

Supplementary Information

Optical absorption of cysteine-ligated CdSe nanoclusters from first-principles calculations

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Coordinates of the lowest-energy structures presented in this paper

Cartesian coordinates of CdSe cluster in gas

Cartesian coordinates of CdSe cluster in toluene

Cartesian coordinates of CdSe cluster in water

Cartesian coordinates of CdSe-Cys clusters in alkaline solution

Cartesian coordinates of CdSe-Cys clusters in gas

Cartesian coordinates of CdSe-Cys clusters in water

Cartesian coordinates of CdSe-Cys clusters in toluene

Table S1 Average bond lengths (in Å) and bond angles (in degree) of (CdSe)₂ calculated with PBE0 functional.

Functional	CCSD(T)	B3LYP	PBE0	M06-2X
Cd-Se	2.606	2.663	2.624	2.645
Cd-Cd	2.842	2.980	2.921	2.970
∠Se-Cd-Se	113.90	111.94	112.36	111.68
∠Cd-Se-Cd	66.10	68.06	67.64	68.31

Table S2 Selected bond lengths (in Å) of (CdSe)₃-Cys complexes optimized with PBE0 functional and 6-31++G(d,p)/Lanl2DZ or 6-311++G(d,p)/SDD basis set.

	N-Cd	S-Cd	Se-Cd
6-31++G(d,p)/Lanl2DZ	2.464	2.855	2.596
6-311++G(d,p)/SDD	2.466	2.860	2.560

Table S3 Bond lengths of the $(\text{CdSe})_N$ clusters ($N = 3, 6$ and 9) in water and gas calculated with PBE0 functional.

N	Water	Gas
	Cd–Se (Å)	Cd–Se (Å)
3	2.656	2.562
6	2.811	2.715
9	2.778	2.639

Table S4 Bond lengths of selected bonds in the (CdSe)_N-Cys complexes calculated with PBE0 functional.

N	Gas		Toluene		Water		Alkaline	
	N-Cd	S-Cd	N-Cd	S-Cd	O-Cd	H-Se	N-Cd	S-Cd
1	2.506	2.883	2.456	2.895	2.443	2.398	2.438	2.600
2	2.463	2.828	2.488	2.870	2.488	2.462	2.425	2.625
3	2.476	2.864	2.452	2.897	2.554	2.546	2.460	2.649
4	2.437	2.954	2.433	3.045	2.626	2.508	2.466	2.633
5	2.399	2.790	2.414	2.933	2.518	2.495	2.413	2.622
6	2.422	2.966	2.436	3.009	2.523	2.474	2.447	2.631
7	2.466	2.834	2.454	2.915	2.542	2.569	2.439	2.612
8	2.507	2.847	2.446	3.181	2.582	2.525	2.473	2.628
9	2.506	2.823	2.430	3.089	2.579	2.506	2.451	2.625
10	2.500	2.850	2.507	2.936	2.649	2.655	2.432	2.612
13	2.427	2.809	2.441	2.893	2.507	2.553	2.453	2.636
16	2.462	3.093	2.487	3.219	2.534	2.574	2.403	2.617
19	2.580	2.866	2.557	2.922	2.568	2.705	2.408	2.616

Table S5 NBO population analysis of (CdSe)_N and (CdSe)_N-Cys calculated with PBE0 functional. Q is atomic net charge, and EC is electronic configuration.

N	(CdSe) _N			(CdSe) _N -Cys		
		Q	EC		Q	EC
1	Cd	1.455	5S ^{0.43} 4d ^{9.99} 5p ^{0.12}	Cd	1.105	5s ^{0.52} 4d ^{9.99} 5p ^{0.37} 6p ^{0.01}
	Se	-1.455	4S ^{1.95} 4p ^{5.50}	Se	-1.431	4s ^{1.89} 4p ^{5.54}
	S			S	-0.651	3s ^{1.78} 3p ^{4.84} 3d ^{0.01} 4p ^{0.01} 5p ^{0.01}
2	Cd	1.321	5S ^{0.44} 4d ^{10.00} 5p ^{0.24} 6p ^{0.01}	Cd	0.963	5s ^{0.50} 4d ^{9.99} 5p ^{0.53} 6p ^{0.01}
	Se	-1.321	4S ^{1.89} 4p ^{5.43}	Se	-1.291	4s ^{1.86} 4p ^{5.43}
	S			S	-0.637	3s ^{1.77} 3p ^{4.84} 3d ^{0.01} 4p ^{0.01} 5p ^{0.01}
3	Cd	1.242	5S ^{0.49} 4d ^{9.99} 5p ^{0.26} 6p ^{0.01}	Cd	0.975	5s ^{0.49} 4d ^{9.99} 5p ^{0.52} 6p ^{0.01}
	Se	-1.252	4S ^{1.87} 4p ^{5.39}	Se	-1.253	4s ^{1.84} 4p ^{5.41}
	S			S	-0.644	3s ^{1.77} 3p ^{4.85} 3d ^{0.01} 5p ^{0.01}
4	Cd	1.257	5S ^{0.50} 4d ^{9.99} 5p ^{0.24} 6p ^{0.01}	Cd	1.007	5s ^{0.49} 4d ^{9.99} 5p ^{0.50} 6p ^{0.01}
	Se	-1.257	4S ^{1.87} 4p ^{5.39}	Se	-1.281	4s ^{1.83} 4p ^{5.45}
	S			S	-0.641	3s ^{1.77} 3p ^{4.84} 3d ^{0.01} 5p ^{0.01}
5	Cd	1.198	5S ^{0.43} 4d ^{10.00} 5p ^{0.36} 6p ^{0.01}	Cd	0.938	5s ^{0.47} 4d ^{9.99} 5p ^{0.58} 6p ^{0.01}
	Se	-1.155	4S ^{1.81} 4p ^{5.34}	Se	-1.164	4s ^{1.81} 4p ^{5.35}
	S			S	-0.626	3s ^{1.75} 3p ^{4.84} 4s ^{0.01} 3d ^{0.01} 5p ^{0.01}
6	Cd	1.138	5S ^{0.46} 4d ^{9.99} 5p ^{0.39} 6p ^{0.02}	Cd	0.924	5s ^{0.49} 4d ^{9.99} 5p ^{0.57} 6p ^{0.02}
	Se	-1.148	4S ^{1.81} 4p ^{5.34}	Se	-1.139	4s ^{1.81} 4p ^{5.33}
	S			S	-0.626	3s ^{1.75} 3p ^{4.84} 3d ^{0.01} 5p ^{0.01}
7	Cd	1.154	5S ^{0.45} 4d ^{9.99} 5p ^{0.39} 6p ^{0.01}	Cd	1.091	5s ^{0.46} 4d ^{9.99} 5p ^{0.44} 6p ^{0.01}
	Se	-1.220	4S ^{1.83} 4p ^{5.39}	Se	-1.220	4s ^{1.84} 4p ^{5.38}
	S			S	-0.636	3s ^{1.76} 3p ^{4.84} 3d ^{0.01} 5p ^{0.01}
8	Cd	1.178	5S ^{0.45} 4d ^{9.99} 5p ^{0.36} 6p ^{0.01}	Cd	1.092	5s ^{0.44} 4d ^{9.99} 5p ^{0.46} 6p ^{0.01}
	Se	-1.170	4S ^{1.81} 4p ^{5.36}	Se	-1.175	4s ^{1.78} 4p ^{5.39}
	S			S	-0.639	3s ^{1.76} 3p ^{4.85} 3d ^{0.01} 4p ^{0.01} 5p ^{0.01}
9	Cd	1.141	5S ^{0.47} 4d ^{9.99} 5p ^{0.38} 6p ^{0.01}	Cd	0.962	5s ^{0.50} 4d ^{9.99} 5p ^{0.52} 6p ^{0.02}
	Se	-1.146	4S ^{1.79} 4p ^{5.35}	Se	-1.153	4s ^{1.79} 4p ^{5.37}
	S			S	-0.636	3s ^{1.76} 3p ^{4.85} 3d ^{0.01} 5p ^{0.01}
10	Cd	1.156	5S ^{0.46} 4d ^{9.99} 5p ^{0.37} 6p ^{0.02}	Cd	0.983	5s ^{0.49} 4d ^{9.99} 5p ^{0.51} 6p ^{0.02}
	Se	-1.151	4S ^{1.79} 4p ^{5.36}	Se	-1.152	4s ^{1.80} 4p ^{5.35}
	S			S	-0.629	3s ^{1.76} 3p ^{4.84} 3d ^{0.01} 4p ^{0.01} 5p ^{0.01}
13	Cd	1.324	5S ^{0.40} 4d ^{9.99} 5p ^{0.24} 6p ^{0.01}	Cd	1.099	5s ^{0.45} 4d ^{9.99} 5p ^{0.44} 6p ^{0.01}
	Se	-1.142	4S ^{1.78} 4p ^{5.36}	Se	-1.147	4s ^{1.78} 4p ^{5.37}
	S			S	-0.635	3s ^{1.76} 3p ^{4.84} 3d ^{0.01} 5p ^{0.02}
16	Cd	1.175	5S ^{0.46} 4d ^{9.99} 5p ^{0.35} 6p ^{0.01}	Cd	1.016	5s ^{0.47} 4d ^{9.99} 5p ^{0.50} 6p ^{0.01}
	Se	-1.178	4S ^{1.80} 4p ^{5.38}	Se	-1.174	4s ^{1.78} 4p ^{5.40}
	S			S	-0.633	3s ^{1.76} 3p ^{4.84} 4s ^{0.01} 3d ^{0.01} 5p ^{0.01}
19	Cd	1.182	5S ^{0.46} 4d ^{9.99} 5p ^{0.35} 6p ^{0.01}	Cd	1.105	5s ^{0.44} 4d ^{9.99} 5p ^{0.44} 6p ^{0.01}
	Se	-1.185	4S ^{1.78} 4p ^{5.40}	Se	-1.163	4s ^{1.77} 4p ^{5.39}
	S			S	-0.631	3s ^{1.76} 3p ^{4.84} 3d ^{0.01} 4p ^{0.01} 5p ^{0.01}

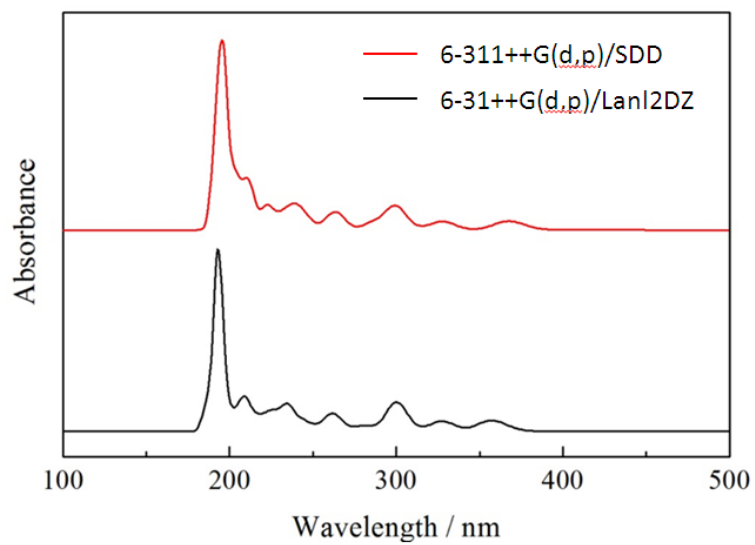


Fig. S1 Optical absorption spectra of (CdSe)₃-Cys calculated with PBE0 functional and 6-31++G(d,p)/LanI2DZ or PBE0/6-311++G(d,p)/SDD basis set..

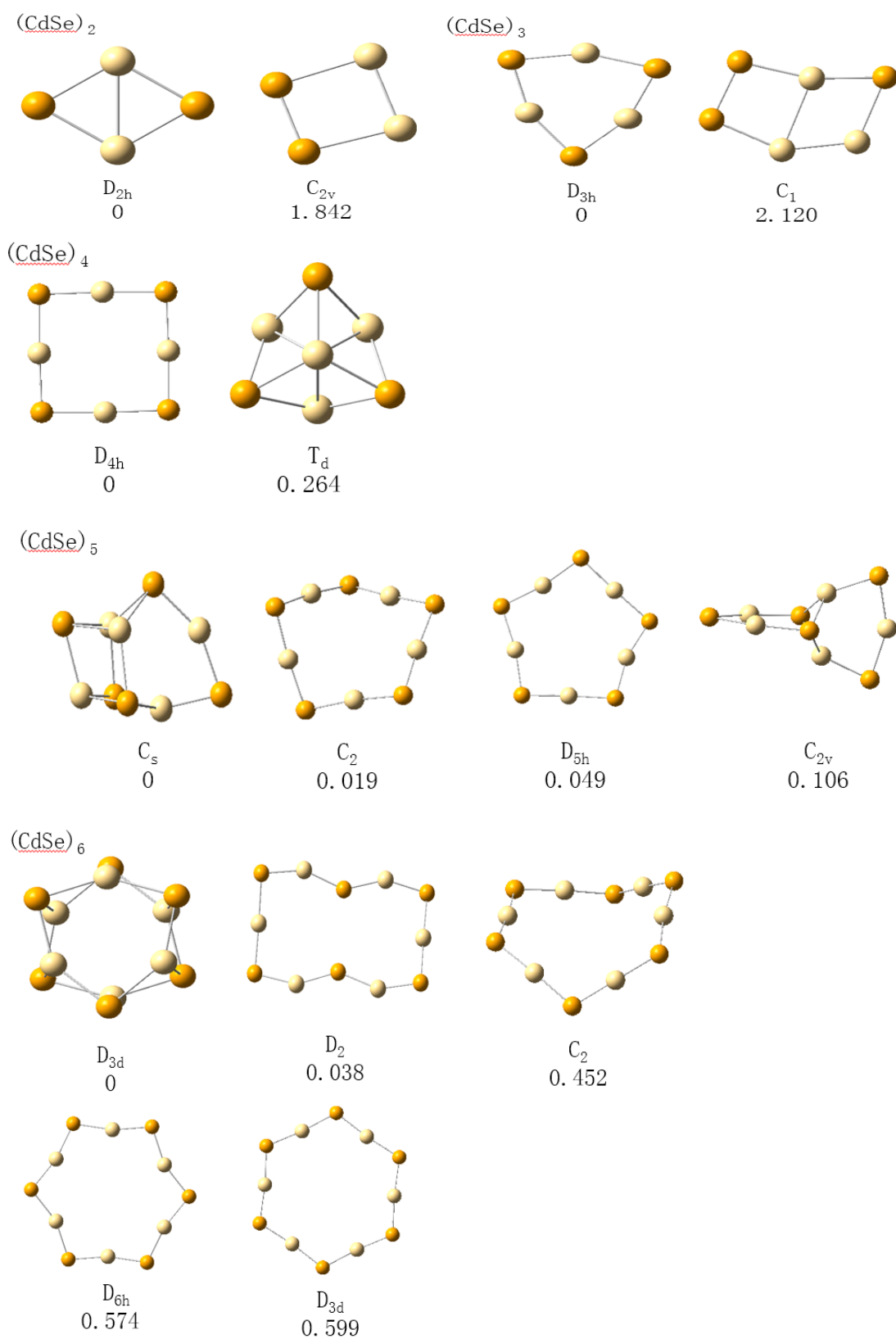


Fig. S2 Structures, symmetry and relative energy (in eV) of the low-lying (CdSe)_N ($N = 2-10, 13, 16$ and 19) clusters in water calculated with PBE0 functional.

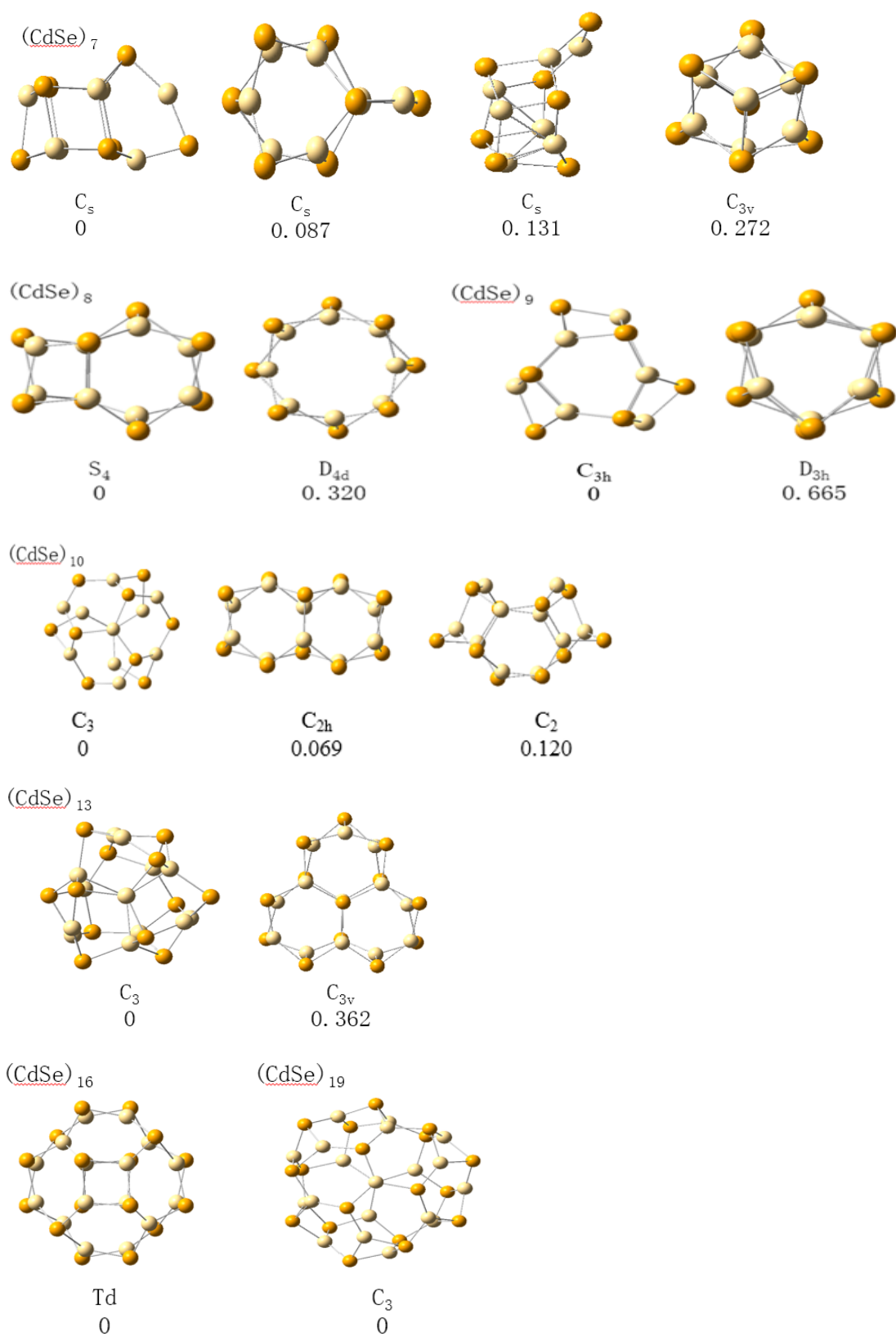


Fig. S2 Structures, symmetry and relative energy (in eV) of the low-lying $(\text{CdSe})_N$ ($N = 2-10, 13, 16$ and 19) clusters in water calculated with PBE0 functional (Continued).

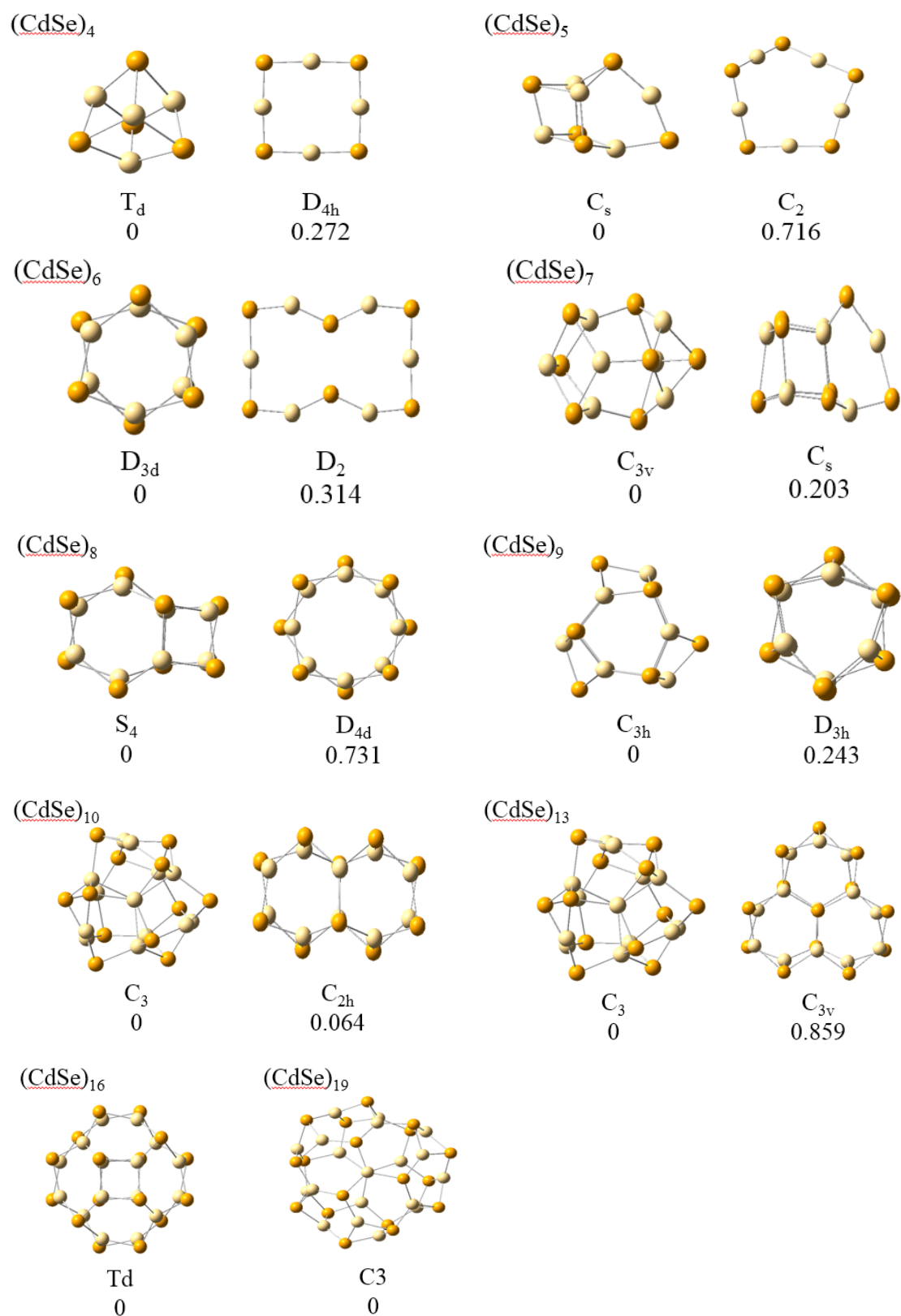


Fig. S3 Structures, symmetry and relative energy (in eV) of the low-lying $(\text{CdSe})_N$ ($N = 4-10, 13, 16$ and 19) clusters in gas calculated with PBE0 functional.

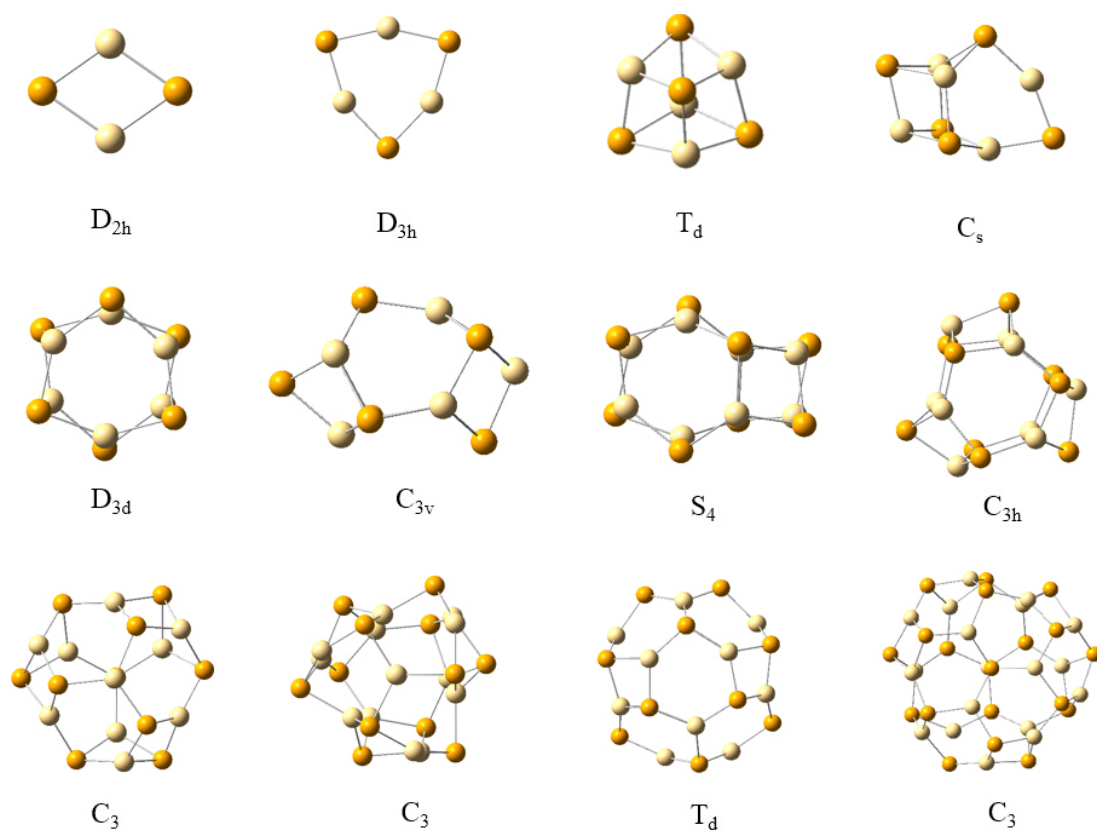


Fig. S4 The lowest-energy structures and symmetry of $(CdSe)_N$ ($N = 2-10, 13, 16$ and 19) clusters in toluene calculated with PBE0 functional.

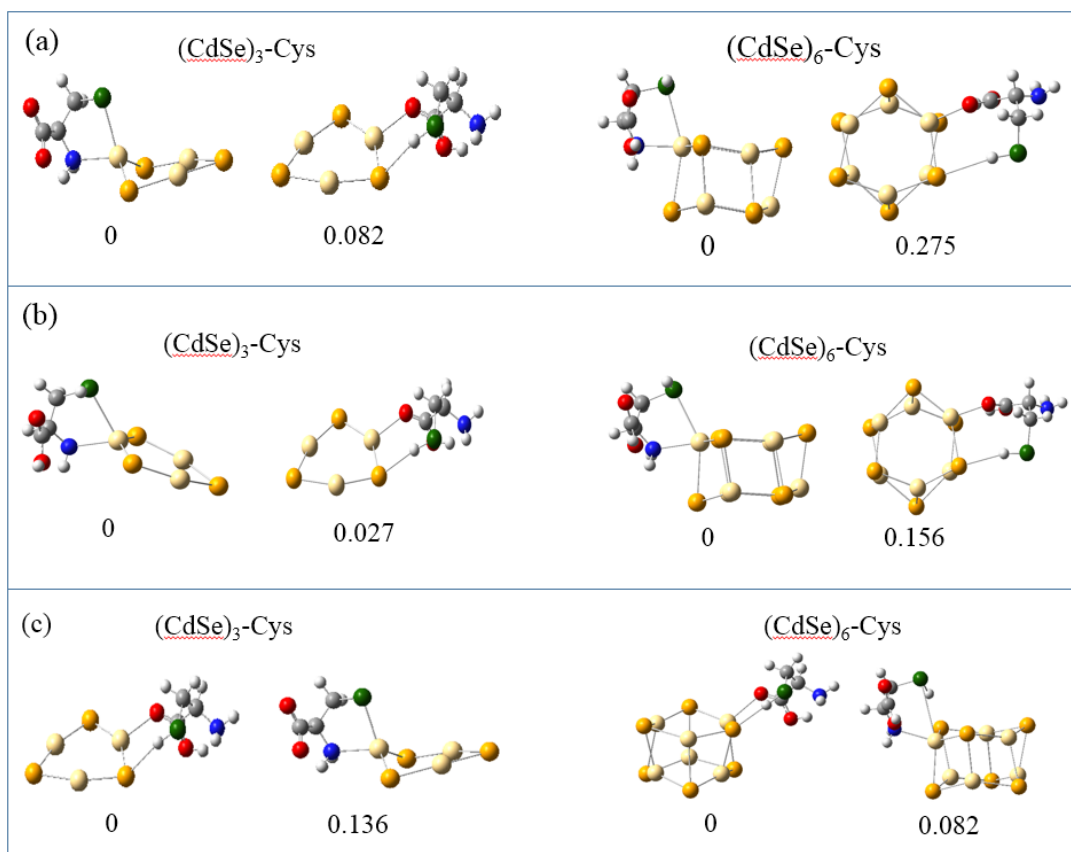


Fig. S5 Comparison of the $(\text{CdSe})_N\text{-Cys}$ ($N = 3, 6$) structures with different adsorption patterns in gas (a), toluene (b) and water (c) with PBE0. The relative energies are given in eV.

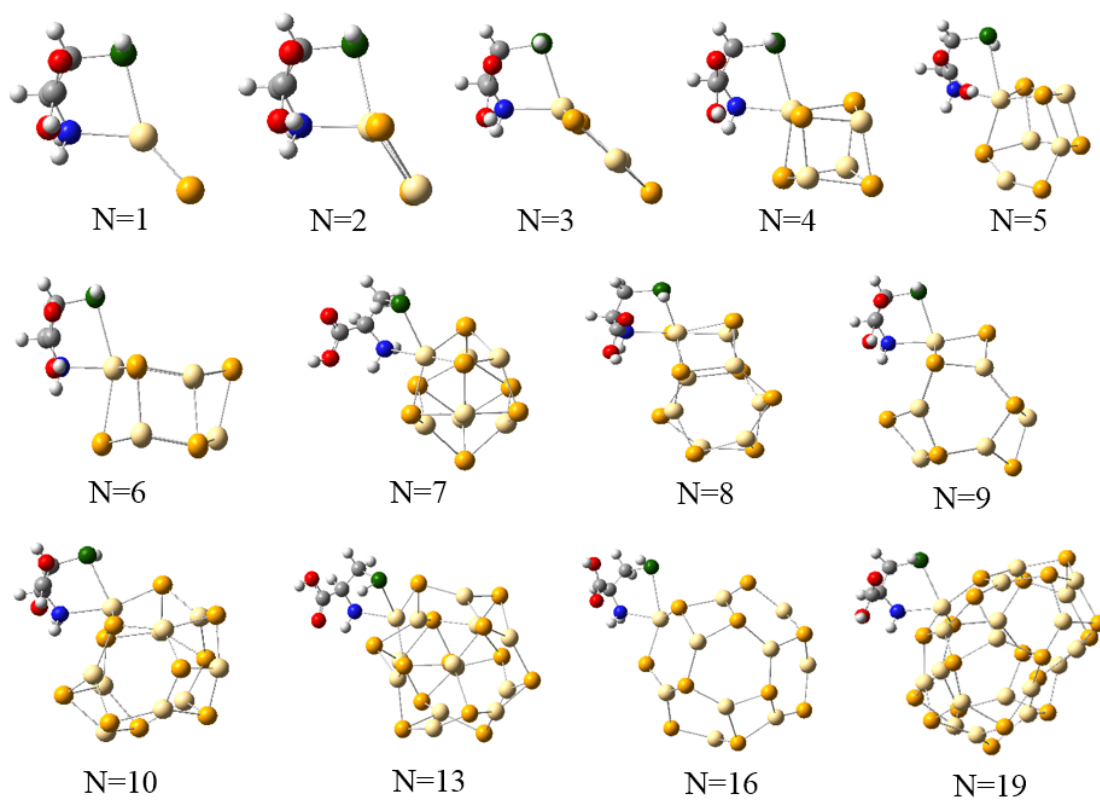


Fig. S6 The lowest-energy structures of $(\text{CdSe})_N\text{-Cys}$ complexes of ($N = 1-10, 13, 16$ and 19) in gas calculated with PBE0 functional.

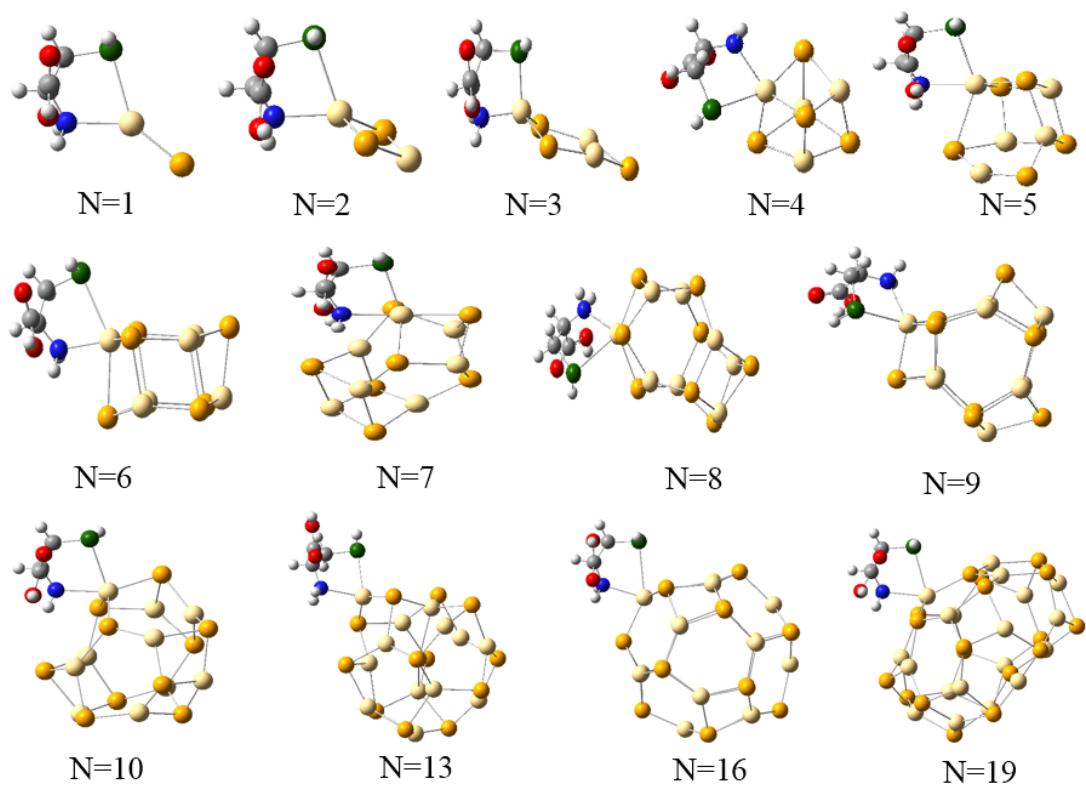


Fig. S7 The lowest-energy structures of $(\text{CdSe})_N\text{-Cys}$ complexes of ($N = 1-10, 13, 16$ and 19) in toluene calculated with PBE0 functional.

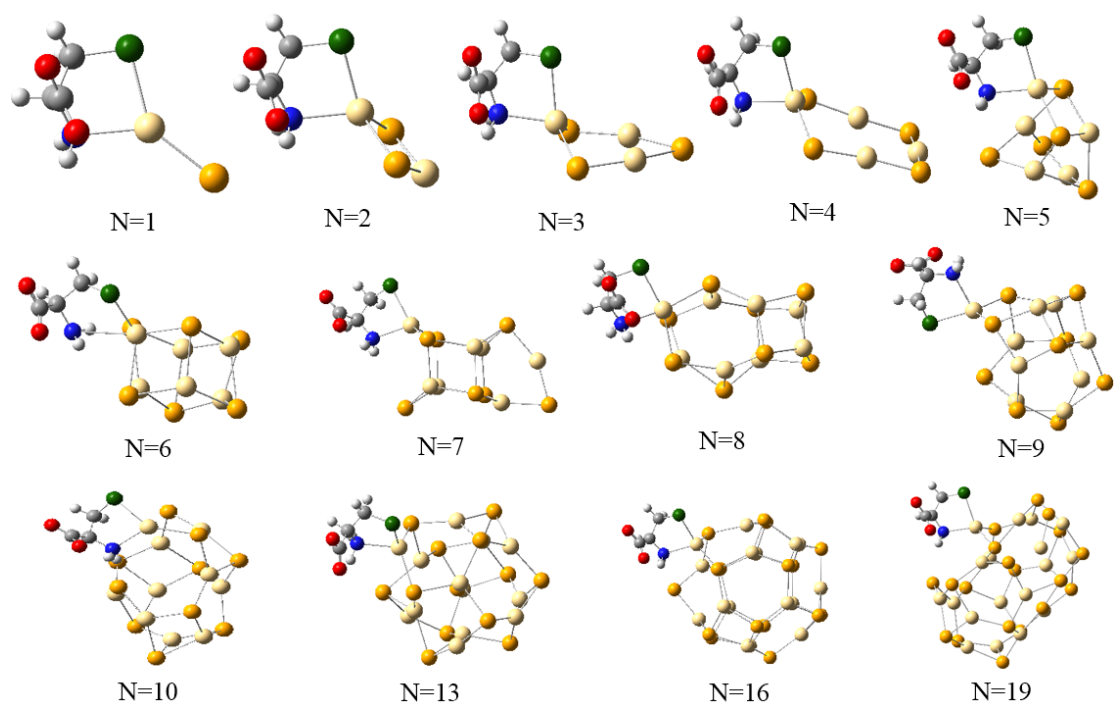


Fig. S8 The lowest-energy structures of $(\text{CdSe})_N\text{-Cys}$ complexes of ($N = 1\text{--}10, 13, 16$ and 19) in alkaline solution calculated with PBE0 functional.

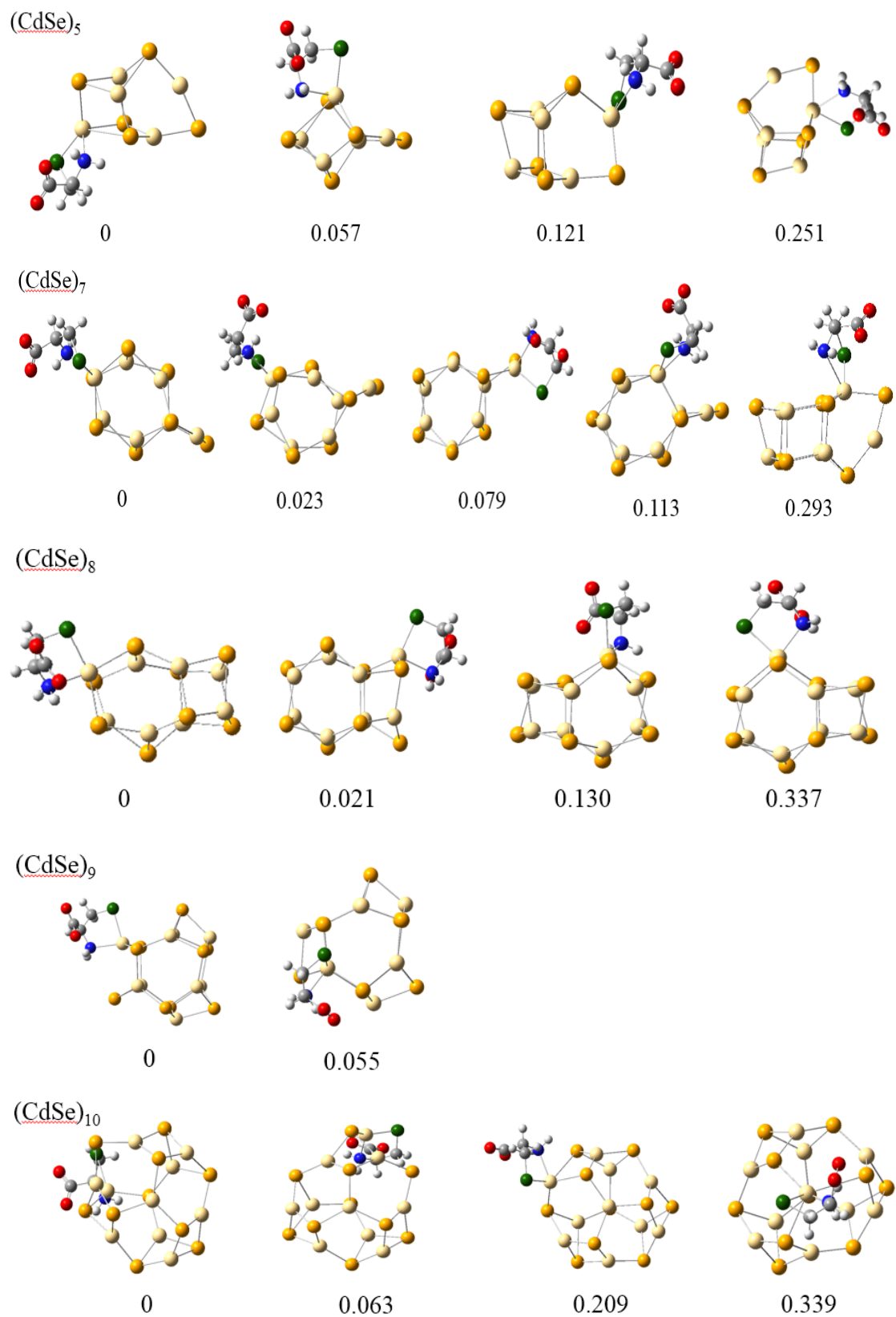


Fig. S9 Structures and relative energy (in eV) of the (CdSe)_N-Cys complexes ($N = 5-10, 13, 16$ and 19) clusters in alkaline solution calculated with PBE0 functional.

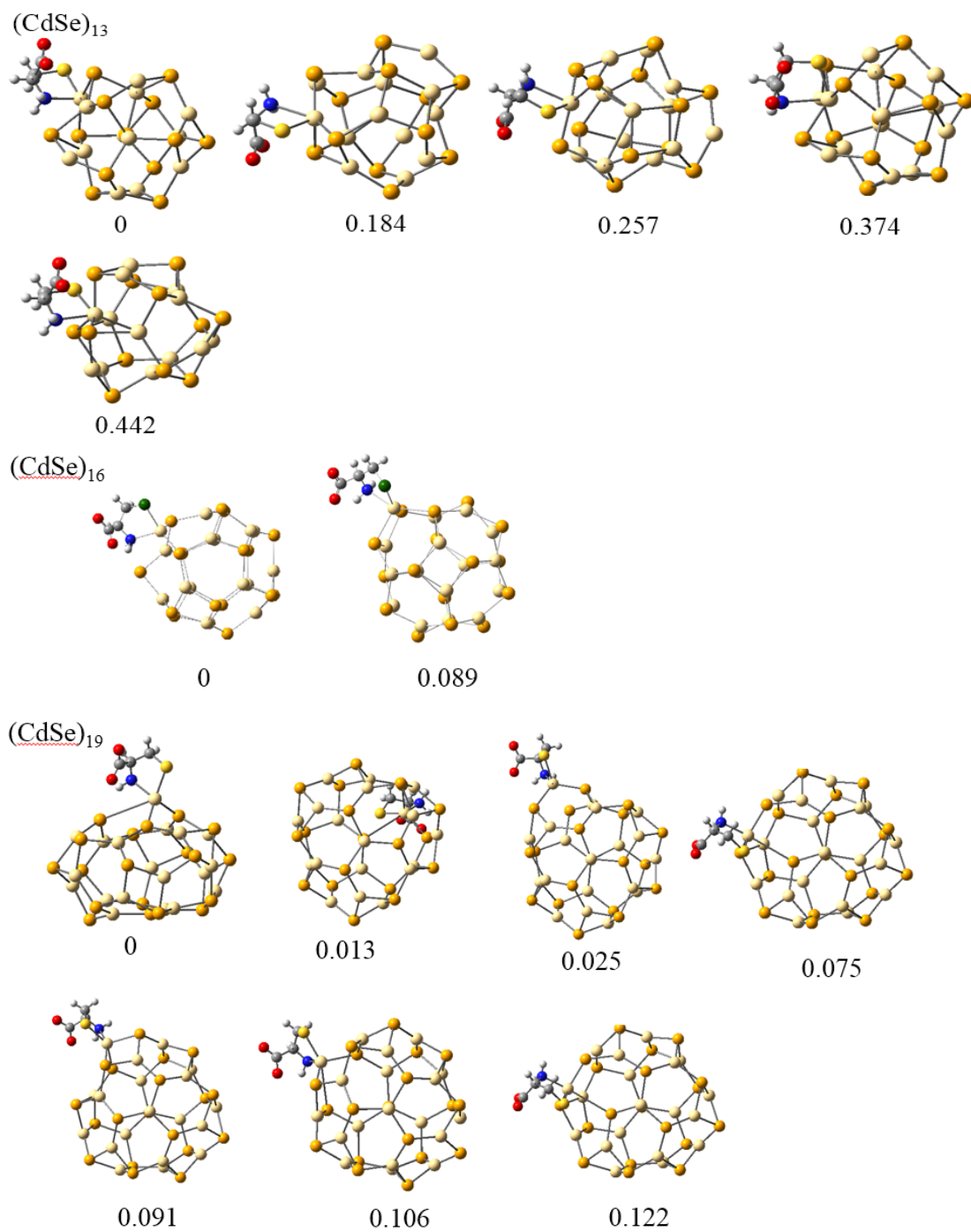


Fig. S9 Structures and relative energy (in eV) of the (CdSe)_N-Cys complexes ($N = 5-10, 13, 16$ and 19) clusters in alkaline solution calculated with PBE0 functional (Continued).

Cartesian coordinates of CdSe cluster in gas

Gas

(CdSe)₁

Se	0.00000000	0.00000000	-1.42680900
Cd	0.00000000	0.00000000	1.01065600

(CdSe)₂

Cd	-0.00002900	-1.46052200	0.00000000
Cd	0.00000000	1.46049900	0.00000000
Se	-2.17985400	-0.00104200	0.00000000
Se	2.17989500	0.00107400	0.00000000

(CdSe)₃

Cd	0.00000000	1.97095100	0.00000000
Cd	1.70689300	-0.98547500	0.00000000
Cd	-1.70689300	-0.98547500	0.00000000
Se	0.00000000	-2.89639600	0.00000000
Se	2.50835300	1.44819800	0.00000000
Se	-2.50835300	1.44819800	0.00000000

(CdSe)₄

Se	-1.52960400	1.52960400	1.52960400
Se	1.52960400	1.52960400	-1.52960400
Se	-1.52960400	-1.52960400	-1.52960400
Cd	1.15895600	1.15895600	1.15895600
Cd	-1.15895600	-1.15895600	1.15895600
Cd	-1.15895600	1.15895600	-1.15895600
Cd	1.15895600	-1.15895600	-1.15895600
Se	1.52960400	-1.52960400	1.52960400

(CdSe)₅

Cd	2.85974800	0.73963000	0.00000000
Cd	0.94601900	-1.91200600	0.00000000
Cd	-0.74893600	1.22764700	1.58841800
Se	-0.74893600	-1.41326200	2.12268500
Se	3.56554500	-1.67806800	0.00000000
Se	1.05645700	2.60139400	0.00000000
Se	-0.74893600	-1.41326200	-2.12268500
Se	-2.95171400	1.59382400	0.00000000
Cd	-2.43002300	-1.06377900	0.00000000
Cd	-0.74893600	1.22764700	-1.58841800

(CdSe)₆

Cd	0.00000000	2.28407600	1.21604400
Cd	1.97806800	-1.14203800	1.21604400
Cd	-1.97806800	-1.14203800	1.21604400
Se	2.50700700	1.44742100	1.53734700
Se	-2.50700700	1.44742100	1.53734700
Se	0.00000000	-2.89484300	1.53734700
Se	0.00000000	2.89484300	-1.53734700
Se	2.50700700	-1.44742100	-1.53734700
Se	-2.50700700	-1.44742100	-1.53734700
Cd	1.97806800	1.14203800	-1.21604400
Cd	-1.97806800	1.14203800	-1.21604400
Cd	0.00000000	-2.28407600	-1.21604400

(CdSe)₇

Se	2.62174700	0.23750000	-2.45342600
Se	2.62301200	2.00590900	1.43191700
Cd	1.22735400	1.97807800	-0.90010400
Cd	3.76039600	0.00021800	-0.00080400
Se	-4.34211400	-0.00024400	-0.00004300
Se	-1.33109400	2.59604000	-1.18143100
Cd	-2.37174600	1.53139500	1.09362800
Cd	-2.37073900	0.18112700	-1.87288800
Cd	1.22758300	-1.76885700	-1.26241900
Cd	-2.37127100	-1.71279000	0.77968500
Cd	1.22842000	-0.20925500	2.16338700
Se	-1.33009400	-0.27465800	2.83860400
Se	-1.33047400	-2.32139900	-1.65715800
Se	2.62313800	-2.24303100	1.02085200

(CdSe)₈

Se	-3.57409800	-1.93024300	0.86091100
Cd	-3.09360000	-0.74160000	-1.46650400
Se	-1.00841100	-0.42511200	-3.11720500
Cd	0.99465400	-1.62539700	-1.88630400
Se	1.00841600	-3.11721500	0.42511500
Cd	-0.99465300	-1.88630900	1.62538800
Se	-1.00840700	0.42511100	3.11720800
Cd	-3.09359500	0.74159900	1.46650500
Se	-3.57410200	1.93024100	-0.86090700
Cd	-0.99465700	1.88630800	-1.62538800
Se	1.00841000	3.11721600	-0.42511400
Cd	0.99465700	1.62539700	1.88630700
Se	3.57409700	-0.86091000	-1.93024400
Cd	3.09359800	-1.46650300	0.74160100

Se	3.57410100	0.86091300	1.93023700
Cd	3.09359000	1.46650500	-0.74160600

(CdSe)₉

Se	2.84841200	3.01799900	0.00000000
Cd	1.91802600	1.46226000	1.98376800
Se	2.62271200	-1.02163100	2.51457300
Se	-0.42659800	2.78215100	2.51457300
Cd	-2.22536800	0.92992900	1.98376800
Cd	0.30734100	-2.39219000	1.98376800
Se	-2.19611400	-1.76052000	2.51457300
Cd	-3.12758100	-1.62536700	0.00000000
Se	-2.19611400	-1.76052000	-2.51457300
Cd	0.30734100	-2.39219000	-1.98376800
Cd	-2.22536800	0.92992900	-1.98376800
Se	2.62271200	-1.02163100	-2.51457300
Cd	1.91802600	1.46226000	-1.98376800
Se	1.18945800	-3.97579700	0.00000000
Se	-4.03787000	0.95779800	0.00000000
Cd	0.15618100	3.52124800	0.00000000
Cd	2.97139900	-1.89588100	0.00000000
Se	-0.42659800	2.78215100	-2.51457300

(CdSe)₁₀

Cd	0.00000000	3.51478300	0.37104200
Se	2.16896300	3.83958800	-1.16587900
Cd	2.10136800	1.31037500	-2.06277300
Se	0.00000000	0.00000000	-3.08893600
Cd	-2.18550300	1.16465100	-2.06277300
Se	-2.43969900	3.47186500	-0.58988300
Se	4.22657200	0.37690900	-0.58988300
Cd	3.04389100	-1.75739100	0.37104200
Se	2.24069900	-3.79817100	-1.16587900
Cd	0.08413400	-2.47502600	-2.06277300
Se	-4.40966200	-0.04141700	-1.16587900
Cd	-3.04389100	-1.75739100	0.37104200
Se	-1.78687400	-3.84877300	-0.58988300
Cd	3.09677100	2.28350600	0.90237400
Cd	0.42918900	-3.82363500	0.90237400
Cd	-3.52596000	1.54012900	0.90237400
Cd	0.00000000	0.00000000	2.67337600
Se	1.07449600	2.45403100	2.64173600
Se	-2.66250200	-0.29647500	2.64173600
Se	1.58800500	-2.15755700	2.64173600

(CdSe)₁₃

Se	3.61722500	2.41316900	-1.47899900
Se	3.73330700	-2.39039600	-1.20470700
Se	3.61736600	0.24765600	2.81865100
Cd	2.91163500	-0.00396700	-2.25247300
Cd	2.81673800	2.08918400	1.11381300
Cd	2.91545000	-1.87397400	1.24561800
Cd	1.15921300	3.44370000	-1.40043000
Cd	1.19168400	-0.45057500	3.67730700
Cd	1.32646000	-2.90032100	-2.23249000
Se	0.85924100	3.99035700	1.23436700
Se	1.01286700	-3.01829900	2.83643500
Se	1.04465500	-0.89920200	-4.03414500
Se	-0.90111600	3.33602000	-3.10803900
Se	-0.73125500	-4.38080200	-1.36960200
Se	-0.93687400	0.98158600	4.44503500
Cd	-0.81148600	0.57822200	-2.80974800
Cd	-0.77420700	-2.74513500	0.87231500
Cd	-0.90873900	2.10692600	1.90779600
Se	-0.19755000	-0.00368900	-0.00131500
Se	-3.44947200	-0.35870400	-2.74888700
Se	-3.56578500	2.39363800	1.07325400
Se	-3.45422800	-2.29444400	1.54675600
Cd	-2.43481100	3.28445000	-1.04634600
Cd	-2.27046200	-2.60943200	-2.41802000
Cd	-2.38606400	-0.85162800	3.37506400
Cd	-3.19468200	-0.07941600	-0.03864300

(CdSe)₁₆

Se	-4.65917700	1.41325200	1.41325200
Se	-4.65917700	-1.41325200	-1.41325200
Se	-2.87413000	2.87413000	-2.87413000
Se	-1.41325200	-1.41325200	-4.65917700
Se	1.41325200	1.41325200	-4.65917700
Se	2.87413000	-2.87413000	-2.87413000
Se	-1.41325200	-4.65917700	-1.41325200
Se	1.41325200	-4.65917700	1.41325200
Se	-2.87413000	-2.87413000	2.87413000
Se	-1.41325200	1.41325200	4.65917700
Se	-1.41325200	4.65917700	1.41325200
Se	2.87413000	2.87413000	2.87413000
Se	1.41325200	-1.41325200	4.65917700
Se	4.65917700	-1.41325200	1.41325200

Se	4.65917700	1.41325200	-1.41325200
Se	1.41325200	4.65917700	-1.41325200
Cd	-1.21597700	4.13217600	-1.21597700
Cd	1.21597700	4.13217600	1.21597700
Cd	-2.52224500	2.52224500	2.52224500
Cd	1.21597700	1.21597700	4.13217600
Cd	-4.13217600	1.21597700	-1.21597700
Cd	-4.13217600	-1.21597700	1.21597700
Cd	-1.21597700	-1.21597700	4.13217600
Cd	-1.21597700	-4.13217600	1.21597700
Cd	2.52224500	-2.52224500	2.52224500
Cd	4.13217600	1.21597700	1.21597700
Cd	-2.52224500	-2.52224500	-2.52224500
Cd	2.52224500	2.52224500	-2.52224500
Cd	-1.21597700	1.21597700	-4.13217600
Cd	1.21597700	-1.21597700	-4.13217600
Cd	1.21597700	-4.13217600	-1.21597700
Cd	4.13217600	-1.21597700	-1.21597700

(CdSe)₁₉

Cd	0.00000000	0.00000000	3.29045600
Se	2.61221800	-0.56176100	3.44729900
Se	-1.79260900	-1.98136700	3.44729900
Cd	-3.28892700	2.72840400	2.54391500
Cd	-3.98378900	-1.47165300	1.99488500
Cd	-0.71840400	-4.21249700	2.54391500
Cd	3.26638300	-2.71423600	1.99488500
Cd	0.71740600	4.18588900	1.99488500
Cd	4.00733100	1.48409200	2.54391500
Se	3.34461800	4.06917900	2.28528800
Se	-5.19632100	0.86193500	2.28528800
Se	1.85170300	-4.93111400	2.28528800
Se	-0.81961000	2.54312800	3.44729900
Se	0.00000000	5.97150800	0.16742400
Se	-4.42043900	4.41318200	0.73685900
Cd	-2.35003700	5.02416600	-0.73478800
Se	-5.17147800	-2.98575400	0.16742400
Se	-1.61170800	-6.03480300	0.73685900
Se	5.17147800	-2.98575400	0.16742400
Cd	-3.17603700	-4.54727500	-0.73478800
Cd	5.52607400	-0.47689100	-0.73478800
Cd	0.85310400	-5.39191900	-0.16939200
Cd	4.24298700	3.43476900	-0.16939200
Cd	-5.09609000	1.95715000	-0.16939200

Se	6.03214700	1.62162100	0.73685900
Se	1.47542300	-4.46886400	-2.58321800
Cd	3.58319700	-2.98992800	-2.00136500
Se	-4.60786100	0.95667900	-2.58321800
Cd	-4.38095200	-1.60817600	-2.00136500
Se	3.13243900	3.51218600	-2.58321800
Cd	0.79775500	4.59810400	-2.00136500
Cd	-0.42072400	-2.57370300	-2.81517700
Se	-2.86814900	-3.47984700	-3.20967700
Se	4.44771000	-0.74396600	-3.20967700
Cd	2.43925500	0.92249400	-2.81517700
Se	-1.57956200	4.22381300	-3.20967700
Cd	-2.01853000	1.65121000	-2.81517700
Se	0.00000000	0.00000000	-2.17148300

Cartesian coordinates of CdSe cluster in toluene

(CdSe)₁

Se	0.00000000	0.00000000	-1.44075700
Cd	0.00000000	0.00000000	1.02460400

(CdSe)₂

Cd	0.00049600	-1.51747500	0.00000100
Cd	-0.00048900	1.51747900	0.00000100
Se	-2.16666100	-0.00071200	-0.00000100
Se	2.16666600	0.00071700	-0.00000100

(CdSe)₃

Cd	0.00000000	2.03231000	0.00000000
Cd	1.80276700	-1.02434500	0.00000000
Cd	-1.80276700	-1.02434500	0.00000000
Se	0.00000000	-2.91241400	0.00000000
Se	2.53713000	1.46439800	0.00000000
Se	-2.53713000	1.46439800	0.00000000

(CdSe)₄

Se	-1.52774900	1.52770700	1.52775200
Se	1.52773400	1.52777500	-1.52780100
Se	-1.52774900	-1.52770700	-1.52775200
Cd	1.19645000	1.19642600	1.19640600
Cd	-1.19643500	-1.19645900	1.19646500
Cd	-1.19643500	1.19645900	-1.19646500
Cd	1.19645000	-1.19642600	-1.19640600
Se	1.52773400	-1.52777500	1.52780100

(CdSe)₅

Cd	2.61642700	1.35698700	0.00002500
Cd	1.43480900	-1.73781200	0.00000000
Cd	-1.05155500	1.03378100	1.64269700
Se	-0.37868900	-1.56786800	2.10138600
Se	3.94638800	-0.81984400	-0.00002500
Se	0.40678700	2.75322200	0.00000200
Se	-0.37869200	-1.56788100	-2.10138200
Se	-3.28458200	0.83658600	-0.00000600
Cd	-2.20266700	-1.66349100	0.00000300
Cd	-1.05153800	1.03377500	-1.64270000

(CdSe)₆

Cd	0.00000000	2.25993400	1.16810000
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Cd	2.09501600	-1.19074800	1.26248600
Cd	-2.09501600	-1.19074800	1.26248600
Se	2.52132000	1.43707400	1.57201000
Se	-2.52132000	1.43707400	1.57201000
Se	0.00000000	-2.88758100	1.55419800
Se	0.00000000	2.88758100	-1.55419800
Se	2.52132000	-1.43707400	-1.57201000
Se	-2.52132000	-1.43707400	-1.57201000
Cd	2.09501600	1.19074800	-1.26248600
Cd	-2.09501600	1.19074800	-1.26248600
Cd	0.00000000	-2.25993400	-1.16810000

(CdSe)₇

Se	2.69312800	0.23038700	-2.47356400
Se	2.61964300	2.01182600	1.43568600
Cd	1.26365400	2.01077600	-0.96491000
Cd	3.86003500	0.01692100	0.00790000
Se	-4.39798700	0.00719800	0.00207900
Se	-1.34447100	2.60836800	-1.16811700
Cd	-2.41403900	1.56819200	1.12735400
Cd	-2.44869500	0.19411900	-1.92709200
Cd	1.29273800	-1.84232600	-1.34089600
Cd	-2.45963600	-1.76392000	0.83066100
Cd	1.24126900	-0.21993900	2.22034100
Se	-1.36987900	-0.29016000	2.86618900
Se	-1.31957800	-2.28953200	-1.62568300
Se	2.64793700	-2.24187600	1.00985300

(CdSe)₈

Se	-3.64532700	-1.94613600	0.85678500
Cd	-3.22251200	-0.74532100	-1.51107000
Se	-1.03376200	-0.43375000	-3.09812900
Cd	1.04997900	-1.68502100	-1.94675600
Se	1.03376200	-3.09813000	0.43374900
Cd	-1.04997800	-1.94675600	1.68502100
Se	-1.03375700	0.43374800	3.09812900
Cd	-3.22251100	0.74531900	1.51107600
Se	-3.64533000	1.94613300	-0.85677900
Cd	-1.04998200	1.94675400	-1.68502100
Se	1.03375800	3.09813000	-0.43375000
Cd	1.04998100	1.68502200	1.94675400
Se	3.64532700	-0.85678000	-1.94613700
Cd	3.22251100	-1.51107100	0.74531800
Se	3.64532900	0.85678400	1.94613200

Cd	3.22251000	1.51107500	-0.74532200
(CdSe) ₉			
Se	2.87450700	2.98843100	0.00000000
Cd	1.94603800	1.48403000	2.06564800
Se	2.66162200	-1.05059400	2.52269300
Se	-0.43805300	2.79534000	2.50953500
Cd	-2.33225600	0.99411100	1.99128000
Cd	0.34838300	-2.48216500	2.03895900
Se	-2.17363500	-1.72904700	2.50197600
Cd	-3.20836000	-1.66688000	0.00000000
Se	-2.17363500	-1.72904700	-2.50197600
Cd	0.34838300	-2.48216500	-2.03895900
Cd	-2.33225600	0.99411100	-1.99128000
Se	2.66162200	-1.05059400	-2.52269300
Cd	1.94603800	1.48403000	-2.06564800
Se	1.21464400	-4.02141000	0.00000000
Se	-4.17294700	0.96906400	0.00000000
Cd	0.18150000	3.63335000	0.00000000
Cd	3.08645500	-1.92590600	0.00000000
Se	-0.43805300	2.79534000	-2.50953500
(CdSe) ₁₀			
Cd	-0.00311500	3.62880900	0.31718800
Se	2.23879500	3.93829500	-1.18163400
Cd	2.24554500	1.38912900	-2.13994200
Se	0.02872200	-0.01154400	-2.84806800
Cd	-2.25187700	1.21107100	-2.07785800
Se	-2.50543700	3.53045100	-0.57628100
Se	4.25717000	0.39380200	-0.53491800
Cd	3.08480400	-1.82803500	0.31100000
Se	2.28055000	-3.91769000	-1.21073000
Cd	0.07096700	-2.63583600	-2.13524300
Se	-4.47630100	-0.04348000	-1.16846200
Cd	-3.10334700	-1.79794500	0.37465900
Se	-1.81624600	-3.92151400	-0.56318000
Cd	3.15353700	2.36579000	0.94435900
Cd	0.46130400	-3.98416400	0.88011500
Cd	-3.62269600	1.58946400	0.92997100
Cd	0.01757400	0.02480700	2.70304800
Se	1.04648700	2.53619100	2.62751700
Se	-2.67533300	-0.28696600	2.63555800
Se	1.56889300	-2.18063300	2.58719100

(CdSe)₁₃

Se	3.62994600	2.46701900	-1.48736300
Se	3.82618500	-2.38948500	-1.24168300
Se	3.69052700	0.23782000	2.85133200
Cd	3.06506700	0.00987300	-2.35261700
Cd	2.95469700	2.17062200	1.17252100
Cd	3.13243700	-1.97407900	1.29679000
Cd	1.15715100	3.52415500	-1.39112100
Cd	1.24507500	-0.53901600	3.73574000
Cd	1.34922000	-2.91682100	-2.17115100
Se	0.92050800	4.03367000	1.28573200
Se	1.08954400	-3.07440000	2.77844300
Se	1.09776400	-0.91559600	-4.03300400
Se	-0.91431100	3.36234000	-3.10769300
Se	-0.73702100	-4.40921800	-1.36218100
Se	-0.87255900	0.94922400	4.46341000
Cd	-0.85994300	0.56549900	-2.89093000
Cd	-0.86552900	-2.76651300	0.92456400
Cd	-0.92848100	2.13413500	1.91769700
Se	-0.35627100	-0.00484400	-0.01739400
Se	-3.49170300	-0.44356800	-2.84277700
Se	-3.61005000	2.44382300	1.05316000
Se	-3.55543400	-2.24823800	1.62896600
Cd	-2.57293100	3.46083000	-1.10592600
Cd	-2.36904000	-2.77688400	-2.57303300
Cd	-2.56033600	-0.81622400	3.54988200
Cd	-3.27540200	-0.07919900	-0.07879600

(CdSe)₁₆

Se	-4.75084400	1.43227100	1.43227100
Se	-4.75084400	-1.43227100	-1.43227100
Se	-2.87427600	2.87427600	-2.87427600
Se	-1.43227100	-1.43227100	-4.75084400
Se	1.43227100	1.43227100	-4.75084400
Se	2.87427600	-2.87427600	-2.87427600
Se	-1.43227100	-4.75084400	-1.43227100
Se	1.43227100	-4.75084400	1.43227100
Se	-2.87427600	-2.87427600	2.87427600
Se	-1.43227100	1.43227100	4.75084400
Se	-1.43227100	4.75084400	1.43227100
Se	2.87427600	2.87427600	2.87427600
Se	1.43227100	-1.43227100	4.75084400
Se	4.75084400	-1.43227100	1.43227100
Se	4.75084400	1.43227100	-1.43227100

Se	1.43227100	4.75084400	-1.43227100
Cd	-1.23742900	4.22641200	-1.23742900
Cd	1.23742900	4.22641200	1.23742900
Cd	-2.64886800	2.64886800	2.64886800
Cd	1.23742900	1.23742900	4.22641200
Cd	-4.22641200	1.23742900	-1.23742900
Cd	-4.22641200	-1.23742900	1.23742900
Cd	-1.23742900	-1.23742900	4.22641200
Cd	-1.23742900	-4.22641200	1.23742900
Cd	2.64886800	-2.64886800	2.64886800
Cd	4.22641200	1.23742900	1.23742900
Cd	-2.64886800	-2.64886800	-2.64886800
Cd	2.64886800	2.64886800	-2.64886800
Cd	-1.23742900	1.23742900	-4.22641200
Cd	1.23742900	-1.23742900	-4.22641200
Cd	1.23742900	-4.22641200	-1.23742900
Cd	4.22641200	-1.23742900	-1.23742900

(CdSe)₁₉

Cd	0.00924200	0.00148700	3.33465100
Se	2.65290400	-0.49715300	3.37885000
Se	-1.85604200	-1.97273200	3.35433100
Cd	-3.43253600	2.73834500	2.65419400
Cd	-4.19359100	-1.51646400	2.05291600
Cd	-0.76957100	-4.27620100	2.56939300
Cd	3.33748600	-2.74345900	2.04816600
Cd	0.77417000	4.30930800	2.03843100
Cd	4.13625800	1.60312100	2.63437500
Se	3.45814100	4.20101200	2.27407800
Se	-5.37486400	0.87255900	2.33152200
Se	1.85615800	-4.95627300	2.33932200
Se	-0.84100200	2.58202800	3.35007600
Se	0.00865900	6.06318800	0.15440300
Se	-4.45183400	4.43384700	0.74046700
Cd	-2.39127500	5.14389800	-0.76330200
Se	-5.24280700	-3.08772400	0.13410000
Se	-1.58129600	-6.05706000	0.66173000
Se	5.18131900	-3.03875500	0.11766700
Cd	-3.27398500	-4.70682900	-0.86056900
Cd	5.67542200	-0.51879900	-0.77936400
Cd	0.95730600	-5.48293600	-0.16974800
Cd	4.40720300	3.51154400	-0.19153900
Cd	-5.27467100	1.98469700	-0.15867700
Se	6.13431900	1.61023800	0.73733900

Se	1.49600400	-4.55988000	-2.63658400
Cd	3.64103200	-3.06107400	-2.10734300
Se	-4.58070400	0.96940200	-2.53939900
Cd	-4.51153800	-1.63923200	-2.02356400
Se	3.12553700	3.50596200	-2.56580200
Cd	0.81903600	4.75200500	-2.08100000
Cd	-0.43948200	-2.62432800	-2.74817400
Se	-2.92869000	-3.45825500	-3.27296700
Se	4.50377500	-0.75522600	-3.25686700
Cd	2.45613200	0.88143500	-2.78100800
Se	-1.57326200	4.22525800	-3.23247800
Cd	-1.94629700	1.62548600	-2.71119100
Se	0.03334500	-0.06243600	-1.92130300

Cartesian coordinates of CdSe cluster in water

(CdSe)₁

Cd	0.00000000	0.00000000	1.05923300
Se	0.00000000	0.00000000	-1.49538700

(CdSe)₂

Cd	-0.00003900	-1.57566200	0.00000000
Cd	0.00000000	1.57538200	0.00000000
Se	-2.20415500	-0.00211500	0.00000000
Se	2.20421000	0.00250900	0.00000000

(CdSe)₃

Cd	0.00000000	0.00000000	1.99869100
Cd	0.00000000	1.81321500	-1.01811300
Cd	0.00000000	-1.81321500	-1.01811300
Se	0.00000000	0.00000000	-2.97842900
Se	0.00000000	2.59970400	1.51571000
Se	0.00000000	-2.59970400	1.51571000

(CdSe)₄

Cd	-2.68044600	-0.00120400	0.00000000
Cd	2.68240100	0.00125400	0.00000000
Cd	0.00000000	2.68017400	0.00000000
Cd	-0.00077800	-2.68030400	0.00000000
Se	-2.63034500	2.62883300	0.00000000
Se	2.62995400	2.63171100	0.00000000
Se	-2.63079400	-2.63142200	0.00000000
Se	2.62952200	-2.62901000	0.00000000

(CdSe)₅

Cd	2.60815500	1.41368800	-0.00155400
Cd	1.48263600	-1.54562600	0.03666800
Cd	-1.03010800	1.18847200	1.49846900
Se	-0.28943800	-1.38015900	2.24263800
Se	4.09341400	-0.74787000	0.06244200
Se	0.34909700	2.80798600	-0.33645500
Se	-0.34381900	-1.79649900	-2.10308500
Se	-3.45429100	0.83366100	0.11838700
Cd	-2.14632000	-1.65630500	0.14470100
Cd	-1.16579500	0.80014500	-1.66689800

(CdSe)₆

Cd	-1.16359800	-1.11786600	2.02612600
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Cd	2.31499800	-1.17433900	-0.05642300
Cd	-1.15931800	-1.15171000	-2.17600200
Cd	1.15931800	1.15171000	2.17600200
Cd	-2.31499800	1.17433900	0.05642400
Cd	1.16359800	1.11786600	-2.02612600
Se	1.48362000	-1.74404500	2.50395000
Se	-2.88349600	-1.65655500	-0.08611300
Se	1.47815900	-1.78984100	-2.61845400
Se	-1.47815900	1.78984100	2.61845400
Se	2.88349500	1.65655500	0.08611300
Se	-1.48362000	1.74404500	-2.50395000

(CdSe)₇

Se	-1.60489000	-3.61727000	-0.02000000
Se	-2.58624000	-0.33824000	2.50147000
Cd	-0.53645000	-2.15830000	1.91695000
Cd	-3.07692000	-1.20606000	0.04500000
Se	4.46380000	2.02764000	0.04000000
Se	1.54228000	-0.55955000	2.33404000
Cd	-0.53995000	1.20094000	-1.83239000
Cd	2.82497000	-0.05963000	-0.02000000
Cd	-0.53995000	-2.12830000	-1.93195000
Cd	2.22705000	3.16575000	-0.26000000
Cd	-0.49995000	1.19594000	1.81239000
Se	-0.39022000	3.20122000	0.03000000
Se	1.49828000	-0.45955000	-2.34404000
Se	-2.67624000	-0.32824000	-2.43147000

(CdSe)₈

Se	0.76766900	2.05933300	3.63307900
Cd	1.58970900	-0.50737400	3.10802000
Se	2.61188600	-1.97589100	1.01443500
Cd	2.61188600	-0.09677800	-0.97081000
Se	1.97589100	2.61188600	-1.01443500
Cd	0.09677800	2.61188600	0.97081000
Se	-2.61188600	1.97589100	1.01443500
Cd	-1.58970900	0.50737400	3.10802000
Se	-0.76766900	-2.05933300	3.63307900
Cd	-0.09677800	-2.61188600	0.97081000
Se	-1.97589100	-2.61188600	-1.01443500
Cd	-2.61188600	0.09677800	-0.97081000
Se	2.05933300	-0.76766900	-3.63307900
Cd	0.50737400	1.58970900	-3.10802000
Se	-2.05933300	0.76766900	-3.63307900

Cd	-0.50737400	-1.58970900	-3.10802000
(CdSe) ₉			
Se	2.94501500	3.04690500	0.00000000
Cd	1.87663000	1.47945700	2.02671600
Se	2.67401800	-1.06489800	2.58111800
Se	-0.46645500	2.91581100	2.57886200
Cd	-2.23278800	0.97847000	1.91419100
Cd	0.32946100	-2.53596200	1.96648400
Se	-2.21491600	-1.74015600	2.56887300
Cd	-3.22692100	-1.68738100	0.00000000
Se	-2.21491600	-1.74015600	-2.56887300
Cd	0.32946100	-2.53596200	-1.96648400
Cd	-2.23278800	0.97847000	-1.91419100
Se	2.67401800	-1.06489800	-2.58111800
Cd	1.87663000	1.47945700	-2.02671600
Se	1.29861400	-4.20743000	0.00000000
Se	-4.21513100	0.98627500	0.00000000
Cd	0.18335900	3.69511600	0.00000000
Cd	3.08316200	-1.89893100	0.00000000
Se	-0.46645500	2.91581100	-2.57886200
(CdSe) ₁₀			
Cd	0.30323800	3.56855000	0.33639500
Se	2.64670600	3.84873200	-1.15021800
Cd	2.19775500	1.22824000	-2.02343400
Se	0.04350200	0.01393300	-3.24213900
Cd	-2.10648900	1.25686000	-2.06356100
Se	-2.18342600	3.71384100	-0.71834200
Se	4.37151200	0.01503700	-0.65370100
Cd	2.96480600	-2.05857200	0.39659200
Se	1.99182600	-4.02698200	-1.29195600
Cd	-0.16926900	-2.44784000	-2.06515800
Se	-4.55264800	0.22393100	-1.19569700
Cd	-3.22487900	-1.52087500	0.47595800
Se	-2.16250300	-3.77590600	-0.57821000
Cd	3.33360200	2.03095300	0.90268400
Cd	0.15883300	-4.01865600	0.86773300
Cd	-3.54206100	1.92341100	0.87690400
Cd	-0.01097500	-0.02966500	2.87364000
Se	1.28585200	2.40680900	2.67963700
Se	-2.76970800	0.04584700	2.72029700
Se	1.42432300	-2.39764700	2.69571600

(CdSe)₁₃

Se	-3.60390500	-1.34766000	-2.74429200
Se	-3.39610600	3.14546100	-0.96286600
Se	-4.12045000	-0.70025600	2.17313100
Cd	-2.51930100	1.15125500	-2.72753500
Cd	-3.23853600	-1.99896300	-0.03288300
Cd	-3.09891400	1.82508800	1.39841100
Cd	-1.17745100	-2.71805500	-2.68402800
Cd	-1.70342100	-0.47667200	3.52120600
Cd	-0.70184400	3.72909100	-1.40369000
Se	-1.42998200	-4.10484100	-0.28862200
Se	-1.39661400	2.27080600	3.58639200
Se	-0.21534000	2.28379400	-3.75502100
Se	1.13560400	-2.23464200	-4.07434500
Se	1.23508100	4.53333300	0.34485800
Se	-0.03720100	-2.59652100	3.99824500
Cd	1.31097900	0.22431700	-2.65851900
Cd	0.82381100	2.18043600	1.92585200
Cd	0.46016900	-2.70756700	1.20367200
Se	0.29856700	-0.00677100	0.07681200
Se	4.04580600	0.75876200	-1.98745500
Se	3.19400600	-3.13996800	0.61971500
Se	3.35532400	1.18418300	2.86370400
Cd	2.44696500	-3.13595200	-1.94116400
Cd	2.98090400	2.97649800	-0.94262200
Cd	1.92653700	-0.75240700	3.97556200
Cd	3.17084600	-0.30735600	0.48071900

(CdSe)₁₆

Se	-4.84473100	1.47272400	1.47272400
Se	-4.84473100	-1.47272400	-1.47272400
Se	-2.92408700	2.92408700	-2.92408700
Se	-1.47272400	-1.47272400	-4.84473100
Se	1.47272400	1.47272400	-4.84473100
Se	2.92408700	-2.92408700	-2.92408700
Se	-1.47272400	-4.84473100	-1.47272400
Se	1.47272400	-4.84473100	1.47272400
Se	-2.92408700	-2.92408700	2.92408700
Se	-1.47272400	1.47272400	4.84473100
Se	-1.47272400	4.84473100	1.47272400
Se	2.92408700	2.92408700	2.92408700
Se	1.47272400	-1.47272400	4.84473100
Se	4.84473100	-1.47272400	1.47272400
Se	4.84473100	1.47272400	-1.47272400

Se	1.47272400	4.84473100	-1.47272400
Cd	-1.23620100	4.23332800	-1.23620100
Cd	1.23620100	4.23332800	1.23620100
Cd	-2.68698600	2.68698600	2.68698600
Cd	1.23620100	1.23620100	4.23332800
Cd	-4.23332800	1.23620100	-1.23620100
Cd	-4.23332800	-1.23620100	1.23620100
Cd	-1.23620100	-1.23620100	4.23332800
Cd	-1.23620100	-4.23332800	1.23620100
Cd	2.68698600	-2.68698600	2.68698600
Cd	4.23332800	1.23620100	1.23620100
Cd	-2.68698600	-2.68698600	-2.68698600
Cd	2.68698600	2.68698600	-2.68698600
Cd	-1.23620100	1.23620100	-4.23332800
Cd	1.23620100	-1.23620100	-4.23332800
Cd	1.23620100	-4.23332800	-1.23620100
Cd	4.23332800	-1.23620100	-1.23620100

(CdSe)₁₉

Cd	-0.06017800	-0.00582500	3.08252500
Se	2.35373800	1.29032900	3.36350800
Se	-0.08769500	-2.73491900	3.35681700
Cd	-4.47047100	0.21096400	2.40685000
Cd	-2.30798800	-3.80092900	2.11890600
Cd	2.19589900	-3.91101000	2.46646800
Cd	4.46243500	0.05177400	2.09345900
Cd	-2.08683900	3.88843000	2.04827800
Cd	2.30654100	3.92254800	2.67847600
Se	0.03903700	5.55772700	2.56380100
Se	-4.72312300	-2.54146100	2.39166600
Se	4.65680200	-2.69428700	2.19559500
Se	-2.33779100	1.51159900	3.43915300
Se	-3.95300000	4.72998900	0.23873200
Se	-6.58466800	0.73148600	0.67405600
Cd	-5.26083100	2.52034800	-0.88330700
Se	-2.19047800	-5.79690500	0.25289700
Se	2.75883100	-6.02164100	0.70441200
Se	6.19715700	1.02122300	0.19169500
Cd	0.44884900	-5.72838200	-0.69157700
Cd	4.86014800	3.23242300	-0.78477800
Cd	4.19786500	-3.85802700	-0.32421900
Cd	1.10744600	5.57296700	0.00633900
Cd	-5.29578900	-1.63305000	-0.18334100
Se	3.80774800	5.24673700	0.69744200

Se	3.99031300	-2.54985200	-2.72501200
Cd	4.86311900	-0.07444300	-1.97944500
Se	-4.24956500	-2.29789100	-2.58538000
Cd	-2.51237700	-4.31171200	-2.05892400
Se	0.22952700	4.73399300	-2.44587000
Cd	-2.37085000	4.10647800	-1.95403600
Cd	1.21640000	-2.38163000	-2.85489000
Se	-0.07029600	-4.77990900	-3.26437400
Se	4.08240700	2.28851300	-3.28869200
Cd	1.42746900	2.24598300	-2.64443900
Se	-3.96828300	2.32958600	-3.33731400
Cd	-2.65406100	-0.04199400	-2.96263200
Se	-0.02744300	-0.06255900	-1.99618500

Cartesian coordinates of CdSe-cys clusters in alkaline solution

(CdSe) ₁			
C	2.54418000	1.14398000	0.37137600
C	2.46761500	-0.31959100	0.80832900
C	2.89086500	-1.30946300	-0.30703600
O	3.96905200	-1.05386600	-0.89871500
O	2.14764000	-2.31158300	-0.48876100
N	1.14245300	-0.67458300	1.32248800
S	1.34896000	1.62899000	-0.93257500
H	2.39552800	1.78291200	1.24991700
H	3.55488100	1.32401600	-0.00296700
H	3.22323400	-0.44544300	1.60091900
H	1.08991400	-0.54913900	2.32804200
H	1.00473700	-1.66292200	1.11035200
Cd	-0.68907300	0.46963700	0.19114800
Se	-3.23478700	0.25430200	0.50529800

(CdSe) ₂			
Cd	-2.71601800	0.41987800	-0.05712400
Se	-1.82304300	-2.07585900	-0.33331000
Se	-0.83483200	2.28218900	0.24252200
Cd	0.34710700	-0.33777200	0.19067800
C	3.43827700	-1.50937500	0.32338100
C	3.44922200	-0.58364200	-0.89487600
C	4.09504900	0.79693600	-0.60897100
O	5.20143700	0.78169000	-0.01393900
O	3.48596900	1.81043900	-1.04615300
N	2.11193000	-0.40849200	-1.47136400
S	2.38598200	-0.95788700	1.72367800
H	3.11345000	-2.50637300	0.00162000
H	4.46796300	-1.59618300	0.67906900
H	4.11605400	-1.05616100	-1.63492100
H	1.92765200	-1.09456600	-2.19575400
H	2.09659500	0.52207900	-1.88957900

(CdSe) ₃			
C	-3.98038700	1.23747000	1.45353200
C	-4.57286200	0.71956300	0.14141900
C	-5.23034900	-0.67738200	0.27173300
O	-6.01445200	-0.83697500	1.24060700
O	-4.97045100	-1.51471800	-0.63455400
N	-3.58888200	0.71561500	-0.94434500
S	-2.56907500	0.27117000	2.11600700
H	-3.66184100	2.27674700	1.30527200
H	-4.78037700	1.23880600	2.19852300
H	-5.40534300	1.39928600	-0.10785100
H	-3.56709000	1.60894900	-1.42537300
H	-3.87818600	-0.00711300	-1.60191700
Cd	-1.31140100	0.14197200	-0.21171800
Cd	2.16171100	1.49361600	0.04812600
Cd	1.94275900	-1.68960900	0.06869600
Se	4.03861900	-0.22802800	0.80602600
Se	-0.02445300	2.50325700	-0.99080500
Se	-0.36611400	-2.33805300	-0.96545200

(CdSe) ₄			
Cd	-3.05807000	-0.65359700	-0.33298900

Cd	3.12434700	-0.91358900	-2.01297100
Cd	0.57356200	1.47454200	-1.18766600
Cd	0.62603600	-3.17537700	-0.67675700
Se	-1.75519400	1.74383900	-0.02797800
Se	2.93499200	1.67952000	-2.35530100
Se	-1.85045800	-3.08762000	0.14482500
Se	3.10235400	-3.50213400	-1.51484800
C	-6.15783200	-1.65267500	-0.66821100
C	-6.19930700	-1.04793100	0.73792200
C	-6.94180200	0.31130900	0.78538600
O	-8.07921500	0.34115900	0.25206300
O	-6.36812900	1.25493500	1.39399400
N	-4.86314200	-0.92116800	1.32603200
S	-5.17628200	-0.70316700	-1.89643000
H	-5.75129600	-2.66915000	-0.59788000
H	-7.18767200	-1.72856000	-1.02650500
H	-6.81430100	-1.72925600	1.34824300
H	-4.63804900	-1.71656000	1.91409200
H	-4.87759800	-0.07934500	1.90215700

(CdSe)₅

Cd	3.62943300	-0.18920000	-0.04309600
Cd	0.99883400	-1.91571100	-0.07950700
Cd	0.36322700	1.31807200	1.77951500
Se	0.21076900	-1.28916900	2.47267500
Se	3.59038400	-2.77534700	-0.56787000
Se	2.79155700	2.28735200	0.33326000
Se	-0.25747600	-0.65236400	-2.23025800
Se	-1.50222700	2.78376300	0.28011400
Cd	-2.52166600	0.43119700	-0.77988600
Cd	0.62167600	1.79876500	-1.37215500
C	-4.46876500	-2.12351900	-0.88727400
C	-4.35967400	-1.91670000	0.62766000
C	-5.68912000	-1.39757100	1.23618800
O	-6.72343900	-2.05394000	0.95602900
O	-5.61804000	-0.38600200	1.98593000
N	-3.24987000	-1.03415900	0.99368400
S	-4.68659800	-0.58007800	-1.85905300
H	-3.56838800	-2.64191500	-1.23935400
H	-5.32526200	-2.77614000	-1.07449200
H	-4.20491900	-2.91413700	1.06769700
H	-2.44211000	-1.52560100	1.37541900
H	-3.61109700	-0.41669000	1.72332500

(CdSe)₆

Cd	2.10990500	1.50390100	-1.46640200
Cd	-2.16893500	0.71629600	-0.48003600
Cd	1.08833100	-2.16655300	-1.17002600
Se	-0.37800300	2.72059000	-1.44663600
Se	3.20600000	-0.87197100	-2.33894800
Se	-1.63767600	-1.99639300	-1.14787400
Se	3.28610900	2.01473000	1.25794200
Se	-1.58392000	0.91582300	2.42576000
Se	1.90018200	-2.77480500	1.68976600
Cd	0.52143500	2.19667300	1.21189800
Cd	3.27310200	-0.64988000	0.62394900
Cd	-0.50412700	-1.43032500	1.49528700
C	-5.37399300	-0.32655400	-1.62093100

C	-6.00096600	-1.12888300	-0.46570200
C	-7.21709500	-0.38887200	0.13482400
O	-8.20488300	-0.24086600	-0.63657800
O	-7.13923700	0.00870600	1.32750000
N	-5.06514800	-1.53771400	0.57235800
S	-4.64062000	1.30294300	-1.19349500
H	-4.59553500	-0.94762800	-2.08047200
H	-6.14926600	-0.15560200	-2.37492900
H	-6.40981100	-2.03456300	-0.94087800
H	-4.99025100	-0.77172800	1.23649600
H	-4.14161600	-1.68692100	0.16827600

(CdSe)₇

Se	-1.90023000	3.51274400	0.48770700
Se	-1.87880500	-0.35321600	-2.49205000
Cd	-0.80984300	2.03461200	-1.48545600
Cd	-3.31305300	-1.01440100	-0.18930200
Se	5.80786400	0.38763100	0.11530500
Se	1.86791300	1.56856300	-2.21783300
Cd	0.78273300	-1.45646600	1.57738200
Cd	3.18545900	1.25289300	0.16587600
Cd	-0.81295000	1.53248900	1.95661700
Cd	4.26036300	-1.72072400	-0.15196900
Cd	0.76907400	-0.96407000	-1.96612800
Se	1.89006500	-2.98603900	-0.45008800
Se	1.85961000	0.92465700	2.56386900
Se	-1.87730300	-1.04480900	2.22474000
C	-6.19091100	-1.73045700	1.08675400
C	-6.41859200	-0.26795800	0.69132400
C	-7.38393900	-0.12584600	-0.51343400
O	-8.47489000	-0.74260300	-0.42766900
O	-7.01261400	0.62711100	-1.45453900
N	-5.16471100	0.44860500	0.42515000
H	-5.64278100	-1.75759300	2.03655300
H	-7.17017500	-2.18581200	1.25388200
H	-6.94153400	0.20303300	1.53834400
H	-5.35511500	1.05679600	-0.37324400
H	-4.89653900	1.03218900	1.21074700
S	-5.28134700	-2.73128500	-0.15551000

(CdSe)₈

Se	-4.92513600	0.13800200	0.69809100
Cd	-3.21894700	-1.95790600	1.25417300
Se	-0.74942400	-2.22804900	2.43983100
Cd	0.25958300	0.28594200	2.57673500
Se	-1.02571800	2.69885100	2.11573500
Cd	-2.76896000	1.81653000	0.22898400
Se	-2.37976900	1.53004000	-2.54763100
Cd	-3.51560700	-0.81211200	-1.73121500
Se	-2.65588400	-3.38037100	-1.18239900
Cd	-0.19288800	-2.39285200	-0.32095100
Se	1.58203600	-1.06246500	-1.89223100
Cd	0.36660100	1.44102700	-2.22469100
Se	2.88442100	1.06090800	2.25018900
Cd	1.40677700	2.90847000	0.73502000
Se	1.82010200	3.69803200	-1.78873500
Cd	3.57014900	-0.41929600	-0.04085600
C	6.72231000	-1.11170600	0.47478700

C	6.13491400	-2.52291800	0.38786000
C	6.50355100	-3.24800900	-0.93166100
O	7.71945500	-3.24620500	-1.24676400
O	5.56295300	-3.81695200	-1.55006300
N	4.68155000	-2.53703700	0.58649600
S	6.05123200	0.08876900	-0.74175900
H	6.55448900	-0.72531400	1.48765300
H	7.80197200	-1.19270300	0.32458100
H	6.62368600	-3.10948200	1.18226600
H	4.31797400	-3.25394600	-0.04348900
H	4.44408700	-2.79724500	1.53788100

(CdSe)₉

Se	2.61999700	-1.23133200	1.93257700
Cd	3.40984700	-0.09582400	-0.43293400
Se	2.07081600	2.27138300	-1.25550000
Se	0.56518800	-3.75102000	-1.67767400
Cd	-1.71080600	-2.37251500	-2.09714400
Cd	-0.56930200	1.85927700	-2.00573600
Se	-2.09548500	0.08468800	-3.42142200
Cd	-4.17598000	-0.06795600	-1.63604000
Se	-4.75256500	0.79050000	0.93626500
Cd	-2.57791900	2.38697500	1.41584600
Cd	-3.44596300	-1.66472300	1.17319900
Se	-0.46846900	2.54245400	3.22852500
Cd	0.30131600	-0.03405400	2.81088100
Se	-1.77703800	4.01779000	-0.71298200
Se	-4.28468000	-2.89524200	-1.17364500
Cd	0.67170800	-2.97550900	0.88894800
Cd	0.56527700	3.36929500	0.76903200
Se	-1.33431900	-2.32266900	2.73332900
C	5.73145000	-0.00840600	-2.75054700
C	6.52745200	0.36008600	-1.49682000
C	7.41851100	-0.79825600	-0.97999800
O	8.13987200	-1.36994100	-1.83500500
O	7.38373300	-1.03334100	0.25848700
N	5.66664600	0.85916200	-0.41975200
S	4.45468100	-1.30635900	-2.51429000
H	5.25065900	0.89817700	-3.13803600
H	6.44233000	-0.35563300	-3.50465500
H	7.23600800	1.14704600	-1.80272700
H	5.60158100	1.87148400	-0.43810700
H	6.10616800	0.57388400	0.45570900

(CdSe)₁₀

Cd	-0.27965900	3.28835200	0.94851900
Se	2.02441900	3.93613300	-0.53361100
Cd	2.11138100	2.11932900	-2.60423100
Se	0.07501700	0.19316500	-2.67862200
Cd	-2.28731000	1.26664300	-1.87552800
Se	-2.71554600	3.51218100	-0.20515000
Se	4.92548900	0.13407400	1.19848700
Cd	3.09768400	-1.84521600	1.23278600
Se	2.45584300	-3.66180200	-0.78628100
Cd	0.27155400	-2.43750300	-1.96151400
Se	-4.59338000	-0.18227700	-1.30838300
Cd	-3.17190400	-1.95376500	0.27892500
Se	-1.75181500	-4.00702600	-0.81542800

Cd	2.97488900	2.01094900	1.21480500
Cd	0.29166600	-4.00995400	1.03911300
Cd	-3.93236600	1.33749400	1.00292800
Cd	-0.23226100	-0.41009200	2.86345800
Se	0.92735900	2.05295900	3.10361100
Se	-2.99449400	-0.60494900	2.72292700
Se	1.27749700	-2.68780800	3.20960800
C	4.05404200	1.77924600	-5.30223200
C	3.11479800	2.94459700	-5.61825900
C	3.73278300	4.34364300	-5.36717700
O	4.90163200	4.52419800	-5.79073700
O	2.98674600	5.20017900	-4.82024200
N	1.83640100	2.82922200	-4.91405000
S	4.48418900	1.54178400	-3.53217100
H	3.60229100	0.85553000	-5.68357700
H	4.97913200	1.94768700	-5.85931600
H	2.94710700	2.90913700	-6.70841200
H	1.20051500	2.20157100	-5.39599000
H	1.42541100	3.76082800	-4.88559200

(CdSe)₁₃

Se	-3.35948100	-3.61450700	1.12372200
Se	-0.58626400	-3.66005200	-3.02287200
Se	-4.48229800	-0.53594300	-2.50250200
Cd	-1.00628800	-3.86749200	-0.23410300
Cd	-4.17712200	-1.11217400	0.14455900
Cd	-1.89934500	-1.28457900	-3.30712300
Cd	-2.43602600	-1.80959100	3.02574200
Cd	-3.07063700	1.87824300	-2.61207200
Cd	1.76758500	-2.65211900	-1.91502300
Se	-4.13877700	0.35798900	2.49379000
Se	-0.89368300	1.17472900	-4.19787400
Se	1.65034300	-3.86204900	0.59030800
Se	-0.05450300	-1.59064600	4.37727800
Se	3.30116700	-0.55380200	-2.67304400
Se	-3.14948600	3.84270000	-0.68209300
Cd	1.34608000	-1.42065100	1.88674800
Cd	1.07497800	1.10961600	-2.22898700
Cd	-2.20092300	2.06410400	1.36142500
Se	-0.37712800	0.17033400	0.12222100
Se	3.38337400	0.50159200	2.07054500
Se	-0.31719300	3.43830600	3.00814300
Se	2.01859700	3.68153600	-1.27153100
Cd	-0.06452600	1.07044400	4.18111600
Cd	4.67601800	-0.29646200	-0.26571100
Cd	-0.57527400	4.30164100	-1.21015200
Cd	1.43840400	2.24192400	1.08791600
C	7.84096200	-0.89943100	-0.97640400
C	7.84531000	0.61550500	-0.76067800
C	8.47819200	1.03101300	0.59157600
O	9.58793600	0.51229500	0.86948300
O	7.85582800	1.89168100	1.27120500
N	6.50963600	1.20537700	-0.89944300
H	7.53444700	-1.10686600	-2.00879500
H	8.86903600	-1.25152900	-0.85793900
H	8.51802800	1.03347800	-1.52735100
H	6.47697600	1.99569200	-0.25449300
H	6.35699400	1.55129600	-1.84110200

S	6.76513000	-1.84416200	0.17056700
(CdSe) ₁₆			
Se	1.48317000	3.88343500	2.59719500
Se	0.04585100	0.83136600	4.98353900
Se	-3.44430100	3.16827400	2.28605600
Se	-3.76556100	-1.73435500	3.65926100
Se	-5.53326100	-0.70734400	0.09140200
Se	-2.57031900	-4.81846900	-0.18721300
Se	0.44961600	-3.78951700	3.71878400
Se	2.44869800	-4.63245100	0.18440200
Se	4.03558600	-0.53185700	2.53523400
Se	3.75525200	3.69710200	-1.62745200
Se	-0.66706300	5.27761300	-1.37034900
Se	0.58435400	1.63511400	-4.60007500
Se	3.99873200	-0.87307900	-2.38490700
Se	0.34127800	-3.28551100	-3.87783100
Se	-3.34946500	-1.48016500	-3.93718100
Se	-3.84467900	2.95756800	-2.62535400
Cd	-2.84094300	3.98623500	-0.25724300
Cd	-1.12597600	3.27970100	-3.24712400
Cd	1.54446300	4.18001600	-0.13591300
Cd	2.66562400	1.50041500	-2.76048000
Cd	-1.00337900	2.89499100	3.44867200
Cd	2.23262600	1.32624000	3.32434300
Cd	5.30999500	-0.53630600	0.03250600
Cd	2.57138200	-2.79090200	2.24851700
Cd	2.27251200	-2.96418200	-1.96011300
Cd	-0.71258800	-0.75356300	-4.33235400
Cd	-1.05790600	-1.54623200	4.20060900
Cd	-4.24002500	0.31436400	-2.07260200
Cd	-4.28548800	0.55825700	2.22916900
Cd	-3.81569500	-2.69467400	1.04195000
Cd	-0.18843100	-4.60674500	1.14918300
Cd	-2.09358300	-3.51256200	-2.55379900
C	8.23285800	-0.31628300	-1.28014800
C	8.08455100	1.10038100	-0.71282500
C	9.04504700	1.35387700	0.47839900
O	10.25622400	1.08164000	0.28465800
O	8.53977600	1.84512000	1.52426700
N	6.70325100	1.41845800	-0.33169000
H	7.66240200	-0.38148200	-2.21490200
H	9.28768500	-0.46964400	-1.52173700
H	8.41662800	1.78672000	-1.50711700
H	6.77045900	1.90848100	0.56287300
H	6.24641100	2.04393700	-0.99228000
S	7.68417000	-1.66077600	-0.15547300
(CdSe) ₁₉			
Cd	0.14435400	1.06715300	4.39780700
Se	1.86035100	0.94585700	2.19409700
Se	0.08702700	-3.97273300	3.97297500
Cd	-4.21647800	0.02895700	2.62653800
Cd	-1.88498700	-4.04350400	2.09944600
Cd	2.35807600	-4.37318300	2.59536100
Cd	4.27373800	-0.37483900	1.89724200
Cd	-2.23012200	4.12848000	2.07982600
Cd	2.20891500	3.63242000	2.24050000

Se	0.11987100	5.49468400	2.40983800
Se	-4.28190200	-2.72798600	2.46147600
Se	4.78516800	-3.00268500	2.37949700
Se	-2.43552600	1.82129800	3.55508200
Se	-4.04001900	4.82066600	0.15579800
Se	-6.36956300	0.54117400	0.91114200
Cd	-5.07233200	2.33579600	-0.64222800
Se	-1.99707000	-5.87327600	0.03605200
Se	2.80820200	-6.09424300	0.38521400
Se	6.09518500	0.93257500	0.29348500
Cd	0.53687000	-5.67297300	-1.02068400
Cd	4.82585200	3.24020400	-0.58441700
Cd	4.26347300	-3.79563900	-0.23245600
Cd	1.16747700	5.49673500	-0.18558800
Cd	-5.13062700	-1.80960500	-0.02196200
Se	3.82096500	5.37766800	0.74320300
Se	4.01972500	-2.48062600	-2.62966500
Cd	4.84761600	0.04393600	-2.03336900
Se	-4.28240300	-2.35558600	-2.55776700
Cd	-2.38271600	-4.28227600	-2.23929600
Se	0.10704300	4.84493600	-2.58874900
Cd	-2.45136400	4.10882200	-1.99228500
Cd	1.33119100	-2.38747600	-3.28206400
Se	-0.01114300	-4.76172500	-3.58328700
Se	4.08308000	2.44369800	-3.15221700
Cd	1.36846800	2.41101400	-2.86242500
Se	-4.09703100	2.30169300	-3.26917000
Cd	-2.75942900	-0.08835300	-2.98814100
Se	-0.00486800	0.01872600	-3.07767600
C	-0.07675200	0.99751200	7.68201700
C	0.29163000	-0.43365600	7.28112000
C	1.80483400	-0.72366200	7.42069000
O	2.30789600	-0.45681800	8.54282300
O	2.39102100	-1.23924600	6.43348500
N	-0.19022100	-0.75569400	5.93503200
H	-1.16967700	1.09282300	7.67702700
H	0.26416200	1.14826300	8.70924000
H	-0.19575700	-1.09164700	8.01967900
H	0.29189300	-1.58207900	5.57872600
H	-1.18151400	-0.97828100	5.96060300
S	0.64338600	2.32524100	6.63630900

Cartesian coordinates of CdSe-cys clusters in gas

(CdSe)₁

C	-2.80673800	-1.09006100	0.51717700
C	-2.50546300	0.36441800	0.86748100
C	-2.59481300	1.24907800	-0.36983700
O	-3.16741300	0.93738600	-1.38639700
O	-1.99282700	2.42560300	-0.17583200
N	-1.19781900	0.50647800	1.50457800
S	-1.58017500	-1.89410100	-0.56430600
H	-2.82774000	-1.69259400	1.43011700
H	-3.78854800	-1.16232100	0.04573000
H	-3.32050800	0.71020400	1.52696600
H	-1.20152800	0.09385600	2.43363800
H	-0.95065700	1.48775400	1.61224100
H	-2.05750500	2.94805100	-0.99063300
Se	3.03284500	0.34535300	-0.19912000
Cd	0.73638600	-0.33674300	0.15232800
H	-1.92526100	-1.24752400	-1.69397400

(CdSe)₂

Cd	-0.65625300	-1.42588600	-0.77009400
Se	0.30117100	1.08061600	-1.26002000
Se	1.41995900	-3.07324700	-0.59960400
Cd	2.21559200	-0.64412200	-1.00962700
C	-4.14583400	-1.12946700	-0.10997800
C	-3.27254200	-0.57069900	1.01000900
C	-2.82145600	0.85375000	0.68338300
O	-3.36619600	1.54786700	-0.14113200
O	-1.76266300	1.20309800	1.41032200
N	-2.08925500	-1.40422200	1.23049000
S	-3.31408300	-1.32761200	-1.72377100
H	-4.50318000	-2.12843500	0.15727500
H	-5.01600400	-0.48667300	-0.25383000
H	-3.21579500	-0.01229900	-2.00131200
H	-3.90493500	-0.50759300	1.91148500
H	-2.34292800	-2.32821000	1.56922100
H	-1.48399400	-0.97409700	1.92556200
H	-1.25366800	1.88951400	0.93361700

(CdSe)₃

C	4.63237700	1.13600100	-0.44515700
C	4.29123400	0.49945900	0.89933800
C	4.36027300	-1.02141600	0.81776900
O	4.91694100	-1.62798900	-0.06563500
O	3.75303800	-1.59165800	1.86036600
N	2.97236000	0.90798100	1.37909000
S	3.45909300	0.79688900	-1.79882500
H	4.64842800	2.22528500	-0.34347100
H	5.62652800	0.81346800	-0.76032500
H	3.73742500	-0.51619400	-1.91294600
H	5.09027600	0.79597500	1.60117000
H	2.94057000	1.90530800	1.57621000
H	2.74299400	0.41562100	2.23846800
H	3.68728700	-2.54587300	1.69674600
Cd	-2.33976700	1.38991200	0.19599200
Cd	-1.65515000	-1.84885200	-0.10495400
Cd	1.11113700	0.46879900	-0.19287600

Se	0.84686200	-2.15042700	-0.36418400
Se	-3.89852200	-0.64806100	0.20003900
Se	-0.19145700	2.72922600	0.10476500
(CdSe) ₄			
Se	0.70324400	2.45248700	-0.60528200
Se	0.77949800	-1.58883500	-2.15344900
Se	-0.55325900	-0.85496000	1.92079000
Cd	2.37505400	0.47625700	-1.42974200
Cd	1.39321200	1.03899800	1.61781500
Cd	-0.92462000	0.20878800	-0.64698800
Cd	1.43242800	-1.98896200	0.44081300
Se	3.60613500	-0.37738700	0.87164400
C	-4.55217300	0.56745900	-1.05416200
C	-4.05257500	-0.86090000	-1.26119800
C	-4.04651200	-1.61454100	0.06391000
O	-4.75435600	-1.32860300	0.99938900
O	-3.19252500	-2.64003200	0.05005900
N	-2.72633900	-0.88162400	-1.87343200
S	-3.45178600	1.61733200	-0.05140200
H	-4.63774900	1.07281600	-2.02088400
H	-5.54231300	0.54715300	-0.59561400
H	-3.68734100	1.00090200	1.12268800
H	-4.79838400	-1.37727200	-1.88967600
H	-2.76000800	-0.54319500	-2.83142800
H	-2.33992100	-1.82328700	-1.90978200
H	-3.14487300	-3.00929200	0.94625200
(CdSe) ₅			
Cd	2.13607400	2.47890300	1.14080100
Cd	1.38491700	0.83934000	-1.76011400
Cd	1.04776300	-0.89469200	1.73128500
Se	2.48676000	-1.37643200	-0.55267000
Se	2.17950800	3.30476100	-1.28697900
Se	1.19234400	1.28412700	3.19257500
Se	-1.08883400	-0.09668200	-2.44889900
Se	-1.29358400	-2.27296300	1.25828900
Cd	0.00680100	-2.21883000	-1.13431300
Cd	-2.13289000	-0.03586100	0.04482000
C	-4.23686400	2.68878900	0.79536100
C	-2.78260200	2.95869200	1.16628200
C	-2.00604300	3.54156500	-0.01587100
O	-2.52956800	3.93711500	-1.03140200
O	-0.70634600	3.55403600	0.24529000
N	-2.11112500	1.74782100	1.64879600
S	-4.50077700	1.36145900	-0.43134700
H	-4.79937900	2.37861700	1.68109900
H	-4.69434800	3.60050600	0.40697700
H	-2.78985000	3.74135500	1.94263900
H	-2.55639100	1.41484500	2.50220500
H	-1.13748100	1.93489000	1.92193500
H	-0.13705000	3.79382400	-0.53091100
H	-3.97677700	2.02180800	-1.48338800
(Cdse) ₆			
Cd	0.95488900	1.93580400	-1.51915000
Cd	-1.97853400	-0.48627200	0.10907300
Cd	1.61000200	-1.94494300	-1.26938500

Se	-1.53358500	2.09311700	-0.61540700
Se	2.66931700	0.15913500	-2.52047600
Se	-0.69111600	-2.82905700	-0.29756900
Se	2.37236400	2.84369400	0.73767100
Se	-0.99397500	-0.13317800	2.98906500
Se	3.21679800	-2.05502000	1.04388300
Cd	0.05524000	1.89644000	1.67698700
Cd	3.39822800	0.45323900	0.19458100
Cd	0.69329400	-1.85429200	1.91384600
C	-5.46388700	-1.12797000	-0.76260800
C	-5.31075900	-0.38994400	0.56592600
C	-5.35280300	1.11703600	0.34496000
O	-5.91263600	1.64261500	-0.58697400
O	-4.73193200	1.78289900	1.32163600
N	-4.08749700	-0.78126000	1.26312500
S	-4.09140300	-0.88154300	-1.93454300
H	-5.50461400	-2.20646200	-0.58293200
H	-6.39859800	-0.82983300	-1.24069600
H	-4.36024100	0.40936200	-2.20766200
H	-6.20788400	-0.61922100	1.16654400
H	-4.14260000	-1.74838700	1.57236600
H	-3.92564700	-0.21433900	2.09406900
H	-4.72803200	2.72557900	1.09285000

(CdSe)₇

C	5.14854600	0.35482100	2.07080300
C	5.05057600	-0.30950100	0.69779300
C	6.11295300	0.23577700	-0.24568500
O	7.10718100	0.82268600	0.11145100
O	5.83967600	-0.04823800	-1.52431300
N	3.71456500	-0.18912200	0.11940500
S	4.75809000	2.13253000	2.09115500
H	4.41830800	-0.09782500	2.74832600
H	6.14696600	0.20753000	2.48669900
H	5.32527800	-1.36929100	0.83760600
H	3.09864300	-0.92340500	0.46781700
H	3.74486500	-0.30553500	-0.89124400
H	6.55308400	0.31115600	-2.07371200
Se	0.78691800	-2.63696300	-0.39795500
Se	-2.92968300	-1.68631800	1.51382100
Cd	-0.27663400	-1.20336700	1.69257300
Cd	-1.91438300	-2.80992800	-0.72694800
Se	1.33980600	4.41018900	0.78251000
Se	1.07168900	0.76259600	2.76786800
Cd	-0.47314700	2.80705200	1.98665200
Cd	2.42255100	1.87581800	0.50674500
Cd	0.15608800	-0.57309800	-2.10276500
Cd	-0.15676700	3.32061100	-1.18421500
Cd	-2.97472800	0.33418300	-0.32428500
Se	-2.49428200	2.88586300	0.15287800
Se	1.60540400	1.60452800	-2.22976400
Se	-2.45972100	-0.99505600	-2.65397100
H	5.79577600	2.52512800	1.32693800

(CdSe)₈

Se	-4.19806200	-0.00831100	0.89477600
Cd	-2.43172200	-1.58926600	2.09211600
Se	0.05497800	-1.39901800	3.06502100

Cd	0.79219200	1.08361800	2.50816500
Se	-0.68287400	3.14791800	1.44263200
Cd	-2.31408400	1.69111900	-0.02008400
Se	-1.93349800	0.64900900	-2.53245000
Cd	-2.93448900	-1.40946300	-1.15199800
Se	-1.98940500	-3.52922900	0.14487300
Cd	0.42026300	-2.38750500	0.51517500
Se	2.16240500	-1.66058100	-1.30459700
Cd	0.70176300	0.38841000	-2.34986100
Se	3.24355100	1.94736700	1.89623800
Cd	1.62087700	3.19202500	0.05529100
Se	2.52041100	2.34013700	-2.27414800
Cd	3.65224100	0.49737500	-0.39849700
C	7.20851000	-0.24268200	-0.46016900
C	6.45441200	-1.40024100	0.18659600
C	6.06565200	-2.45174300	-0.84514200
O	6.44360600	-2.46175200	-1.99259400
O	5.27038000	-3.38171600	-0.30969500
N	5.25725100	-0.93940000	0.88478300
S	6.22321100	0.79944300	-1.58328000
H	7.56921300	0.43767700	0.31708100
H	8.07668700	-0.62225500	-1.00247800
H	7.16099500	-1.90156100	0.87061600
H	5.49076400	-0.36055400	1.68860700
H	4.71212800	-1.72852800	1.22178600
H	6.09525300	-0.11630600	-2.56246000
H	4.96288100	-3.96639200	-1.02002000

(CdSe)₉

Se	-1.35127300	3.57783400	0.37797900
Cd	-0.99613400	1.96034300	-1.76431300
Se	-2.47937200	-0.11780900	-2.30109200
Se	1.54976400	2.67466200	-2.46214300
Cd	2.75002900	0.33783500	-2.15686300
Cd	-0.67417600	-2.10421000	-1.93831100
Se	1.85569400	-2.18399600	-2.73127100
Cd	3.02172000	-2.45999200	-0.33663800
Se	2.29649800	-2.43663900	2.24094100
Cd	-0.33437600	-2.29780000	1.92492500
Cd	3.10541500	0.13604000	1.77823900
Se	-2.01535300	-0.36735400	2.81206300
Cd	-0.61818500	1.76305200	2.25288800
Se	-1.86526100	-3.41106700	0.05155400
Se	4.66740100	-0.26054900	-0.37190600
Cd	1.38231400	3.38654000	0.11387500
Cd	-3.13506500	-0.90973800	0.29948600
Se	2.01768000	2.42616500	2.53207900
C	-6.59936800	-0.20901400	0.93765400
C	-5.95270100	1.01936300	0.30427100
C	-6.10458600	1.00231700	-1.21123300
O	-6.78871300	0.21491300	-1.82238600
O	-5.41387500	1.99178100	-1.78017000
N	-4.54176000	1.13201900	0.66569100
S	-5.80066800	-1.80326000	0.55921700
H	-6.56006700	-0.12227100	2.02762100
H	-7.64884800	-0.26981500	0.64311600
H	-6.53101200	1.89511700	0.64670000
H	-4.43845600	1.31126200	1.66212700

H	-4.09735600	1.90941500	0.17855000
H	-5.46837300	1.88408600	-2.74251700
H	-6.14267700	-1.83101800	-0.74340000

(CdSe)₁₀

Cd	-0.08186000	4.16476400	-1.06358400
Se	0.95767700	4.79227900	-3.43375700
Cd	0.46023800	2.48260700	-4.85818000
Se	-2.00547800	1.33535900	-4.23160300
Cd	-3.27626600	2.15797400	-2.05004700
Se	-2.60468700	4.18906300	-0.33184700
Se	3.17372600	1.49644800	-4.45393100
Cd	2.45237900	-0.73554100	-3.31266500
Se	0.77121100	-2.42731300	-4.58360000
Cd	-1.51681900	-1.22309300	-3.80394900
Se	-4.64729400	0.66079600	-0.28253000
Cd	-2.72465000	-1.18178700	-0.04753300
Se	-2.25303100	-3.01889800	-1.87363500
Cd	2.78964800	3.08856600	-2.37848000
Cd	0.41365000	-3.02943100	-1.90569500
Cd	-2.69753200	1.97360900	1.15853600
Cd	1.12133500	0.39202600	0.43154100
Se	2.01073500	2.89125300	0.16924000
Se	-1.11057200	-0.06881300	1.84221200
Se	2.39170900	-1.66134600	-0.76030100
C	0.77002700	2.81262300	-8.44772300
C	0.21706700	1.42917500	-8.11999800
C	-1.30482100	1.42743500	-8.16762900
O	-1.97649800	2.33865700	-8.58468900
O	-1.80532300	0.26841100	-7.72357900
N	0.67877600	0.94833800	-6.82030200
S	0.29954100	4.08152900	-7.21211300
H	1.85996500	2.76562200	-8.50551800
H	0.38281300	3.13154900	-9.41692700
H	0.53830500	0.75804500	-8.93477500
H	1.68750300	0.80500900	-6.82601700
H	0.26160900	0.04552300	-6.59749100
H	-2.77165200	0.34783300	-7.71459000
H	1.54070800	4.51003600	-6.92157700

(CdSe)₁₃

Se	-4.80422100	-1.26293500	-1.32347400
Se	-3.32347800	3.29476700	-0.53063600
Se	-3.46389400	0.18654100	3.02176100
Cd	-3.65498000	1.01826400	-2.00082500
Cd	-3.54270400	-1.60101700	1.06536500
Cd	-2.10659300	1.86937800	1.32437600
Cd	-2.66429100	-2.78123200	-1.87548800
Cd	-0.93919700	-0.18047800	3.62006300
Cd	-1.27501300	3.33117700	-2.27678600
Se	-2.09195600	-3.83076000	0.55998200
Se	0.23475500	2.32072600	2.85228500
Se	-2.12458400	1.63764700	-4.17261200
Se	-1.08226400	-2.85882300	-4.02537800
Se	1.19423900	4.16073400	-1.71169400
Se	1.07074500	-1.89066100	3.54785500
Cd	-0.35735600	-0.21204600	-3.42876000
Cd	1.21181000	2.33515700	0.26249500

Cd	0.23353200	-2.57319700	1.01109100
Se	-0.36268700	-0.03670900	-0.46563800
Se	2.37253000	-0.14261600	-3.73129200
Se	2.45038300	-3.36895600	-0.46203200
Se	3.70799700	1.12098700	0.54412900
Cd	0.85602800	-3.46397600	-2.46146600
Cd	2.61662700	2.40233600	-3.14570100
Cd	2.20085100	0.28492200	2.55590900
Cd	2.60806600	-0.72744000	-1.08505600
C	4.57643400	5.08251400	-3.53423900
C	5.52245500	4.08679700	-2.84689500
C	6.65261000	3.65021200	-3.76808800
O	7.25088100	4.69032600	-4.35803900
O	6.97789100	2.49950600	-3.93869900
N	4.84808400	2.89942900	-2.33151700
H	3.83782100	5.44335200	-2.81078800
H	5.14039500	5.93845000	-3.90930000
H	6.00632000	4.64846600	-2.03362400
H	5.42504500	2.08180300	-2.53584600
H	4.73979600	2.93133200	-1.31825300
S	3.56559100	4.39187500	-4.88606600
H	4.56350100	3.86283900	-5.62123600
H	7.98029000	4.34737200	-4.89745400

(CdSe)₁₆

Se	-4.98313300	2.10477300	0.57387200
Se	-4.90282300	-0.71846500	-2.25342100
Se	-2.22739600	3.21441000	-3.28477700
Se	-1.12514000	-1.27372800	-4.81721300
Se	2.04322500	1.08596100	-4.25685200
Se	2.46431800	-3.34015900	-2.24615000
Se	-2.24235400	-4.41582900	-1.68470900
Se	-0.08049200	-4.90962400	1.62237000
Se	-4.21503400	-2.39404600	2.27361200
Se	-2.41216500	1.60625700	4.35138500
Se	-1.34161900	4.80488200	1.23119100
Se	2.29328700	2.44177400	3.44299900
Se	-0.06650600	-1.61937700	4.70353600
Se	3.71057400	-2.08253500	2.31490800
Se	4.56984400	0.64549900	-0.46416600
Se	1.92887500	4.35597400	-1.02551500
Cd	-0.73999500	4.22380300	-1.32221400
Cd	1.17308400	3.89329900	1.51594200
Cd	-2.93646400	2.86083100	2.08258900
Cd	0.20978500	0.99632400	4.26717500
Cd	-4.01254400	1.79404400	-1.91235700
Cd	-4.84208600	-0.57949800	0.43485000
Cd	-2.50797700	-1.03366700	3.80289900
Cd	-2.46933700	-3.90801600	0.95263900
Cd	1.45450300	-3.34154300	3.18013700
Cd	3.54865400	0.57481100	2.02313100
Cd	-2.78613500	-2.15718100	-2.94726500
Cd	2.88021800	2.05352600	-1.93530000
Cd	-0.63595500	1.30185800	-4.23191200
Cd	1.34936300	-1.47017300	-3.77557000
Cd	0.34708100	-4.30897400	-0.94803000
Cd	3.64796500	-1.88510300	-0.35301100
C	4.16913200	-5.42785300	4.48685600

C	3.17518700	-5.15631700	5.61956700
C	2.24077200	-6.32072200	5.90051100
O	2.86644400	-7.50373500	5.83462100
O	1.07635200	-6.19435400	6.19276700
N	2.35946000	-3.97211000	5.38159300
H	4.79799700	-4.54364000	4.34165700
H	4.81716700	-6.26559300	4.75184500
H	3.77573400	-5.05284500	6.54013300
H	1.52221400	-4.00226700	5.96319400
H	2.86810900	-3.12769600	5.62777700
S	3.41085400	-5.71616200	2.86208600
H	2.22139200	-8.18666200	6.07509600
H	2.78526200	-6.86791600	3.17115700

(CdSe)₁₉

Cd	0.33733000	-0.73490600	3.59778300
Se	-2.06552900	-2.03779200	3.25675900
Se	0.82267800	1.94463900	3.62853900
Cd	4.51233000	-0.78899300	1.63000900
Cd	2.64931400	3.00150200	1.99962700
Cd	-1.44758400	3.13926300	3.06677600
Cd	-3.88331600	-0.39009300	2.21604200
Cd	2.08384200	-4.12863900	0.74498100
Cd	-2.05742600	-4.18141700	1.74791700
Se	-0.01410300	-5.73890400	0.97552700
Se	5.02342400	1.84513600	1.81326800
Se	-3.94705000	2.16162800	2.93447500
Se	2.48994100	-2.19379800	2.51940000
Se	3.49839900	-4.83462100	-1.39600300
Se	6.23861100	-1.13875300	-0.44925200
Cd	4.77375500	-2.56799100	-2.07018800
Se	2.50926600	5.20734000	0.52281500
Se	-2.05239200	5.39585300	1.68106900
Se	-5.76163300	-0.91958700	0.40645300
Cd	-0.10626000	5.42768700	-0.06223000
Cd	-4.74628100	-2.93527700	-1.05599800
Cd	-3.74233300	3.55467200	0.64867000
Cd	-1.36675400	-5.33512500	-1.31499000
Cd	5.28076500	1.35899600	-0.81990400
Se	-3.78026600	-5.16873100	-0.10633300
Se	-4.01586800	2.94217500	-1.92349400
Cd	-4.75932900	0.42044300	-1.69513800
Se	4.05083800	2.28179700	-2.99097100
Cd	2.42496800	4.05122000	-1.90036000
Se	-0.71596100	-4.30738500	-3.67935500
Cd	1.85451900	-3.85552100	-3.28141000
Cd	-1.42455400	2.64073300	-2.58409200
Se	-0.01035700	4.86708100	-2.71391100
Se	-4.34040000	-1.62662400	-3.39589400
Cd	-1.70678000	-1.82309800	-3.38103500
Se	3.44677800	-1.96997400	-4.36006200
Cd	2.34414700	0.25263000	-3.45642700
Se	-0.20037000	0.25695400	-2.61244600
C	-0.81518300	-1.25161700	7.12641100
C	0.65603900	-1.61364400	6.93610200
C	1.55770200	-0.46021100	7.34847800
O	1.27106700	0.34661300	8.19978400
O	2.72652200	-0.47223100	6.69670800

N	0.93852500	-2.04780400	5.56917400
S	-1.38942100	0.14393000	6.11318300
H	-1.44137000	-2.09926800	6.83240900
H	-1.00567300	-1.03470800	8.17906900
H	-0.68726700	1.08800100	6.76825800
H	0.88328100	-2.41610600	7.65979400
H	0.46831100	-2.93075300	5.38266600
H	1.93397600	-2.21139100	5.42733000
H	3.25057800	0.28213500	7.00786600

Cartesian coordinates of CdSe-cys clusters in water

(CdSe)₁

C	3.62794400	0.93748100	0.06995900
C	3.18517000	0.48600100	1.46681400
C	1.72496900	0.02818000	1.47352900
O	1.27389900	-0.77341600	0.66408900
O	1.01282000	0.55541800	2.43836200
N	3.32934700	1.48069500	2.52258600
S	2.95184500	2.55176100	-0.44541800
H	4.71599400	1.03715500	0.06571300
H	3.35454000	0.17987500	-0.66845600
H	3.77093200	-0.40536400	1.72480600
H	3.37941200	2.42001800	2.13414600
H	4.14416300	1.31950800	3.10179700
H	1.69743200	1.13432300	2.91002200
Se	-0.04113700	1.53559800	-2.52432100
Cd	-0.55979100	-0.37675700	-0.90101800
H	1.81177300	2.10746700	-1.11352300

(CdSe)₂

Cd	-2.11523300	-2.33138700	-0.48069100
Se	0.34735800	-3.03821700	-1.37554000
Se	-2.67245900	0.20390300	-1.27718200
Cd	-0.12394600	-0.38692700	-2.00966600
C	3.48797900	-0.95284600	1.31298800
C	4.01574400	0.00328500	0.23852900
C	2.99448200	0.19577000	-0.88541100
O	1.81210300	0.42820500	-0.67659100
O	3.51218300	0.10540000	-2.08766200
N	5.27849500	-0.37578400	-0.38087700
S	3.47161200	-2.70754200	0.81854500
H	4.14142600	-0.89756600	2.18700800
H	2.48538800	-0.64625000	1.61913000
H	2.33180900	-2.70063700	0.04150400
H	4.12371800	0.99137500	0.70374400
H	6.06761100	0.12655500	0.00700800
H	5.44174700	-1.37583300	-0.28021400
H	4.48344700	-0.08738200	-1.88672800

(CdSe)₃

C	4.92280100	-0.41849200	1.67875600
C	5.22563000	0.63313600	0.60825600
C	3.94640100	1.08424400	-0.10271800
O	2.91214700	1.35072800	0.49081700
O	4.07485800	1.17359300	-1.40750200
N	6.18403400	0.24372900	-0.41681500
S	4.50897100	-2.06750700	1.02102400
H	5.81326500	-0.56662800	2.29463100
H	4.11751500	-0.06371500	2.32529900
H	3.25842300	-1.79560800	0.53461800
H	5.59713500	1.52752400	1.12458900
H	7.11703700	0.58807200	-0.22542400
H	6.22026100	-0.77011600	-0.50599200
H	5.02632300	0.87241800	-1.55080500
Cd	-1.47707900	-2.04219300	0.08390200
Cd	-2.82978100	1.08559800	0.18297900
Cd	0.58074700	0.94985600	-0.47056200

Se	-1.10213600	2.99331000	-0.34626200
Se	-3.98554100	-1.27634400	0.47153100
Se	1.03121600	-1.67764600	-0.69378500
(CdSe) ₄			
Cd	3.52798500	-0.24173000	-0.93850300
Cd	0.46191800	-0.19332500	-5.27937000
Cd	2.39004600	2.34977200	-3.50449800
Cd	1.88728200	-3.00490300	-3.03864800
Se	3.90317100	2.33044700	-1.36858100
Se	0.87782400	2.36534700	-5.64614400
Se	3.59969700	-2.90261100	-1.03540200
Se	0.04642000	-2.74953200	-4.91295400
C	1.69469000	-2.52113600	3.22412700
C	2.67992500	-1.43807100	3.67033000
C	3.28124000	-0.70197500	2.46836400
O	2.61712200	-0.30696700	1.52373600
O	4.58160900	-0.52071200	2.56334500
N	3.78300200	-1.88948500	4.50821700
S	2.47856700	-3.99932600	2.50029600
H	1.14197400	-2.87996500	4.09588900
H	0.97710500	-2.09961600	2.51710800
H	2.80604500	-3.48397600	1.27110400
H	2.10564600	-0.67769300	4.21524200
H	3.60895100	-1.73482400	5.49377300
H	3.96436000	-2.88045100	4.35899800
H	4.79822200	-0.96806900	3.43971000
(CdSe) ₅			
Cd	-2.12926300	1.42610700	3.66930200
Cd	0.54130400	0.63806400	2.05758500
Cd	-1.97715600	-2.30946800	2.59977600
Se	0.79198500	-2.11184800	2.63687500
Se	0.23541400	2.57492700	3.93115900
Se	-3.94632400	-0.33623700	2.81169800
Se	-0.42926400	0.63128300	-0.59099600
Se	-2.74679400	-3.30659100	-0.02866400
Cd	-0.18190800	-2.14338500	-0.05886400
Cd	-2.95048900	-0.46270200	0.11095500
C	-2.88188700	2.73619100	-3.85328200
C	-3.76190400	1.51951100	-4.15252200
C	-3.75448900	0.51703400	-2.99303000
O	-3.89385200	0.84574000	-1.82281000
O	-3.60422200	-0.72706300	-3.38257800
N	-3.42942500	0.78256600	-5.36460100
S	-1.09047800	2.41273100	-3.94972300
H	-3.07955200	3.50836500	-4.60073100
H	-3.13196700	3.14181000	-2.87081700
H	-0.94196700	1.75074700	-2.76135900
H	-4.79826800	1.87419700	-4.22064700
H	-4.02534800	1.02876900	-6.14544100
H	-2.45869100	0.94301300	-5.62749700
H	-3.51659400	-0.62644600	-4.38479000
(CdSe) ₆			
Cd	0.87019700	2.20861100	-1.59498900
Cd	-2.26429200	0.17270400	0.05653400
Cd	1.59478400	-1.60026300	-0.99028300

Se	-1.78981900	2.59434500	-1.19846500
Se	2.72769300	0.42261900	-2.47670600
Se	-0.95795600	-2.25634700	-0.20265500
Se	2.18978500	3.42575100	0.99469400
Se	-1.67333700	0.77609400	2.85651400
Se	2.87486700	-1.54222500	1.68237700
Cd	-0.43802700	2.72674500	1.35552000
Cd	3.08089600	0.90378900	0.43068700
Cd	0.23485400	-0.99028100	2.07543500
C	-4.98325400	-3.68895300	-1.73454500
C	-5.75551400	-3.00626300	-0.60051200
C	-4.95338800	-1.85838100	0.02486800
O	-4.38982500	-0.99690800	-0.63594300
O	-4.95386300	-1.87903700	1.33702700
N	-6.18341200	-3.87979300	0.48381600
S	-3.65550300	-4.80940500	-1.18299600
H	-5.67264100	-4.31774000	-2.30320300
H	-4.57522700	-2.93502300	-2.41105700
H	-2.73524100	-3.86416700	-0.81781000
H	-6.63583300	-2.52937500	-1.04961000
H	-5.61200000	-4.72259100	0.51101200
H	-7.15773500	-4.14533900	0.40873000
H	-5.50627300	-2.70238600	1.53578500

(CdSe)₇

C	6.03922300	2.19914100	-2.78341900
C	6.52405300	2.90191900	-1.51666900
C	5.48844700	2.85176100	-0.38862300
O	4.79980400	1.87025600	-0.15366100
O	5.44343800	3.95542300	0.32324800
N	6.93035100	4.29299900	-1.66814200
S	4.67787300	3.05994300	-3.64090400
H	6.86683500	2.14845400	-3.49494500
H	5.72776300	1.17865200	-2.55162700
H	7.38322100	2.33280000	-1.13604000
H	6.39886400	4.74639100	-2.40863000
H	7.91724500	4.38637500	-1.87614500
H	6.09014300	4.55494600	-0.16102100
Se	0.23387800	-3.15878100	-0.54150100
Se	-3.15374500	-1.73379800	1.83530800
Cd	-0.35978500	-1.59044000	1.67196100
Cd	-2.56389400	-2.96877000	-0.67708600
Se	1.42026100	4.28400500	1.04258900
Se	1.13683300	0.40746800	2.76784900
Cd	-0.51608000	2.56620800	2.18938100
Cd	2.38217000	1.65472700	0.60108900
Cd	-0.22133000	-0.84581500	-2.01987200
Cd	-0.11037600	3.15377500	-1.04616900
Cd	-3.18019100	0.25034500	-0.11483100
Se	-2.52626600	2.87989300	0.29320600
Se	1.61305900	1.19751300	-2.05343000
Se	-2.91100900	-0.96203100	-2.65587900
H	3.64198000	2.47515800	-2.97566400

(CdSe)₈

Se	-4.79021600	0.60324200	1.16795700
Cd	-3.44903700	-1.78406300	1.43831300
Se	-0.88274700	-2.55530100	2.17482600

Cd	0.42088000	-0.17696200	2.46423700
Se	-0.58281200	2.44250600	2.47101500
Cd	-2.52798000	2.14339400	0.60597200
Se	-2.39571300	2.04939700	-2.18164600
Cd	-3.97015900	-0.11337700	-1.49383400
Se	-3.54477400	-2.81600900	-1.28636600
Cd	-0.90561800	-2.40040300	-0.64107400
Se	1.07976600	-1.29204700	-2.16058700
Cd	0.27686900	1.38281400	-2.19184500
Se	3.13062600	0.43314800	2.09374100
Cd	1.77174700	2.63972600	0.94515900
Se	2.15858400	3.25859300	-1.63340100
Cd	2.98770500	-0.53889600	-0.40077700
C	4.67222900	-2.81836900	-4.63871100
C	5.57149500	-1.62815800	-4.29343400
C	5.10337900	-0.90905500	-3.02273000
O	4.77677700	-1.49388000	-1.99954000
O	5.10829500	0.39932500	-3.13410600
N	5.71433900	-0.62039000	-5.33577300
S	3.04946100	-2.36412800	-5.33396500
H	5.16098000	-3.41749600	-5.41085600
H	4.53399800	-3.44793300	-3.75738300
H	2.43763000	-1.97268000	-4.17738300
H	6.56235600	-2.03048900	-4.04648900
H	6.56312000	-0.73753700	-5.87555900
H	4.91665500	-0.64383700	-5.96866300
H	5.41037500	0.53264600	-4.08834000

(CdSe)₉

Se	2.71500700	-1.12729400	2.23385800
Cd	2.57732700	-0.45460900	-0.47040800
Se	2.20121800	2.18734500	-1.15961500
Se	1.22986800	-2.75980700	-1.39736000
Cd	-1.21725700	-1.88047700	-2.22635400
Cd	-0.43599500	2.24206200	-2.11967600
Se	-1.97689300	0.48642200	-3.55244400
Cd	-3.92449300	0.18081100	-1.63859400
Se	-4.54254800	0.94762800	0.93901900
Cd	-2.39216700	2.55278500	1.43509900
Cd	-3.20237800	-1.48347100	1.20806800
Se	-0.35079700	2.51316100	3.30802400
Cd	0.33742400	-0.12554000	3.23113200
Se	-1.38438300	4.28983000	-0.47921900
Se	-3.67532000	-2.66804300	-1.24308600
Cd	0.71540600	-2.90555200	1.32213000
Cd	0.88603700	3.36931100	0.96968000
Se	-1.39988300	-2.36565900	3.04225700
C	5.10615900	-3.74046300	-3.59670400
C	5.23439000	-2.29864800	-4.09502700
C	4.41720800	-1.32766700	-3.23233900
O	4.45331600	-1.32402000	-2.01105000
O	3.69471000	-0.49008300	-3.94178200
N	4.85347700	-2.07768500	-5.48416400
S	3.50843400	-4.53202600	-3.97713700
H	5.86005400	-4.35646900	-4.09301900
H	5.29037600	-3.77790300	-2.52108000
H	2.74034100	-3.87275200	-3.05790500
H	6.28022500	-1.99745800	-3.95585200

H	5.65280100	-2.02186600	-6.10337000
H	4.23332300	-2.81639700	-5.81059700
H	3.91026000	-0.77194500	-4.88773900

(CdSe)₁₀

Cd	5.62199700	6.28316100	-1.65388400
Se	6.63731300	7.07410100	-4.11243300
Cd	6.04349100	4.61750500	-5.37786800
Se	3.61237300	3.32005400	-5.10627500
Cd	2.36978300	4.20955800	-2.82597000
Se	2.99272500	6.30619800	-0.98160000
Se	8.71129500	3.58958100	-5.37606000
Cd	8.02566100	1.20398700	-4.31448600
Se	6.46594000	-0.65801400	-5.61158700
Cd	4.17555200	0.64603500	-4.76221600
Se	0.91344500	2.64295400	-1.06591100
Cd	2.95740400	0.76335400	-0.90074600
Se	3.25372600	-1.13092500	-2.80298700
Cd	8.44129700	5.05055600	-3.08839500
Cd	6.04418800	-1.30419700	-2.86992100
Cd	2.89485500	3.98015200	0.45949700
Cd	6.79169300	2.33864900	-0.41267000
Se	7.76733100	4.95895500	-0.43978800
Se	4.51901400	1.85637100	1.10572300
Se	8.02892100	0.22184700	-1.67961800
C	5.54198800	8.57258100	-8.56878800
C	6.15825300	7.46077500	-9.41818700
C	6.46392400	6.21353900	-8.58301600
O	5.70279700	5.77481500	-7.73692000
O	7.61098300	5.64593500	-8.89064400
N	7.36875100	7.80841400	-10.14962200
S	6.70136400	9.34948500	-7.39404300
H	5.20511800	9.37636600	-9.22812200
H	4.67400000	8.19174800	-8.02701800
H	5.39450600	7.13955500	-10.13898300
H	7.87987000	8.54772900	-9.67165500
H	7.17421700	8.10969800	-11.09684900
H	7.98169000	6.26523500	-9.59034300
H	6.63925500	8.42065200	-6.40119800

(CdSe)₁₃

Se	-4.72497500	-0.97751200	-1.55973000
Se	-2.75788700	3.45400900	-0.44002100
Se	-4.00807600	0.46542200	3.07802400
Cd	-3.14745200	1.19219500	-2.08191800
Cd	-4.06436900	-1.45928800	1.14497300
Cd	-1.89191200	1.68784700	1.43082500
Cd	-2.74575100	-2.92315400	-1.66368100
Cd	-1.47750200	-0.06669400	4.01680100
Cd	-0.33018300	3.10521700	-1.73443400
Se	-2.73060300	-3.89654000	0.95257300
Se	0.14539000	2.27658700	3.53031600
Se	-1.00983300	1.46489700	-3.86802700
Se	-0.80199700	-3.21821400	-3.54594700
Se	2.21500300	3.62235700	-0.85042000
Se	0.05560700	-2.27698600	4.47966600
Cd	0.23386000	-0.70352000	-2.64487000
Cd	1.64235300	1.72272100	1.21510400

Cd	-0.23715200	-2.87811000	1.72232300
Se	-0.14982500	-0.32649400	0.22636800
Se	3.09765400	-0.99778400	-2.58359100
Se	2.10271800	-4.18328200	0.72296300
Se	3.97854800	0.14461300	2.06737100
Cd	0.92122800	-3.96479100	-1.64930300
Cd	3.21089300	1.68892100	-2.41479000
Cd	1.79856600	-0.35116200	3.64396600
Cd	2.96860200	-1.58928000	0.16569200
C	6.87399300	-0.28809500	-5.24422700
C	6.29132700	0.95004500	-5.93090200
C	5.15194200	1.56122900	-5.10931500
O	5.22679500	1.75605600	-3.90361400
O	4.09636400	1.86650300	-5.82591800
N	5.78873200	0.74537300	-7.28311400
S	5.80031300	-1.75985800	-5.30804900
H	7.79461900	-0.57662100	-5.75729500
H	7.12188300	-0.05486700	-4.20671200
H	4.88743900	-1.38746800	-4.36215200
H	7.07831400	1.71458300	-5.95034300
H	6.44452000	1.04988700	-7.99211000
H	5.56391500	-0.23511100	-7.44100200
H	4.37536800	1.56886000	-6.75135100

(CdSe)₁₆

Se	1.53753700	-1.26647000	4.70731500
Se	-1.53375300	1.47173200	4.70430000
Se	2.79374600	3.18361600	2.79594500
Se	-1.70617300	4.97732800	1.46489800
Se	1.23585400	5.02720200	-1.53834600
Se	-3.07979800	3.02389700	-2.99022400
Se	-4.91289000	1.46015900	1.34350200
Se	-4.89536500	-1.48133200	-1.64806700
Se	-2.90636100	-2.86070500	2.78988300
Se	1.59940400	-4.68205300	1.38607000
Se	4.79510300	-1.09956200	1.30673300
Se	2.94262800	-2.68482200	-3.02410300
Se	-1.39381800	-4.70902100	-1.54520300
Se	-1.45434900	-1.37014800	-4.93616900
Se	1.27820600	1.68505200	-4.93301700
Se	4.75132200	1.82103800	-1.67405700
Cd	4.13364600	1.58611400	1.03688500
Cd	4.20160200	-0.89739300	-1.40862000
Cd	2.80159300	-2.50558700	2.59151300
Cd	1.30040700	-4.04960000	-1.31894600
Cd	1.16412200	1.42016400	4.07204500
Cd	-1.15852200	-1.21802400	4.07070300
Cd	-1.14014800	-4.12977600	1.16492100
Cd	-4.26589900	-1.23516600	1.05965500
Cd	-2.64130200	-2.56756400	-2.75824300
Cd	1.23142100	-1.01068500	-4.30621600
Cd	-2.75634400	2.68784700	2.54953300
Cd	2.47528100	2.88785300	-2.75970400
Cd	1.00908100	4.44012100	1.18139500
Cd	-1.45820700	4.36981200	-1.24990300
Cd	-4.33899100	1.23749200	-1.37622300
Cd	-1.40999700	1.32081200	-4.29650800
C	4.32492000	-7.08771300	4.45191400

C	5.56610500	-6.20260900	4.56578500
C	5.32288100	-4.80080500	3.99447500
O	4.30371300	-4.16221400	4.19347300
O	6.34256600	-4.34392400	3.29504100
N	6.78087600	-6.72514100	3.95382400
S	3.91646900	-7.59289300	2.74688300
H	4.50052800	-8.01441700	5.00371300
H	3.46475800	-6.58447000	4.89770700
H	5.75544800	-6.04360800	5.63565200
H	6.55834600	-7.34702200	3.17950100
H	7.36169500	-7.22649800	4.61496600
H	6.98658300	-5.11551900	3.31799200
H	3.22352900	-6.48285200	2.36628700

(CdSe)₁₉

Cd	-0.10914100	-1.47129800	2.86844400
Se	-2.66839400	-2.43676200	2.70420900
Se	0.68562500	1.00102100	3.88724500
Cd	4.31636200	-1.81665900	1.58273000
Cd	2.83744500	2.05851900	2.51066900
Cd	-1.47001700	2.64357600	3.42974100
Cd	-4.39378200	-0.45977000	1.82945200
Cd	1.54929000	-5.00190100	-0.04694600
Cd	-2.73531500	-4.44485900	0.85329600
Se	-0.90578700	-6.23062500	-0.20694100
Se	5.20026700	0.73422200	2.15709000
Se	-4.13185600	1.95380400	3.14607900
Se	1.92895200	-3.11083700	1.91482200
Se	3.06075200	-5.55981100	-2.25558800
Se	6.08694300	-2.16286900	-0.57170800
Cd	4.56981300	-3.25460900	-2.52913600
Se	2.86229600	4.45984200	1.18714800
Se	-1.68549500	5.16778200	2.27950900
Se	-6.28462100	-0.46770500	-0.14607700
Cd	0.29205100	5.16343900	0.41467400
Cd	-5.32299900	-2.38852700	-1.91325200
Cd	-3.63732200	3.61008500	0.97064300
Cd	-2.20178900	-5.14628600	-2.41791700
Cd	5.42114200	0.52816800	-0.63868100
Se	-4.66869600	-4.90502300	-1.14696300
Se	-3.76025400	3.48729400	-1.75884800
Cd	-4.94769900	1.07319100	-2.03039300
Se	4.40968900	1.94606600	-2.74330300
Cd	2.85058300	3.75963300	-1.47814000
Se	-1.14895500	-4.02438200	-4.66333600
Cd	1.50584200	-4.03729900	-4.00839100
Cd	-1.16726500	2.86055000	-2.50594100
Se	0.53104400	5.01999200	-2.34293600
Se	-4.57964300	-0.80553800	-4.05548800
Cd	-1.90557400	-1.44569800	-3.93206500
Se	3.33420500	-2.08312300	-4.72924500
Cd	2.43392200	0.18562900	-3.48938200
Se	-0.19996300	0.22639700	-2.51825900
C	1.67069600	-4.45380600	6.61549000
C	1.17827200	-3.16357500	7.27835800
C	0.84639300	-2.14020900	6.21000700
O	0.19821300	-2.45530300	5.22015800
O	1.27775900	-0.92074500	6.45568600

N	2.13184000	-2.66703900	8.25161500
S	3.16497500	-4.27914100	5.58174400
H	1.92435600	-5.17316400	7.39895200
H	0.87214400	-4.88863500	6.01200400
H	2.56010500	-3.90796100	4.42104900
H	0.19678500	-3.41143200	7.72401100
H	2.16011700	-3.29793600	9.04628600
H	1.84185000	-1.76079800	8.60380600
H	1.03453000	-0.30517600	5.70450100

Cartesian coordinates of CdSe-cys clusters in toluene

(CdSe) ₁			
C	-2.86633200	-1.08899000	0.51274700
C	-2.58026600	0.36773400	0.86259200
C	-2.74598600	1.26470200	-0.35622700
O	-3.43230300	0.98531000	-1.31133800
O	-2.07737600	2.41195500	-0.22292900
N	-1.25542800	0.53335500	1.46176300
S	-1.67214700	-1.84977100	-0.63351000
H	-2.83035300	-1.69949700	1.41929500
H	-3.86737500	-1.17855500	0.08829700
H	-3.37283900	0.68874800	1.55919200
H	-1.23986300	0.11966600	2.39088700
H	-1.04162500	1.52110600	1.58009600
H	-2.22860900	2.95896300	-1.01026400
Se	3.06294900	0.03416300	-0.20740900
Cd	0.65574500	-0.33643200	0.18724900
H	-2.05962700	-1.18131700	-1.73580100
(CdSe) ₂			
Cd	-0.39317700	-1.68112800	-0.48018600
Se	1.21490300	0.49455600	-0.75987900
Se	1.19147400	-3.84229200	-0.28927200
Cd	2.66239700	-1.67834700	-0.54107500
C	-3.94225500	-1.19038900	-0.15521300
C	-3.20160400	-0.57533000	1.02743200
C	-2.83575300	0.87925000	0.75671800
O	-3.31072000	1.54500200	-0.13478800
O	-1.96124900	1.33636600	1.65155200
N	-2.00790300	-1.34312600	1.38197200
S	-2.97377100	-1.34538200	-1.69021200
H	-4.25079700	-2.20921000	0.09564300
H	-4.84170400	-0.61173300	-0.37218800
H	-2.88374600	-0.02768600	-1.94965900
H	-3.91955400	-0.54088000	1.86450000
H	-2.26751100	-2.24262400	1.77799700
H	-1.47002000	-0.84837300	2.08937100
H	-1.69801300	2.23707600	1.40402600
(CdSe) ₃			
C	4.51326400	1.13783300	0.06331400
C	3.74470600	0.48237700	1.20631800
C	4.01282700	-1.01401900	1.26732600
O	4.96036800	-1.55796100	0.74771800
O	3.09947700	-1.65053200	2.00344500
N	2.30995000	0.74606200	1.12418900
S	4.00977600	0.62611000	-1.61067900
H	4.35724700	2.21986400	0.09255300
H	5.58148800	0.94848500	0.18124200
H	4.43742000	-0.64680000	-1.51946000
H	4.17264600	0.88402500	2.14131800
H	2.11891300	1.73292200	1.28379200
H	1.81513300	0.22549300	1.84390200
H	3.29937100	-2.59995300	1.99586400
Cd	-1.97958800	1.99107300	-2.34606200
Cd	-1.83152300	-1.41788400	-2.51003800

Cd	1.15274300	0.36172900	-1.02985400
Se	0.39937000	-2.13554800	-1.45667700
Se	-3.67755200	0.25747500	-3.25960600
Se	0.14789000	2.81867000	-1.17542100

(CdSe)₄

Se	0.68750800	2.34470400	-0.99652200
Se	0.82174800	-1.90743100	-1.83377800
Se	-0.35852700	-0.57062900	2.11113400
Cd	2.42945500	0.29048900	-1.55816000
Cd	1.50022500	1.35992800	1.45837700
Cd	-0.87729400	0.07628400	-0.58248800
Cd	1.62955400	-1.92970300	0.78459200
Se	3.75170400	-0.12369300	0.81852100
C	-4.53384700	0.61621600	-0.95602800
C	-4.07970700	-0.80223000	-1.29398600
C	-4.17069000	-1.69956700	-0.06790200
O	-4.97642700	-1.54007100	0.81989200
O	-3.29413300	-2.70471000	-0.10890700
N	-2.73700100	-0.81907300	-1.87058200
S	-3.44989700	1.50163400	0.20717400
H	-4.54420100	1.22376100	-1.86554400
H	-5.54927400	0.59123700	-0.55760500
H	-3.76122300	0.77930900	1.29908600
H	-4.82151000	-1.21344700	-1.99954400
H	-2.74512400	-0.37629100	-2.78594400
H	-2.40440400	-1.77130600	-2.01101800
H	-3.39209800	-3.23210800	0.69955400

(CdSe)₅

Cd	2.99699400	2.13709400	0.77330600
Cd	2.46345000	0.01845800	-1.73264200
Cd	1.24624100	-1.28102000	1.73363500
Se	2.54500600	-2.41609900	-0.39871100
Se	4.27051300	1.94808200	-1.44866800
Se	1.10750900	1.34486400	2.37927100
Se	-0.27047400	0.19783600	-2.24682400
Se	-1.38464900	-2.00707300	1.27864100
Cd	-0.10176800	-2.30714800	-1.10370700
Cd	-1.32339700	0.54776400	0.25827800
C	-4.47227700	2.28687400	0.72510200
C	-3.28724700	3.09482000	1.25063900
C	-2.78159600	4.05229300	0.18163200
O	-3.49408600	4.55206100	-0.65813200
O	-1.47666900	4.31012900	0.30043300
N	-2.22321700	2.22523400	1.74302600
S	-4.05789600	1.13543200	-0.62306100
H	-4.87462300	1.66236700	1.52750100
H	-5.26273100	2.96038600	0.39108000
H	-3.67559300	3.74569500	2.05199400
H	-2.52976000	1.72876800	2.57643500
H	-1.38601600	2.74269200	2.00850200
H	-1.22500300	4.94271800	-0.39142600
H	-3.84845300	2.06476600	-1.57384500

(CdSe)₆

Cd	1.32620100	1.97354500	-1.51486200
Cd	-1.96072200	-0.12293600	-0.00595600

Cd	1.62826900	-2.06159300	-1.35819700
Se	-1.18291100	2.40615300	-0.67336500
Se	2.92737400	0.02997900	-2.48621300
Se	-0.85359900	-2.58038500	-0.49036900
Se	2.78141100	2.64117500	0.83628900
Se	-0.95348400	0.02482200	2.89669400
Se	3.10286400	-2.36875900	1.04007100
Cd	0.28775000	2.08190800	1.70403800
Cd	3.62208100	0.15630700	0.25411500
Cd	0.57088600	-1.90136500	1.85532700
C	-5.37760300	-1.21785200	-0.72270000
C	-5.31286200	-0.45211100	0.59692300
C	-5.68494000	1.00905200	0.39942600
O	-6.40842500	1.40736600	-0.48481900
O	-5.16197700	1.79513400	1.34310500
N	-4.00595900	-0.58766100	1.23324400
S	-4.16654300	-0.68655400	-1.97398600
H	-5.16192600	-2.27442500	-0.54063200
H	-6.38117900	-1.14593900	-1.14492000
H	-4.73912300	0.50260300	-2.23962300
H	-6.11396100	-0.85849000	1.23813400
H	-3.87458700	-1.53902800	1.56813100
H	-3.91202400	0.01749600	2.04621600
H	-5.44062300	2.70875300	1.17311100

(CdSe)₇

C	5.18063300	0.27909800	2.07414700
C	5.04537600	-0.31041900	0.67164100
C	6.10844800	0.24955800	-0.26136900
O	7.14958200	0.74159400	0.11150600
O	5.78245300	0.09398900	-1.54722300
N	3.70244600	-0.13077100	0.12684000
S	4.85300600	2.06611600	2.18900500
H	4.44188800	-0.18480300	2.73363000
H	6.17613300	0.07477700	2.47166400
H	5.29495900	-1.38205200	0.75505700
H	3.07582100	-0.86173000	0.46426200
H	3.70902600	-0.21488300	-0.88747600
H	6.50063600	0.44825800	-2.09463800
Se	0.83045200	-2.64372200	-0.26637900
Se	-2.99141500	-1.71004300	1.51562400
Cd	-0.31127300	-1.18513000	1.79115500
Cd	-1.88530000	-2.91466200	-0.68025300
Se	1.32855400	4.49117900	0.72275300
Se	1.04450600	0.85486100	2.77507900
Cd	-0.51327600	2.91930300	1.97722800
Cd	2.46271700	1.94906500	0.52532400
Cd	0.19240300	-0.65941600	-2.10555800
Cd	-0.15879100	3.41216100	-1.29995600
Cd	-3.07072500	0.29120900	-0.37810800
Se	-2.49998400	2.86879800	0.06751600
Se	1.59756800	1.57671000	-2.22184000
Se	-2.43624900	-1.14087500	-2.67642700
H	5.90802400	2.46465000	1.45297700

(CdSe)₈

Se	-4.54243700	0.31073400	0.38093500
Cd	-3.20542300	-1.80221100	1.38300500

Se	-0.82811000	-2.12566400	2.62042600
Cd	0.34082100	0.26113600	2.87140600
Se	-0.75547400	2.71369800	2.10284000
Cd	-2.39238900	1.95973900	0.14639100
Se	-1.69972200	1.40879600	-2.48579300
Cd	-3.18320400	-0.76271700	-1.82877500
Se	-2.64385300	-3.24970800	-0.95265900
Cd	-0.14998200	-2.67842600	-0.03960700
Se	1.88827900	-1.66087400	-1.41880800
Cd	0.91205500	0.78634600	-2.25613200
Se	2.96827200	0.85916700	2.58133500
Cd	1.72468300	2.80378300	1.03093500
Se	2.85075000	2.47103700	-1.36230800
Cd	3.53979400	0.05311200	-0.02651700
C	7.07183200	-0.35108600	-1.36973200
C	6.86839900	-0.93117700	0.02811300
C	6.56616100	-2.41900900	-0.04854200
O	7.03928700	-3.15619800	-0.88272800
O	5.75950700	-2.82956500	0.93397000
N	5.83752900	-0.20935100	0.77009800
S	5.58707700	-0.39000300	-2.42103700
H	7.35069000	0.70354800	-1.28891700
H	7.88753300	-0.87576100	-1.86963300
H	7.84299600	-0.87193500	0.54209400
H	6.14823800	0.74058600	0.95945200
H	5.67116300	-0.63687100	1.67871300
H	5.59332600	-1.71715200	-2.64379600
H	5.62768400	-3.78637900	0.84155200

(CdSe)₉

Se	-0.14065400	4.20841800	-0.25436900
Cd	-0.15420000	2.30835100	-2.20214900
Se	-2.07858000	0.50224000	-2.45693800
Se	2.57743500	2.10277600	-2.68781700
Cd	3.05431600	-0.46657500	-2.06386900
Cd	-0.97164800	-1.91833000	-1.92111300
Se	1.52736800	-2.74057100	-2.43139200
Cd	2.49267500	-3.11666300	0.06451200
Se	1.55145800	-2.58242300	2.54830900
Cd	-0.95645100	-1.78897200	2.01376300
Cd	3.03044300	-0.30451500	2.01119400
Se	-2.11951900	0.66445900	2.43707200
Cd	-0.24834200	2.41702200	1.77629200
Se	-2.61486900	-2.75578600	0.06597500
Se	4.59455800	-1.27316400	0.02290300
Cd	2.46520300	3.21080100	-0.20988300
Cd	-3.34648600	-0.08344200	0.06709400
Se	2.45464500	2.27254100	2.35060700
C	-6.84822100	0.85255500	0.84399900
C	-6.53682400	0.97495000	-0.64657500
C	-6.98592400	-0.27623000	-1.38555600
O	-7.95730800	-0.92429200	-1.06861200
O	-6.21858700	-0.55319800	-2.44116900
N	-5.12576700	1.27286400	-0.88195200
S	-5.94526100	-0.48397100	1.68838700
H	-6.55633400	1.77497300	1.35427000
H	-7.92091800	0.71339700	0.98668300
H	-7.18191500	1.77680500	-1.04364600

H	-4.92918700	2.23554500	-0.61922700
H	-4.88417200	1.18745200	-1.86867900
H	-6.56743500	-1.34652800	-2.87762500
H	-6.61718500	-1.50228800	1.12023100

(CdSe)₁₀

Cd	-0.04715200	4.23153100	-0.96976500
Se	0.97211600	4.83625500	-3.39308500
Cd	0.51620100	2.54511700	-4.87263800
Se	-1.78233200	1.26880900	-3.91629600
Cd	-3.35060200	2.28229500	-1.97961200
Se	-2.60706200	4.24990700	-0.19957200
Se	3.16785400	1.46457500	-4.43606600
Cd	2.44075500	-0.82379200	-3.34542200
Se	0.77216500	-2.58732400	-4.58032100
Cd	-1.53965000	-1.38678400	-3.80128000
Se	-4.75604400	0.72142900	-0.24753300
Cd	-2.87216700	-1.21246500	-0.02969400
Se	-2.27104100	-3.10984500	-1.79635200
Cd	2.84973300	3.11579200	-2.35239800
Cd	0.44356300	-3.21900300	-1.86207100
Cd	-2.80981600	2.00433900	1.28733300
Cd	1.16715200	0.39653900	0.48597400
Se	2.08138900	2.92612300	0.23754900
Se	-1.16148400	-0.07045400	1.80453800
Se	2.39291600	-1.71105900	-0.75474400
C	0.75311400	2.84685200	-8.52686900
C	0.22793500	1.46049600	-8.16898000
C	-1.29028800	1.40482800	-8.24917600
O	-1.98417300	2.26459600	-8.73908100
O	-1.76572100	0.25644100	-7.75553000
N	0.68781600	1.01978300	-6.85533100
S	0.25660600	4.13776100	-7.32531600
H	1.84359100	2.81783500	-8.57532700
H	0.36974800	3.13141500	-9.50789000
H	0.57906200	0.78095700	-8.96418000
H	1.69638500	0.87595000	-6.86032600
H	0.27184900	0.12319400	-6.61002400
H	-2.73311600	0.27656700	-7.82191100
H	1.48283900	4.62964800	-7.08133900

(CdSe)₁₃

Se	-4.71808200	-1.03236000	-1.81333600
Se	-3.18926800	3.38528900	-0.44524000
Se	-3.84110700	-0.05373600	2.81178800
Cd	-3.44963900	1.29142600	-2.21455400
Cd	-3.94366600	-1.75788700	0.74931800
Cd	-2.22415800	1.68783300	1.40571900
Cd	-2.61283400	-2.69073100	-2.25079000
Cd	-1.42061400	-0.58821100	3.73541700
Cd	-0.90728900	3.55306700	-1.90444400
Se	-2.39709900	-3.92157200	0.18998500
Se	-0.10167200	1.93063500	3.28790000
Se	-1.49320100	1.97486400	-4.03213000
Se	-0.70539800	-2.63865500	-4.17149600
Se	1.55862600	4.10651300	-1.00075200
Se	0.54289400	-2.39986400	3.71204200
Cd	0.07337800	-0.07825800	-3.24925400

Cd	1.29593800	2.13979900	0.87660100
Cd	-0.04424100	-2.82122200	1.02180800
Se	-0.24383400	-0.11472800	-0.27692800
Se	2.82918700	-0.14367900	-3.11158000
Se	2.30205100	-3.67193600	-0.23013300
Se	3.67849700	0.77236900	1.41448200
Cd	1.12862900	-3.48706700	-2.53153200
Cd	3.00936100	2.43524300	-2.52558200
Cd	1.91970200	-0.12310300	3.23040100
Cd	2.77752800	-0.95665300	-0.47277200
C	4.52876400	5.18472000	-4.05630700
C	5.62067000	4.46178500	-3.26455200
C	6.51686100	3.58108200	-4.12003900
O	6.77267100	4.12321700	-5.31312600
O	6.97606100	2.52881300	-3.74160900
N	5.09568500	3.65071200	-2.16997200
H	3.94528400	5.81263000	-3.37633800
H	4.98184500	5.83442400	-4.80674800
H	6.28819200	5.25389600	-2.88612700
H	5.81214300	2.98813200	-1.87638200
H	4.87173600	4.23831300	-1.37086700
S	3.29466200	4.11656600	-4.86310700
H	4.13096900	3.47153100	-5.69805100
H	7.39222800	3.54286500	-5.78328100

(CdSe)₁₆

Se	-5.00237700	1.93714600	0.72467600
Se	-4.93777700	-0.98087200	-2.06517000
Se	-2.52695000	3.13710200	-3.30868800
Se	-1.21257500	-1.33319200	-4.84861500
Se	1.90547300	1.15697500	-4.43344100
Se	2.60729000	-3.22037800	-2.32634400
Se	-2.01919600	-4.47675600	-1.50569300
Se	0.29919400	-4.89670300	1.74444100
Se	-3.94616200	-2.48678400	2.54498800
Se	-2.23770000	1.69838000	4.41547800
Se	-1.46112400	4.92487800	1.16963600
Se	2.36961200	2.74027100	3.25699300
Se	0.27821300	-1.44851300	4.84346100
Se	3.86451900	-1.79646900	2.16392800
Se	4.64099100	0.92877000	-0.69051700
Se	1.71742800	4.50934700	-1.27802400
Cd	-1.00695900	4.34242200	-1.44647200
Cd	1.15615700	4.22721700	1.36696000
Cd	-3.00036700	2.96808600	2.18253900
Cd	0.43045000	1.18871600	4.28027400
Cd	-4.28294500	1.65498300	-1.87929800
Cd	-4.83216200	-0.78847000	0.65440500
Cd	-2.25770400	-1.00959400	4.04728800
Cd	-2.20945100	-4.02959400	1.18051300
Cd	1.77754500	-3.18652000	3.25534300
Cd	3.77407100	0.89964700	1.88747700
Cd	-2.78715700	-2.33533700	-2.91772400
Cd	2.88792800	2.27579300	-2.20358200
Cd	-0.80464200	1.30909400	-4.29984100
Cd	1.34213800	-1.46159400	-3.91964800
Cd	0.63008600	-4.32621500	-0.87613700
Cd	3.94425700	-1.69063800	-0.54739400

C	4.16412100	-5.72197400	4.81749100
C	2.97624800	-5.38915800	5.72063700
C	1.81983900	-6.36951600	5.61799200
O	2.22695900	-7.62556500	5.40666800
O	0.66184400	-6.05484400	5.76498600
N	2.45332000	-4.04946400	5.48814200
H	4.95116200	-4.97977800	4.98031300
H	4.57147600	-6.69855900	5.08537300
H	3.33956300	-5.50408100	6.75727100
H	1.56627400	-3.92999300	5.97556500
H	3.08979500	-3.34902300	5.85803200
S	3.82356900	-5.66188100	3.03333400
H	1.44094300	-8.19432300	5.39584700
H	2.99447900	-6.72080400	2.99017300

(CdSe)₁₉

Cd	0.17619900	-0.32532200	3.61001100
Se	-2.41927100	-1.45722400	3.20086000
Se	0.20296100	2.34413200	2.76098800
Cd	4.44503400	-0.05403200	1.81001100
Cd	2.22366600	3.64781000	1.55765000
Cd	-2.09385400	3.63567500	2.46047000
Cd	-4.26505900	-0.05746100	1.79885300
Cd	2.24256600	-3.78864200	1.23252800
Cd	-2.17370300	-3.79547600	1.97670000
Se	0.03835900	-5.30134200	1.51387600
Se	4.68820200	2.62695000	1.66079500
Se	-4.56723000	2.55782300	2.21518800
Se	2.52358100	-1.61369700	2.79480900
Se	3.78266300	-4.53000600	-0.83908700
Se	6.31558900	-0.53207300	-0.13406800
Cd	5.03858700	-2.25540200	-1.68155800
Se	2.00001200	5.76155600	-0.08484200
Se	-2.61531400	5.75981300	0.78202400
Se	-5.96240800	-0.94291800	-0.10958200
Cd	-0.61297400	5.77769800	-0.94628400
Cd	-4.76210400	-3.08884400	-1.31356700
Cd	-4.27898600	3.81146000	-0.17146500
Cd	-1.19718900	-5.33756200	-0.93431700
Cd	5.32109700	1.90211700	-0.90767700
Se	-3.69843700	-5.07520500	0.07865100
Se	-4.15596900	2.79859000	-2.66392700
Cd	-4.86001900	0.26206500	-2.28266800
Se	4.01453400	2.55307600	-3.18127800
Cd	2.28460500	4.44770800	-2.43282000
Se	-0.36970200	-4.45472700	-3.34892300
Cd	2.19862600	-3.86577400	-2.94758200
Cd	-1.50559900	2.64694800	-3.29069100
Se	-0.17077700	4.95316400	-3.51645100
Se	-4.22526700	-1.97302600	-3.74336700
Cd	-1.55147000	-2.01268600	-3.58485100
Se	3.73826300	-1.93999500	-4.06789200
Cd	2.45141200	0.37562300	-3.66673300
Se	-0.19004400	0.28252400	-3.02655400
C	0.02880200	-0.50419100	7.33933000
C	0.58462800	-1.81290900	6.78959400
C	2.10605700	-1.81801600	6.75977100
O	2.81463300	-0.90354200	7.11574000

O	2.56766000	-2.98771400	6.31226100
N	0.07596900	-2.09837600	5.44953500
S	0.20484400	0.93849700	6.24488600
H	-1.04860400	-0.60837300	7.49640900
H	0.48631400	-0.28234600	8.30552500
H	1.54137000	1.05546300	6.35228400
H	0.30210500	-2.60372300	7.50468900
H	-0.92440000	-2.28906200	5.47610400
H	0.53351700	-2.92164700	5.06474100
H	3.53244800	-2.93012000	6.23240100