corresponds to the final reacted state, featuring a PbS quantum dot and its byproducts.

Element	X	Y	Z	Element	X	Y	Z
Pb	-2.102088	-0.954089	-1.093897	H	3.954533	-3.534788	-0.480409
O	-2.8447	2.49749	-1.012512	O	0.924583	-0.516744	-2.4523
O	-1.127303	-3.497096	1.131466	H	1.598801	-0.935602	-1.887325
O	-0.892205	1.624828	-0.512528	H	1.164814	0.422574	-2.364389
O	0.073441	-1.719624	0.65608	S	-3.521967	-0.660833	0.814668
C	-1.750128	2.478225	-0.276575	Si	-2.285385	-4.477045	1.95996
C	-0.284383	-2.549585	1.494862	Si	-4.444777	3.116264	-0.803802
C	0.216643	-2.497756	2.910307	C	-4.423919	4.87472	-1.449314
C	-1.574214	3.479916	0.82891	C	-5.458952	1.977184	-1.876409
H	-2.14381	4.395081	0.660102	C	-4.94137	3.002006	0.99224
H	-1.928037	3.012705	1.756258	C	-1.399248	-6.059784	2.427563
H	0.181022	-3.471971	3.400672	C	-3.590839	-4.751137	0.657536
H	-0.425554	-1.802877	3.464522	C	-2.965213	-3.55403	3.434922
H	-0.512073	3.70877	0.937415	H	-6.025373	3.1517	1.074637
H	1.23587	-2.106033	2.911501	H	-4.450312	3.749742	1.622245
O	0.96266	0.764931	1.246739	H	-4.704833	2.000515	1.371694
H	0.748009	-0.197397	1.131563	H	-2.26823	-3.504985	4.277256
H	0.318891	1.220521	0.642885	H	-3.239451	-2.537236	3.130849
Pb	3.208553	1.182647	0.528316	H	-3.874292	-4.062025	3.779833
O	1.800348	3.518525	-0.069059	H	-4.057687	-3.792506	0.40425
O	3.22868	-1.399991	1.608173	H	-4.36783	-5.432769	1.024402
O	2.272532	1.911403	-1.546846	H	-3.158475	-5.183377	-0.251924
O	3.102303	-0.936755	-0.573622	H	-2.103329	-6.760593	2.893938
C	1.740242	3.047602	-1.226904	H	-0.976127	-6.546796	1.541472
C	3.132175	-1.770696	0.416841	H	-0.58655	-5.878884	3.140233
C	3.0457	-3.240259	0.056756	H	-4.06399	4.905503	-2.484045
C	1.021931	3.78718	-2.338377	H	-3.785016	5.527178	-0.844078
H	0.611438	4.73022	-1.974315	H	-5.438227	5.29323	-1.433252
H	1.717012	3.97812	-3.162335	H	-5.08848	1.967657	-2.907705
H	2.198208	-3.407081	-0.614836	H	-6.508366	2.295327	-1.891681
H	2.942611	-3.853813	0.953558	H	-5.412533	0.957321	-1.477314
H	0.216835	3.156127	-2.729175				

Single Point Energy: -2670.21356045 Ha

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