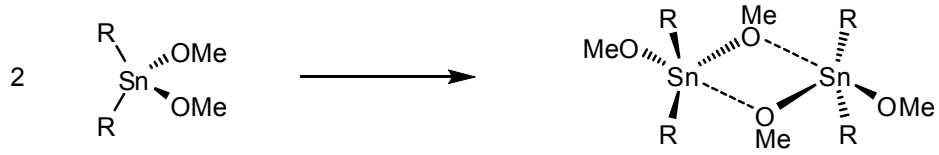
Table S-2 Dependence of energy change in the dimerization on the alkyl chain length [a]



Method	R	*E* / au		BSSE / kcal mol^{-1}	ΔE_{corr} / kcal mol^{-1} [b]
		monomer	dimer		
B3LYP	Me	-313.584983	-627.204401	3.47	-18.14
	Et	-392.220321	-784.473231	3.59	-16.86
	Bu	-549.511298	-1099.052037	3.69	-14.78
MP2	Me	-312.538685	-625.131236	11.72	-22.08
	Et	-390.891436	-781.843256	14.02	-23.88
	Bu	-547.620444	-1095.306616	16.85	-24.39

[a] All calculations were performed using LANL2DZ for Sn and 6-311+G* for C, H, O atoms. [b] Corrected by BSSE.

Table S-3 Single point calculation performed by various levels of theory in dimerization of **1** to **2a** [a]

Method	E / au		BSSE / kcal mol^{-1}	ΔE_{corr} / kcal mol^{-1} [b]
	1	**2a**		
B3LYP	-313.584784	-627.202968	3.48	-17.48
B3LYP [c]	-313.584983	-627.204401	3.47	-18.14
HF	-311.516521	-623.066039	4.47	-16.24
HF [c]	-311.519844	-623.072424	4.27	-16.27
MP2	-312.538685	-625.131236	11.72	-22.08
MP3	-312.579878	-625.213521	11.84	-21.89
MP4(SDQ)	-312.604548	-625.260901	11.74	-20.77

[a] All calculations were performed using LANL2DZ for Sn and 6-311+G* for C, H, O atoms. The geometries of **1** and **2a** were optimized by MP2 except otherwise mentioned.
[b] Corrected by BSSE. [c] The geometry was optimized by the same level of theory.

Table S-4 Calculation results at MP2/6-311+G*-LANL2DZ(Sn) in dimerization of **1** to **2** [a]

	E / au	H / au	S / cal mol^{-1} K^{-1}	G / au	BSSE / kcal mol^{-1}	$T\Delta S$ / kcal mol^{-1}	ΔH_{corr} [b] / kcal mol^{-1}	ΔG_{corr} [b] / kcal mol^{-1}	Sn–O / Å	
									Sn_a–O_a Sn_b–O_b	Sn_a–O_b Sn_b–O_a
1	-312.538685	-312.366962	118.644	-312.423333					1.9489	
2a	-625.131236	-624.785640	192.460	-624.877084	11.72	-13.37	-20.73	-7.37	2.0274	2.2358
2b	-625.125813	-624.780253	183.390	-624.867387	13.11	-16.07	-15.97	0.10	2.0208 (Sn_a–O_a) 2.0551 (Sn_b–O_b)	2.2497 (Sn_a–O_b) 2.1991 (Sn_b–O_a)
2c	-625.122337	-624.776597	179.881	-624.862064	14.73	-17.12	-12.05	5.06	2.0494	2.2052
2d	-625.122416	-624.776740	179.343	-624.861951	14.84	-17.28	-12.02	5.25	2.0601	2.1870
2e	-625.125516	-624.780066	189.986	-624.870334	13.47	-14.10	-15.48	-1.38	2.0885 (Sn_a–O_a) 2.1573 (Sn_b–O_b)	2.1497 (Sn_a–O_b) 2.0829 (Sn_b–O_a)

[a] The calculated thermodynamic parameters (H, S, G) are at 298.15 K and 1 atm. [b] Corrected by BSSE.

Table S-5 Calculation results at MP2/6-31G*-LANL2DZ(Sn) in trimerization of **1** to **3** [a]

	E / au	H / au	S / cal mol^{-1} K^{-1}	G / au	BSSE / kcal mol^{-1}	$T\Delta S$ / kcal mol^{-1}	ΔH_{corr} [b] / kcal mol^{-1}	ΔG_{corr} [b] / kcal mol^{-1}
1	-312.375036	-312.201283	116.858	-312.256806				
3a	-937.223514	-936.697604	239.054	-936.811187	33.94	-33.25	-24.89	8.36
3g	-937.222514	-936.696684	240.296	-936.810856	33.95	-32.88	-24.31	8.57
3m	-937.221455	-936.695678	239.319	-936.809386	36.25	-33.17	-21.37	11.80
3s	-937.211771	-936.685822	246.625	-936.803001	31.16	-30.99	-20.28	10.71
3w	-937.209479	-936.683579	243.627	-936.799334	34.37	-31.89	-15.66	16.23

[a] The calculated thermodynamic parameters (H, S, G) are at 298.15 K and 1 atm. [b] Corrected by BSSE.

Table S-6 Calculation results at MP2/6-311+G*-LANL2DZ(Sn) in dimerization of **4** to **5** [a]

	E / au	*H* / au	*S* / cal mol^{-1} K^{-1}	*G* / au	BSSE / kcal mol^{-1}	$T\Delta S$ / kcal mol^{-1}	ΔH_{corr} [b] / kcal mol^{-1}	ΔG_{corr} [b] / kcal mol^{-1}	Sn–O / Å
4	-237.446801	-237.282249	112.825	-237.335856					1.9637
5a	-474.930614	-474.599351	167.438	-474.678906	12.17	-17.36	-9.70	7.66	2.0376 (Sn_a–O_a, Sn_b–O_b) 2.3344 (Sn_b–O_a, Sn_b–O_a)
5b	-474.923602	-474.592290	168.483	-474.672342	13.26	-17.04	-4.18	12.86	2.1403 (Sn_a–O_a, Sn_b–O_a) 2.1661 (Sn_b–O_b, Sn_a–O_b)
5c	-474.912592	-474.581186	173.578	-474.663658	7.69	-15.53	-2.78	12.75	1.9994 (Sn_a–O_a) 1.9956 (Sn_b–O_b) 2.6431 (Sn_a–O_b)

[a] The calculated thermodynamic parameters (*H*, *S*, *G*) are at 298.15 K and 1 atm. [b] Corrected by BSSE.

Table S-8 Calculation results at MP2/6-311+G*-LANL2DZ(Si) in dimerization of the silicon analogs (**6** and **8**) [a]

	E / au	*H* / au	*S* / cal mol^{-1} K^{-1}	*G* / au	BSSE / kcal mol^{-1}	$T\Delta S$ / kcal mol^{-1}	ΔH_{corr} [b] / kcal mol^{-1}	ΔG_{corr} [b] / kcal mol^{-1}	Si–O / Å
6	-313.079443	-312.904815	105.853	-312.955109					1.7063, 1.7072
7	-626.174803	-625.823911	177.972	-625.908471	7.81	-10.06	-1.15	8.90	1.7051 (Si_a–O_a, Si_b–O_b) 3.4006, 3.4158 (Si_b–O_a, Si_b–O_a)
8	-237.987888	-237.820369	97.180	-237.866542					1.7247
9	-475.990136	-475.653277	159.038	-475.728841	6.41	-10.53	-1.46	9.07	1.7328 (Si_a–O_a, Si_b–O_b) 3.7380, 3.7426 (Si_b–O_a, Si_b–O_a)

[a] The calculated thermodynamic parameters (*H*, *S*, *G*) are at 298.15 K and 1 atm. [b] Corrected by BSSE.

Table S-9-1 Calculation results at MP2/6-311+G*-LANL2DZ(Sn) in dimerization of the distannoxane (**10**) [a]

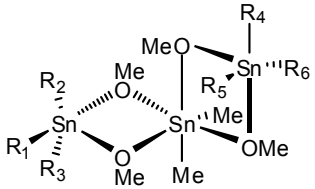
	E / au	H / au	S / cal mol^{-1} K^{-1}	G / au	BSSE / kcal mol^{-1}	$T\Delta S$ / kcal mol^{-1}	ΔH_{corr} [b] / kcal mol^{-1}	ΔG_{corr} [b] / kcal mol^{-1}
10	-1160.203628	-1160.031568	144.798	-1160.100366				
11	-2320.494067	-2320.147373	230.042	-2320.256674	27.76	-17.76	-25.10	-7.34

[a] The calculated thermodynamic parameters (H, S, G) are at 298.15 K and 1 atm. [b] Corrected by BSSE.

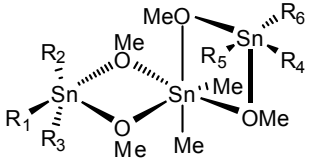
Table S-9-2 Calculation results at MP2/6-311+G*-LANL2DZ(Sn) in dimerization of the distannoxane (**12**) [a]

	E / au	*H* / au	*S* / cal mol^{-1} K^{-1}	*G* / au	BSSE / kcal mol^{-1}	$T\Delta S$ / kcal mol^{-1}	ΔH_{corr} [b] / kcal mol^{-1}	ΔG_{corr} [b] / kcal mol^{-1}
12	-776.199840	-776.015745	147.533	-776.085842				
13a	-1552.516322	-1552.145298	235.089	-1552.256996	22.29	-17.88	-49.13	-31.24
13b	-1552.503739	-1552.132538	231.035	-1552.242310	26.25	-19.09	-37.16	-18.07

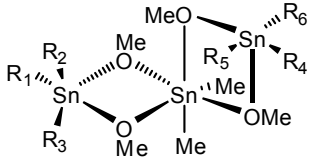
[a] The calculated thermodynamic parameters (*H*, *S*, *G*) are at 298.15 K and 1 atm. [b] Corrected by BSSE.



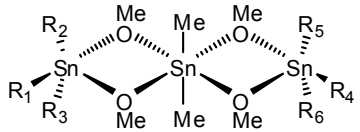
3a-3f



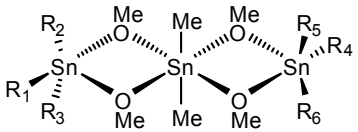
3g-3l



3m-3r



3s-3v



3w-3z

Table S-10 Relative enthalpies and free energies of the trimer **3** calculated using B3LYP/6-31G*-LANL2DZ(Sn) [a]

	R_1	R_2	R_3	R_4	R_5	R_6	*H*(relative) / kcal mol^{-1}	*G*(relative) / kcal mol^{-1}
3a	OMe	Me	Me	OMe	Me	Me	0	0
3b	OMe	Me	Me	Me	OMe	Me	1.34	2.52
3c	OMe	Me	Me	Me	Me	OMe	2.10	3.16
3d	Me	OMe	Me	Me	OMe	Me	2.40	4.71
3e	Me	OMe	Me	Me	Me	OMe	3.29	5.05
3f	Me	Me	OMe	Me	Me	OMe	4.35	6.14
3g	OMe	Me	Me	OMe	Me	Me	0.23	0.94
3h	OMe	Me	Me	Me	OMe	Me	2.60	3.74
3i	OMe	Me	Me	Me	Me	OMe	3.52	5.11
3j	Me	OMe	Me	Me	OMe	Me	4.17	5.69
3k	Me	OMe	Me	Me	Me	OMe	5.01	6.65
3l	Me	Me	OMe	Me	Me	OMe	6.06	7.04
3m	OMe	Me	Me	OMe	Me	Me	1.18	1.25
3n	OMe	Me	Me	Me	OMe	Me	3.27	4.35
3o	OMe	Me	Me	Me	Me	OMe	4.34	3.52
3p	Me	OMe	Me	Me	OMe	Me	6.20	7.12
3q	Me	OMe	Me	Me	Me	OMe	*b*	*b*
3r	Me	Me	OMe	Me	Me	OMe	7.92	6.65
3s	OMe	Me	Me	OMe	Me	Me	4.41	3.40
3t	OMe	Me	Me	Me	OMe	Me	6.63	5.20
3u	Me	OMe	Me	Me	OMe	Me	9.98	10.51
3v	Me	OMe	Me	Me	Me	OMe	8.73	7.94
3w	OMe	Me	Me	OMe	Me	Me	6.44	4.76
3x	OMe	Me	Me	Me	OMe	Me	9.31	8.16
3y	Me	OMe	Me	Me	OMe	Me	*c*	*c*
3z	Me	OMe	Me	Me	Me	OMe	12.14	12.35

[a] The calculated enthalpies and free energies are at 298.15 K and 1 atm.
[b] The geometry changed to **3h** during the optimization calculation. [c] The geometry changed to **3t** during the optimization calculation.

Table S-11 Relative enthalpies and free energies of the trimer **3** calculated using B3LYP/6-31+G*-LANL2DZ(Sn) [a]

	R_1	R_2	R_3	R_4	R_5	R_6	*H*(relative) / kcal mol^{-1}	*G*(relative) / kcal mol^{-1}
3a	OMe	Me	Me	OMe	Me	Me	0	0
3g	OMe	Me	Me	OMe	Me	Me	0.09	-0.48
3m	OMe	Me	Me	OMe	Me	Me	1.12	1.25
3s	OMe	Me	Me	OMe	Me	Me	3.34	2.26
3w	OMe	Me	Me	OMe	Me	Me	5.90	2.58

[a] The calculated enthalpies and free energies are at 298.15 K and 1 atm.

Table S-12 Relative enthalpies and free energies of the trimer **3** calculated using B3LYP/6-311+G*-LANL2DZ(Sn) [a]

	R_1	R_2	R_3	R_4	R_5	R_6	*H*(relative) / kcal mol^{-1}	*G*(relative) / kcal mol^{-1}
3a	OMe	Me	Me	OMe	Me	Me	0	0
3g	OMe	Me	Me	OMe	Me	Me	0.09	-0.24
3m	OMe	Me	Me	OMe	Me	Me	0.96	0.85
3s	OMe	Me	Me	OMe	Me	Me	3.22	2.00
3w	OMe	Me	Me	OMe	Me	Me	5.27	1.60

[a] The calculated enthalpies and free energies are at 298.15 K and 1 atm.

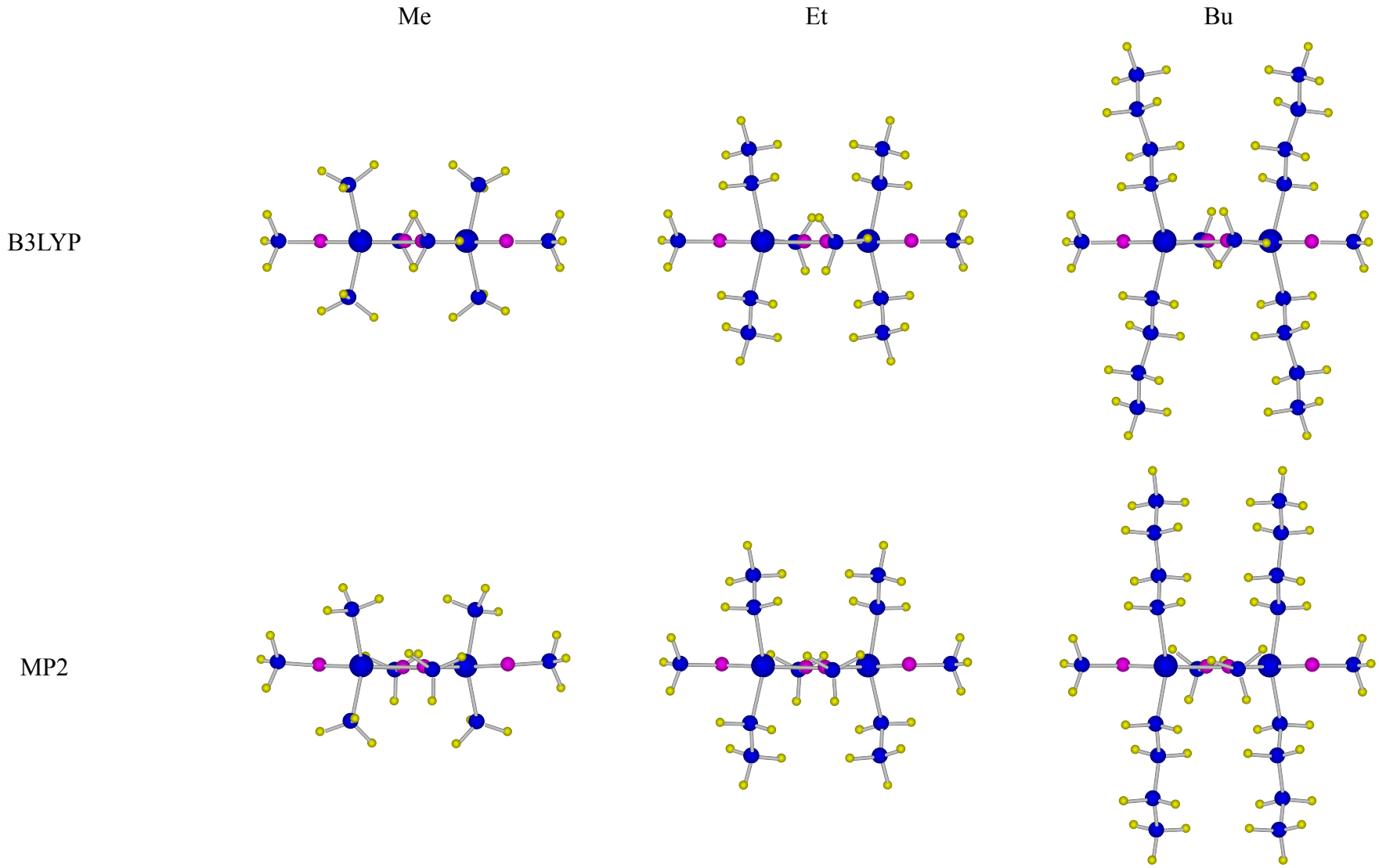


Figure S-6 Optimized structures of dialkyltin dimethoxides using 6-311+G*-LANL2DZ(Sn).

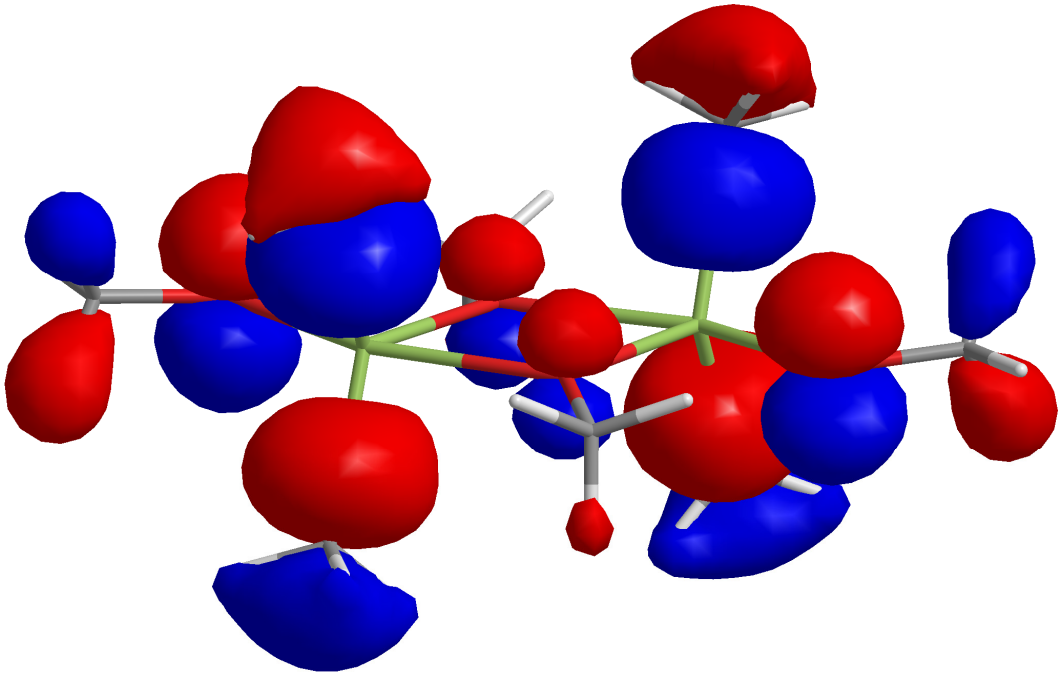


Figure S-7 HOMO of **2a** calculated using MP2/6-311+G*-LANL2DZ(Sn). The isocontour value is 0.03.

Optimized coordinates and energies

Optimized coordinates and energies from Gaussian Archive entries in output files are shown below. "HF", "MP2", "ZeroPoint", and "Thermal" mean electronic energy, electronic energy including MP2 correlation energy, zero-point correction, and thermal correction to energy in hartrees, respectively.

Dimethyltin dimethoxide monomer (1)

B3LYP/6-31G-LANL2DZ(Sn)*

Sn,0.571287576,-0.5634426413,-0.5171162852\O,-1.3523018679,-0.362406925,-0.5498246545\O,1.4239092448,1.1714289746,-0.570935524\C,1.5544780994,2.0503803691,0.5253527103\C,1.1435164715,-1.5759118707,1.278709817\C,1.0557906875,-1.4678021496,-2.3698869842\C,-2.1392733985,0.0915751445,0.530396579\H,2.3175691295,2.8008599131,0.2826189181\H,1.8724243015,1.5423552152,1.4512359372\H,0.6164720347,2.5857780013,0.7417269745\H,0.8309710231,-1.0190967738,2.1670947173\H,2.2305138335,-1.6972761903,1.3144384217\H,0.6815132657,-2.5671971336,1.315442556\H,0.8813016711,-0.7532365593,-3.1791671916\H,2.1066151191,-1.7703608323,-2.3954964618\H,0.4307221116,-2.3484929816,-2.5422093561\H,-3.192689248,-0.1204420477,0.3075565024\H,-2.0430096018,1.1775349366,0.6879792736\H,-1.894359453,-0.4093694492,1.4820990503

HF=-313.4907336

ZeroPoint=0.1560453

Thermal=0.1693675

B3LYP/6-31+G-LANL2DZ(Sn)*

Sn,0.6081566955,-0.6157221485,-0.5073831272\O,-1.3205889184,-0.3627473777,-0.5106676229\O,1.4862532328,1.1200692636,-0.5139421983\C,1.4892081594,2.0682526503,0.5355266133\C,1.1638002006,-1.6635571396,1.2782390677\C,1.0619952104,-1.4789693687,-2.3879073819\C,-2.1035527414,0.1703944338,0.5396524209\H,2.232973317,2.8396197899,0.3002289592\H,1.7608741298,1.6241987819,1.5074925627\H,0.5106592844,2.5612563377,0.6426714489\H,0.8698598921,-1.1053982819,2.1730285272\H,2.2481817455,-1.8132273848,1.3096729256\H,0.6764765671,-2.6437039685,1.3114083412\H,0.7100199035,-0.8139252505,-3.1821984647\H,2.1417257109,-1.6170824743,-2.5005165915\H,0.5669097205,-2.4485840808,-2.4988639668\H,-3.16036144,-0.0094659425,0.3064906455\H,-1.9590499334,1.2566909654,0.6453359488\H,-1.8880897364,-0.3032218047,1.5117468922

HF=-313.5112207

ZeroPoint=0.1554341

Thermal=0.1688032

B3LYP/6-311+G-LANL2DZ(Sn)*

Sn,-0.3890100176,-0.0004469944,0.0417474435\O,0.5429223522,1.5931775839,-0.5937860228\O,0.5490576317,-1.5879131245,-0.6002119203\C,1.8327284712,-2.0530101157,-0.2467959817\C,-0.3619764485,-0.0048778794,2.1857150758\C,-2.2377460859,-0.0017234025,-0.9881510555\C,1.8278534199,2.0577691088,-0.2443443708\H,1.9547101602,-3.0655795668,-0.6428052581\H,1.9824764059,-2.0994505204,0.8418330056\H,2.6264211132,-1.4261163378,-0.6743401664\H,0.6610064405,-0.0017374028,2.5659062873\H,-0.8661326191,-0.8933641774,2.5704066639\H,-0.8729048721,0.8781030805,2.5741189935\H,-2.0446984145,-0.0059958164,-2.0612594453\H,-2.8219729334,-0.8874298801,-0.7351557027\H,-2.8191841095,0.8876458205,-0.7416855438\H,1.9461873568,3.0731517677,-0.634210472\H,2.6200418459,1.4349126429,-0.6804724838\H,1.9835544942,2.0971481673,0.8437334861

HF=-313.5849828

ZeroPoint=0.1546555

Thermal=0.1680554

HF/6-31G-LANL2DZ(Sn)*

Sn,0.3638699977,-0.0007875688,0.0280835553\O,-0.5296268131,-1.5502956526,-0.6175459814\O,-0.52260404,1.5530587725,-0.6169034121\C,-1.7594145418,2.0702353372,-0.2462821954\C,0.2821556359,-0.0008969406,2.1577658407\C,2.2793628466,-0.0046274614,-0.8612819291\C,-1.7681405575,-2.0630060939,-0.2464196974\H,-1.8496992857,3.0791622688,-0.6332191308\H,-1.882131927,2.1176977384,0.8356713185\H,-2.5803799357,1.4819905328,-0.6512236868\H,-0.7421395698,0.0009744621,2.5146094689\H,0.7790326035,0.8775433383,2.555768634\H,0.7757776451,-0.8812306715,2.5556385887\H,2.1795461554,-0.0050953086,-1.9405495242\H,2.8415932254,0.8755762278,-0.5700879141\H,2.8389209599,-0.8861812037,-0.5690548544\H,-1.8627189659,-3.0711473191,-0.6343757481\H,-2.58712123,-1.4710965521,-0.6500332551\H,-1.8901130253,-2.1111490911,0.8355813531

HF=-311.4427819

ZeroPoint=0.1662544

Thermal=0.1791439

HF/6-31+G-LANL2DZ(Sn)*

Sn,0.3768531555,0.0091870142,0.0327357716\O,-0.5685217999,-1.5239902495,-0.5957509762\O,-0.5344721143,1.5763863937,-0.5600229337\C,-1.8045975219,2.0581509127,-0.2576825706\C,0.3695400852,-0.0160302056,2.163751792\C,2.2415206652,0.0040242895,-0.9583031559\C,-1.80175976,-2.0494687509,-0.2219130074\H,-1.8963364033,3.0671361638,-0.6440718564\H,-1.9862178048,2.0934897775,0.8163202833\H,-2.5821358834,1.449823123,-0.7146590594\H,-0.6433390037,0.0079046055,2.5526409421\H,0.9001420632,0.8448969323,2.557818493\H,0.8521507962,-0.9129277727,2.5389145153\H,2.0775489306,-0.0232186753,-2.0296610053\H,2.8082989689,0.8975749797,-0.7204159494\H,2.8279743331,-0.8644533284,-0.6787109717\H,-1.9103306093,-3.0336146708,-0.6640046217\H,-2.6240243229,-1.4296091746,-0.5731125033\H,-1.8929761682,-2.1560948368,0.8586959755

HF=-311.4555977

ZeroPoint=0.1655953

Thermal=0.178648

HF/6-311+G-LANL2DZ(Sn)*

Sn,0.3838813799,-0.0000163235,0.0349406947\O,-0.5737843863,-1.5469484586,-0.5441336454\O,-0.5735998622,1.5470804671,-0.5439975622\C,-1.8148981953,2.0821681827,-0.2306119851\C,0.444408832,-0.0001150362,2.1613609542\C,2.1935377384,-0.0000681286,-1.0421001777\C,-1.8150754008,-2.0820065032,-0.2306677069\H,-1.8911738933,3.0739930701,-0.6616116312\H,-1.9647667582,2.1743213666,0.8450299339\H,-2.6258714958,1.4785908867,-0.6328057535\H,-0.5568857842,0.0000261436,2.5764019995\H,0.961351006,0.8781467485,2.5309273096\H,0.9610763737,-0.8785681905,2.5308563681\H,1.9721576598,-0.0003171767,-2.101853252\H,2.7817147446,0.8804938346,-0.8138484473\H,2.7819075874,-0.8804053244,-0.8134770708\H,-1.8914321741,-3.0738001373,-0.6617250339\H,-2.6260596713,-1.4783684894,-0.6327478033\H,-1.9648504476,-2.1742237334,0.8449818158

HF=-311.5198438

ZeroPoint=0.1644711

Thermal=0.1776142

MP2/6-31G-LANL2DZ(Sn)*

Sn,0.573395968,-0.5497659798,-0.5400395718\O,-1.3460160453,-0.3194665356,-0.5735910925\O,1.4659989552,1.1649648544,-0.5749048711\C,1.5247512278,2.0382846482,0.5440141771\C,1.1139045967,-1.5721723855,1.2502544608\C,1.0663006689,-1.4849929056,-2.3663330012\C,-2.0991738526,0.125611637,0.5456932152\H,2.2755954001,2.8057669739,0.3360115778\H,1.8161194919,1.521111017,1.4696651748\H,0.5642077687,2.5401934781,0.7213765637\H,0.8193669856,-1.0138064639,2.1416820783\H,2.1954417086,-1.723300043,1.2881963286\H,0.6287569248,-2.5505169862,1.2887058656\H,0.737968969,-0.864453387,-3.2023968668\H,2.145565537,-1.6292428108,-2.4508291252\H,0.5771155582,-2.4578615764,-2.4498949664\H,-3.1568261282,-0.0593587269,0.3378211498\H,-1.9697513838,1.2015465384,0.7235734395\H,-1.8372713508,-0.4076643461,1.4710104638

HF=-311.4396013

MP2=-312.375036

ZeroPoint=0.1598082

Thermal=0.1728092

MP2/6-31+G-LANL2DZ(Sn)*

Sn,0.60792414,-0.6296001908,-0.5134162962\O,-1.3111895188,-0.3159507478,-0.5474956903\O,1.5507013538,1.0711669273,-0.4801924047\C,1.5270039759,2.0109700855,0.5901980572\C,1.0847445122,-1.6998668272,1.2714738644\C,1.0628902985,-1.4771129872,-2.3924369071\C,-2.0744582714,0.2662732828,0.5051025214\H,2.3247580563,2.7380087624,0.4139319421\H,1.7045773043,1.535899449,1.5658413005\H,0.5705606086,2.5481220923,0.628160302\H,0.7903938339,-1.1364478171,2.1616754035\H,2.1611874822,-1.886847331,1.3291138804\H,0.5636288189,-2.6616662382,1.2912754712\H,0.1407969165,-1.5877437112,-2.9693014136\H,1.7409902922,-

0.8108459387,-2.9323780033\H,1.5368758353,-2.4578252311,-2.2978487519\H,-3.1319027493,0.0941201615,0.2854652326\H,-1.9053349983,1.3489176391,0.5686222367\H,-1.8486968909,-0.1846943796,1.482224255

HF=-311.4518358

MP2=-312.4057436

ZeroPoint=0.1587144

Thermal=0.1718747

MP2/6-311+G-LANL2DZ(Sn)*

Sn,-0.4043512058,-0.0089451051,0.0368449505\O,0.5032883947,1.6174356878,-0.537025333\O,0.5612424489,-1.5532178533,-0.6567504633\C,1.8684454887,-1.9641226706,-0.3105661155\C,-0.3570388614,-0.0882654194,2.1642222929\C,-2.2432061612,-0.003626011,-0.9849283823\C,1.7968291794,2.0461771482,-0.162375346\H,2.0205781398,-2.9755023351,-0.6947843458\H,2.0287307947,-1.9881730737,0.7763626939\H,2.628487303,-1.3120109102,-0.7580913523\H,0.6702307543,-0.0840422534,2.5343333277\H,-0.8423213614,-0.9969715874,2.5264851555\H,-0.8734825902,0.7731198239,2.5929120555\H,-2.2828439731,-0.8672890543,-1.6504111692\H,-3.096878806,-0.0443046137,-0.3068934549\H,-2.3144100714,0.9054600661,-1.5839441521\H,1.9149271869,3.086149651,-0.4756578047\H,2.5774218218,1.452077998,-0.6532506638\H,1.9576857096,2.0003134658,0.9237606396

HF=-311.5165214

MP2=-312.5386845

ZeroPoint=0.157534

Thermal=0.1707787

Dimethyltin dimethoxide dimer (2a)

B3LYP/6-31G-LANL2DZ(Sn)*

Sn,1.7573569026,0.1761275408,-0.0129609415\O,0.2519383923,-1.1781977617,0.0155309313\C,2.220119688,1.1264839419,1.8426571542\O,3.0334625028,-1.3403158174,-0.017286968\C,2.137359862,1.0602256128,-1.9184005711\C,0.4201768278,-2.5935517811,0.1387083014\C,4.4234881569,-1.1555391247,-0.0662542755\Sn,-1.7647937687,-0.1605644347,-0.011586146\O,-0.2593563668,1.1937914503,0.0143325287\C,-2.2263131334,-1.1087685251,1.8454421488\O,-3.0408998481,1.3558756085,-0.0168151608\C,-2.1460683873,-1.0468744109,-1.9157437864\C,-0.4275110951,2.6092868886,0.1359880788\C,-4.4309583782,1.1710466307,-0.0646344866\H,2.0089505471,2.1988835,1.8149908417\H,3.2720609006,0.9785090892,2.1027341572\H,1.6077999444,0.6779835539,2.6320356764\H,1.620813562,0.4703670367,-2.6829145632\H,1.7743228093,2.0893077149,-1.9768996101\H,3.2067931111,1.0470517912,-2.1485669803\H,0.2857179636,-2.9038985503,1.1823110131\H,1.4210234896,-2.8750405275,-0.1894146303\H,-0.3310627829,-3.0991044693,-0.4801036946\H,4.9196745424,-2.1356860808,-0.033764161\H,4.8135511534,-0.5686968636,0.785481727\H,4.7604773955,-0.6531150813,-0.9910763253\H,-2.0151496419,-2.1811971626,1.8188826266\H,-3.2780831924,-0.9605031532,2.1060454594\H,-1.6134750262,-0.659343655,2.6338920514\H,-1.7831727657,-

2.0760624843,-1.9732521017\H,-3.215643071,-1.0338643999,-2.1452606329\H,-1.6299359026,-0.4579740487,-2.6812751712\H,0.3233242294,3.114123337,-0.4838985996\H,-0.2923673587,2.9208366878,1.1791437573\H,-1.4285718803,2.8904005399,-0.1918029907\H,-4.9271203009,2.1512324958,-0.0329544955\H,-4.8204513099,0.5851991341,0.7880466113\H,-4.768569771,0.6675457779,-0.9886437722

HF=-627.0152079

ZeroPoint=0.3158184

Thermal=0.3425428

B3LYP/6-31+G-LANL2DZ(Sn)*

Sn,1.7656461459,0.1866725736,-0.015521416\O,0.2698065956,-1.1806608293,0.0308369041\C,2.2412690521,1.1513013575,1.8328347334\O,3.0677665172,-1.3228514315,-0.0276405382\C,2.131160598,1.0527902263,-1.9342701522\C,0.4402601707,-2.5970376856,0.1662033279\C,4.4651408306,-1.1680161806,-0.0687830365\Sn,-1.773082886,-0.1711125652,-0.0141301052\O,-0.2772129169,1.1962726912,0.0296432305\C,-2.2474675466,-1.1335975324,1.8356611998\O,-3.07521131,1.3383971426,-0.0271275889\C,-2.1398802742,-1.0394532003,-1.9316288203\C,-0.4475759817,2.6128054586,0.163483653\C,-4.4726128332,1.1835154955,-0.0671554019\H,2.2287744152,2.2414930934,1.7355550101\H,3.2313591145,0.8395742042,2.1790450958\H,1.5037214755,0.8684473775,2.5915077455\H,1.7165210409,0.3872691121,-2.6994952755\H,1.6650704034,2.0358682696,-2.0417461715\H,3.2067531159,1.1469470385,-2.1165747029\H,0.2512196676,-2.8991711059,1.2040495617\H,1.4588328,-2.8758099171,-0.1088085309\H,-0.2746479478,-3.1080371175,-0.4907717379\H,4.9339077982,-2.16162234,-0.0452264982\H,4.8563801082,-0.5992188001,0.7937928521\H,4.8090984715,-0.6621420151,-0.9882649358\H,-2.2350330327,-2.2239013776,1.7396385309\H,-3.2373275186,-0.8214723467,2.1821707611\H,-1.509414672,-0.8498604399,2.5935126185\H,-1.6738811201,-2.0226654273,-2.0382691332\H,-3.2155947478,-1.13379922,-2.1131139996\H,-1.7257319614,-0.3748313149,-2.6979007825\H,0.2668928689,3.1230433754,-0.4945602902\H,-0.2578417832,2.9161401209,1.2008527856\H,-1.4663321982,2.891259846,-0.1111699572\H,-4.9413639427,2.1771485884,-0.0444342447\H,-4.8632745921,0.6157163941,0.7963394559\H,-4.8171859252,0.6765784813,-0.9858211468

HF=-627.0499902

ZeroPoint=0.3141139

Thermal=0.3412235

B3LYP/6-311+G-LANL2DZ(Sn)*

Sn,1.7566056645,0.2250474036,-0.0006885011\O,0.2814562196,-1.174835656,0.0003552853\C,2.1583129405,1.1520327092,1.8857059569\O,3.0789670614,-1.2782480169,0.0002112418\C,2.1575137552,1.1495786044,-1.8883727319\C,0.4608347484,-2.5956247936,0.0011556099\C,4.4754615817,-1.1433079019,0.0007657118\Sn,-1.7640254085,-0.2094782945,0.0007070364\O,-0.2888802258,1.1904084883,-0.0009172592\C,-2.1645338112,-1.1343181069,1.888410437\O,-3.0863922697,1.293808339,0.0007353412\C,-2.1661353411,-1.1361467141,-1.8856735246\C,-0.4682663511,2.6111963847,-0.001754945\C,-4.4828871869,1.1589022569,0.0024866225\H,2.3298967641,2.2250958656,1.7797360569\H,3.0397553698,0.7038829126,2.3459783284\H,1.3063331883,1.0107174631,2.552858557\H,1.3082968108,1.0005106067,-2.5573815754\H,2.3213893228,2.2240659474,-1.7848980923\H,3.0431589465,0.7062131802,-2.3451989013\H,-0.0095431348,-

3.0235813738,0.8916873813\H,1.523430944,-2.8291522691,0.0032151034\H,-0.0061000109,-3.0242546553,-0.8908548358\H,4.9310960622,-2.140013384,0.0027858087\H,4.8518177177,-0.6098850622,0.8885159577\H,4.8527336268,-0.6130569338,-0.8884840576\H,-2.336230333,-2.207490767,1.7837330111\H,-3.0456532392,-0.6856278476,2.3487736333\H,-1.3121047061,-0.9923059051,2.5548402779\H,-2.3300473631,-2.2105022449,-1.7808957635\H,-3.0520210439,-0.6932113025,-2.3424517195\H,-1.3173161526,-0.9879074143,-2.555371123\H,-0.002344633,3.0386864848,-0.8948417147\H,0.0031147593,3.0402964993,0.8876949503\H,-1.5308613038,2.8447202711,0.0011881401\H,-4.9384986609,2.1556196671,0.0038193004\H,-4.8585902081,0.6264051372,0.8910693618\H,-4.8608361003,0.6277404223,-0.8859313665

HF=-627.2044013

ZeroPoint=0.3126666

Thermal=0.3397017

HF/6-31G-LANL2DZ(Sn)*

Sn,-1.728523037,-0.2909367608,-0.0318137336\O,-0.3637970913,1.1545517501,0.0010013574\C,-2.0960907875,-1.2581768186,1.8261810913\O,-3.1177182715,1.0730533326,-0.047463039\C,-2.0309150683,-1.2349688067,-1.9133522885\C,-0.6624439516,2.5342891363,0.0043090236\C,-4.4848325872,0.8605300413,-0.0728236885\Sn,1.7284427764,0.2909388688,0.0319824215\O,0.3637390709,-1.1545698387,-0.0008693193\C,2.0310453291,1.2345825186,1.9136841343\O,3.117661071,-1.0730333777,0.0474399095\C,2.0959638665,1.2585024336,-1.8258616158\C,0.6624692371,-2.534287992,-0.0046540484\C,4.4847749631,-0.8604703632,0.0725001238\H,-1.7121665577,-2.2706642253,1.8461714771\H,-3.1574565987,-1.2825954071,2.0456460337\H,-1.6062486427,-0.6976623326,2.6166667884\H,-1.5129318838,-0.6655220197,-2.6791295377\H,-1.6473372573,-2.2476146524,-1.9320785031\H,-3.0838671573,-1.255417598,-2.1704965533\H,0.2674708138,3.0904636925,0.0244040509\H,-1.2491182709,2.7974290374,0.8724562006\H,-1.2177783703,2.8084115228,-0.8808963162\H,-5.0005871138,1.8164086534,-0.0758168025\H,-4.8384116146,0.3043425312,0.7971873685\H,-4.8075203076,0.315502788,-0.9616991563\H,1.6460174793,2.2466591278,1.9332350494\H,3.0841975219,1.2564375425,2.1699200037\H,1.5146014648,0.6639828088,2.6796393779\H,1.7125836212,2.2712063291,-1.8454155525\H,3.1572736962,1.2824187948,-2.0456409911\H,1.6055630069,0.6985174108,-2.6163772096\H,-0.2674393894,-3.0905091571,-0.023678365\H,1.2189027068,-2.8084547268,0.8798317973\H,1.2480954463,-2.7973287863,-0.8735541519\H,5.0005515166,-1.8163366303,0.0756947859\H,4.8076083147,-0.3151645718,0.9611531859\H,4.8381845942,-0.3045426102,-0.7977448248

HF=-622.9150556

ZeroPoint=0.3359906

Thermal=0.3622575

HF/6-31+G-LANL2DZ(Sn)*

Sn,1.7300492572,0.3047433376,-0.0319304305\O,0.3799233007,-1.1543018309,0.0009839482\C,2.0865351922,1.2662042584,1.829678742\O,3.1388345059,-1.0490719963,-0.0473505155\C,2.0219156027,1.2415293134,-1.9172187019\C,0.6845773393,-2.5330388839,0.0050464451\C,4.511542004,-0.869489822,-0.0725519966\Sn,-1.7299066626,-0.3048235689,0.0319203999\O,-0.3798067273,1.1542476849,-0.0010511651\C,-2.021795271,-1.2416616516,1.9171796504\O,-3.1386778388,1.0490081268,0.0475312816\C,-2.0867500793,-

1.2660390497,-1.8297434492\C,-0.6845687871,2.5329617979,-0.0048666115\C,-4.5113974474,0.8694690946,0.0723878002\H,1.7062214137,2.2804670516,1.8520993527\H,3.1469669955,1.2874168897,2.0565579899\H,1.58978334,0.7047986233,2.615852373\H,1.4990988985,0.6695055002,-2.6784423926\H,1.6401945506,2.2552492902,-1.9400761508\H,3.0739613465,1.260149084,-2.1804725282\H,-0.2428884417,-3.0944870982,0.0246194344\H,1.2720598126,-2.7926407124,0.8745035851\H,1.2421616545,-2.8044010744,-0.8803558279\H,5.0009838829,-1.8391659966,-0.0739826632\H,4.8738528547,-0.3207523984,0.7982570085\H,4.8431611311,-0.3336277372,-0.9633719613\H,-1.6388624739,-2.2549114321,1.9404678877\H,-3.0739769527,-1.2614904766,2.1798082095\H,-1.5001594611,-0.6688418375,2.6786168844\H,-1.7030412883,-2.2789730727,-1.8537883442\H,-3.1475426485,-1.2906423648,-2.0546218592\H,-1.5934832333,-0.7022160081,-2.6163862312\H,0.242843665,3.0944778696,-0.0247810322\H,-1.2418024644,2.804217503,0.8807935231\H,-1.2724379106,2.7926019439,-0.8740456077\H,-5.0007901571,1.8391687176,0.0748364501\H,-4.8431629828,0.332644233,0.9625777062\H,-4.8736178407,0.3217153948,-0.7990732414

HF=-622.9378212

ZeroPoint=0.3348848

Thermal=0.3612654

HF/6-311+G-LANL2DZ(Sn)*

Sn,1.7186177009,0.330498998,-0.0321119403\O,0.3828523756,-1.1491837748,0.0012522307\C,2.073240797,1.2733498595,1.8350727843\O,3.1294538196,-1.0271864757,-0.0471918635\C,2.0079753975,1.2474107908,-1.923310674\C,0.6917988877,-2.5247387284,0.0053331295\C,4.5051263688,-0.9151875174,-0.071638248\Sn,-1.7186159252,-0.3304967152,0.0320659402\O,-0.3828496422,1.1491820836,-0.0013299439\C,-2.0080106771,-1.2473606221,1.9232810281\O,-3.1294429612,1.0271994335,0.0471527971\C,-2.0732191086,-1.2734106116,-1.835090096\C,-0.691795569,2.5247375681,-0.0054679688\C,-4.5051147137,0.9152055945,0.0716872579\H,1.6628929495,2.2736317675,1.8810483808\H,3.1343350767,1.3214801118,2.0487400172\H,1.6046831633,0.6827666617,2.6154534673\H,1.5123626717,0.6464591097,-2.6786622532\H,1.5963900482,2.247213669,-1.9686779208\H,3.0609630443,1.2919535994,-2.1745445029\H,-0.231592872,-3.0930827719,0.0253784761\H,1.281165812,-2.7833470552,0.8733157962\H,1.2505431403,-2.7954113573,-0.8790745702\H,4.9514787335,-1.9054519584,-0.0728409602\H,4.8954729622,-0.38380663,0.798223741\H,4.865159566,-0.3953424128,-0.9613226314\H,-1.5961070147,-2.2470240221,1.9688125985\H,-3.0610346523,-1.292236442,2.1743124045\H,-1.5127533105,-0.646169363,2.6786735798\H,-1.6634289957,-2.2739345649,-1.8807822317\H,-3.1342779328,-1.3209696401,-2.0490545378\H,-1.6040884285,-0.6832369634,-2.61543669\H,0.2316033652,3.0930774919,-0.0253544771\H,-1.2507005818,2.7954158524,0.878831624\H,-1.2810073247,2.7833351085,-0.8735650872\H,-4.9514673619,1.9054701722,0.0726977932\H,-4.8651004006,0.3955505716,0.96150067\H,-4.8955061599,0.3836388348,-0.7980421562

HF=-623.0724236

ZeroPoint=0.3329289

Thermal=0.3592357

MP2/6-31G-LANL2DZ(Sn)*

Sn,1.7421575652,0.2248428567,0.0341878067\O,0.2691645935,-1.1627381952,0.0530441485\C,2.1611833316,1.1433512957,1.9063949707\O,3.0329138248,-1.2767548292,0.0119248337\C,2.1283628576,1.1804660971,-1.8285232766\C,0.4864272784,-2.5775660779,-0.0822020858\C,4.4240156741,-1.0253675906,0.0043380723\Sn,-1.7496617932,-0.2092100453,0.0356998809\O,-0.2766352449,1.1783655641,0.0519604848\C,-2.1670382211,-1.1256454365,1.9092793064\O,-3.0404109189,1.2923805321,0.0126582138\C,-2.1372737382,-1.1669739608,-1.8256220664\C,-0.4938982243,2.5930339575,-0.0849598132\C,-4.4315234558,1.0410361101,0.0056509453\H,3.2346766253,1.1714144717,2.1069966993\H,1.6902142936,0.5488821103,2.6943521439\H,1.7635737358,2.1577547926,1.9655511563\H,1.5175784023,0.704463167,-2.6010296862\H,1.8695002663,2.2407168364,-1.8005426345\H,3.175988461,1.0810949401,-2.1208463967\H,-0.3932355101,-3.0974024588,0.3078532418\H,1.374183609,-2.8708591693,0.4744597262\H,0.6240494036,-2.8421416121,-1.1343290499\H,4.9541323191,-1.9831866986,-0.0284986178\H,4.7631712252,-0.4900356267,0.9050982973\H,4.7458766009,-0.4398105458,-0.8714116808\H,-3.2401593148,-1.1508703998,2.1122061072\H,-1.6927853482,-0.5320093186,2.6958898805\H,-1.7719012764,-2.1410427392,1.9680983678\H,-1.8774563336,-2.2269687172,-1.7969254279\H,-3.1853321786,-1.0687932954,-2.1167980203\H,-1.527840597,-0.6911854789,-2.5993282847\H,-0.6317044776,2.8563297647,-1.1373850825\H,0.3858488155,3.1133313653,0.3042960144\H,-1.3815459935,2.8870000409,0.4715182621\H,-4.9616322362,1.9989062622,-0.0257628794\H,-4.770203509,0.5046884214,0.9059968546\H,-4.7538725117,0.4564836099,-0.8705774119

HF=-622.9088158

MP2=-624.7990576

ZeroPoint=0.3224561

Thermal=0.3490615

MP2/6-31+G-LANL2DZ(Sn)*

Sn,1.7481399411,0.215499922,0.0016047392\O,0.2688465822,-1.1670030671,0.0045231739\C,2.1720717471,1.1645729823,1.863022199\O,3.0551285208,-1.2907773902,0.0299336185\C,2.1528639306,1.1587577012,-1.8658833342\C,0.4516223398,-2.5904281491,-0.1271904216\C,4.4516489625,-1.0569992779,0.1261202912\Sn,-1.7555740124,-0.1998901266,0.003024721\O,-0.2762821032,1.182623537,0.0034097043\C,-2.1782226258,-1.146988545,1.8657414481\O,-3.0625783687,1.3063856009,0.0306082595\C,-2.1615349718,-1.1451855423,-1.8631633469\C,-0.4591351819,2.6059029216,-0.1297887448\C,-4.459023331,1.0726864759,0.1280741889\H,2.9945715858,1.882017893,1.7691698737\H,2.4716289575,0.4047922437,2.5916528164\H,1.2916570184,1.6899098846,2.2411736327\H,1.326712531,0.9675596798,-2.557803306\H,2.2486527812,2.2429236186,-1.7494085699\H,3.0753082959,0.7709384294,-2.3071428908\H,-0.3455677995,-3.092094141,0.4315203195\H,1.4268134935,-2.8721830707,0.2693945513\H,0.3917763812,-2.8778068607,-1.1818255634\H,4.9621054941,-2.0252429896,0.1611554921\H,4.7181687338,-0.4996110453,1.0374372897\H,4.8407450975,-0.5019368326,-0.7417899242\H,-3.0005861592,-1.8647540414,1.7731502471\H,-2.4775570124,-0.3864863667,2.5937096323\H,-1.297452026,-1.6716831719,2.2439578957\H,-2.2569476155,-2.2292539473,-1.7454813432\H,-3.0844232251,-0.7580666124,-2.3041098637\H,-1.3359743746,-0.954496132,-2.555928736\H,-0.3994008831,2.8921532882,-1.1847378934\H,0.338084653,3.1082075455,0.4283050714\H,-1.4343007257,2.8880200157,0.2666022858\H,-4.969473014,2.0409587339,0.1624094545\H,-4.7248652657,0.5163021464,1.0402020391\H,-4.8487403515,0.5166546898,-0.738936007

HF=-622.9302142

MP2=-624.8606869

ZeroPoint=0.3198108

Thermal=0.3467572

MP2/6-311+G-LANL2DZ(Sn)*

Sn,-1.7280277821,-0.3329396518,-0.0018148967\O,-0.350698142,1.1538443274,-0.0532487826\C,-2.0495928222,-1.2547725183,1.886570295\O,-3.12924995,1.0928825151,0.0346661365\C,-2.089154867,-1.3088148042,-1.8526332875\C,-0.6256666767,2.5549243688,-0.1355131389\C,-4.5043189736,0.8065711177,0.1301766275\Sn,1.7282693833,0.3323336894,-0.0067296948\O,0.3509216564,-1.1553208165,-0.0252754513\C,2.0459066108,1.2848595129,1.8671972286\O,3.1309723371,-1.0913627657,0.0509679699\C,2.0898871371,1.2768113679,-1.8734473088\C,0.6252670473,-2.5548630002,-0.1328015814\C,4.5052354186,-0.8019404785,0.1489939674\H,-2.8545987448,-1.9935042292,1.8443101503\H,-2.3397719758,-0.4888823224,2.6094829729\H,-1.1433663753,-1.7477979961,2.2401123972\H,-1.3837946373,-0.9328576233,-2.5975378241\H,-1.945244305,-2.3881206165,-1.7705000793\H,-3.1021776832,-1.1167220806,-2.210839637\H,0.1631570943,3.0998041435,0.3926430781\H,-1.5924468768,2.7713471471,0.3151392598\H,-0.6427738487,2.875400521,-1.1812695395\H,-5.0553473853,1.7484337231,0.2117412676\H,-4.7491740834,0.2006537261,1.0159255754\H,-4.8851349538,0.276486787,-0.7558433227\H,2.8150673606,2.0593862307,1.8032430196\H,2.3837679541,0.5394451618,2.5906378772\H,1.1252912376,1.7402618088,2.2339734125\H,1.8984740728,2.3504948576,-1.8208189209\H,3.1171047245,1.1191919041,-2.2073884174\H,1.4166175204,0.853211331,-2.6225545866\H,0.6198004351,-2.8613820029,-1.1829382628\H,-0.1515886137,-3.1076063693,0.4049385031\H,1.6014198278,-2.775066686,0.2952588055\H,5.0567948331,-1.74166053,0.249497854\H,4.744794761,-0.1808198441,1.0256647009\H,4.8901050285,-0.2863984549,-0.7437844748

HF=-623.0660394

MP2=-625.1312363

ZeroPoint=0.3174409

Thermal=0.3446519

Dimethyltin dimethoxide dimer (2b)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,-1.7858620672,0.0082570433,-0.3000926985\O,-0.2608155823,1.3201852561,0.120225195\O,-2.0934361964,-1.4160360816,1.019824262\C,-3.3370395619,1.4061294292,0.2456896503\C,-2.0821276159,-0.4958177935,-2.3469267321\C,-0.3871987458,2.7020931437,0.4211061565\C,-3.2184658035,-1.5072901035,1.8698991756\Sn,1.7024972149,0.2216758071,0.1176265037\O,0.1716566815,-0.9877404067,-0.4092750971\C,1.8526855491,0.6521237273,2.1904259118\O,2.9555593161,-1.3144973631,-0.1186706994\C,2.3913951122,1.5431144797,-1.4024742276\C,0.2475098728,-2.4191560025,-0.5454154872\C,4.3522507004,-1.1788443045,-0.0058685918\H,-3.1730175301,1.8594545934,1.2260921402\H,-4.3033618597,0.8947824077,0.2751271021\H,-3.4175120268,2.2114889322,-0.4896051298\H,-1.1247395651,-0.5519053059,-2.8672352849\H,-2.5711618487,-1.4703449987,-2.427082966\H,-2.7161203245,0.2417512791,-

2.844391832\H,0.5815053569,3.1897980939,0.2754090483\H,-0.7006341111,2.854857322,1.4586191462\H,-1.1118486284,3.1844128586,-0.2399902874\H,-3.0194023661,-2.2885840664,2.6083088663\H,-4.1298129554,-1.7839424028,1.3228832237\H,-3.4172377278,-0.5727421612,2.4099500707\H,1.6960347759,1.714276525,2.3901157628\H,2.8222497823,0.3564362946,2.595833556\H,1.0750408451,0.0907702518,2.7141995699\H,1.5674711731,2.132097571,-1.8074023631\H,3.1576426673,2.2291473163,-1.0307871892\H,2.8342506852,0.9560132802,-2.2100608787\H,-0.2484782713,-2.7056012552,-1.4774107422\H,-0.2696699844,-2.8789415579,0.2964404942\H,1.2930676176,-2.7192543183,-0.5775528212\H,4.8191786559,-2.1360272304,-0.2567303544\H,4.6671543414,-0.9137525057,1.0147180936\H,4.7598731258,-0.4202400892,-0.6915819158

HF=-623.0586363

MP2=-625.1258131

ZeroPoint=0.3179171

Thermal=0.3446162

Dimethyltin dimethoxide dimer (2c)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,-1.7127297876,-0.2375608142,0.3237841458\O,-0.0401155471,-1.0889085636,-0.4992512714\O,-2.4338254615,1.3696321036,-0.5589435056\C,-3.0719566533,-1.7348470295,-0.4249289834\C,-1.8030162354,-0.2607344996,2.4471763114\C,0.0735224647,-2.4449365054,-0.9365404903\C,-3.6240757521,1.4144920484,-1.3190257706\Sn,1.7127337617,0.2375571571,-0.3237758604\O,0.0401031715,1.0889249363,0.4992139036\C,1.8030773448,0.2607160504,-2.4471639287\C,3.0719607809,1.7348293126,0.4249660052\O,2.4338043209,-1.3696295318,0.5589859562\C,-0.0735670098,2.4449773367,0.936416139\C,3.624062221,-1.4144935301,1.3190568386\H,-2.888525862,-1.9844287184,-1.4726795592\H,-4.0995685623,-1.3707000308,-0.3416322024\H,-3.0044041081,-2.6568340194,0.1588478471\H,-0.9584645402,-0.8301100259,2.8438158967\H,-1.737930508,0.7558560811,2.8397262829\H,-2.7290643747,-0.715970508,2.8056782381\H,-0.0616884378,-2.5039050183,-2.0212712527\H,-0.6841664868,-3.0688134465,-0.4578045318\H,1.0603137428,-2.8135428116,-0.6577520719\H,-3.6597598011,2.3794078884,-1.8321342695\H,-4.5210172716,1.3329553763,-0.6905252441\H,-3.6692151659,0.6246103596,-2.0794816135\H,1.7379914111,-0.7558770736,-2.8397078146\H,2.7291394861,0.7159407894,-2.8056444184\H,0.9585413555,0.8300969817,-2.8438291367\H,3.0044367742,2.6568130111,-0.1588190937\H,4.0995698694,1.3706674123,0.3416985533\H,2.8885074096,1.9844199499,1.4727104156\H,0.0616338902,2.5040202149,2.0211438956\H,-1.0603664806,2.8135419067,0.6575968431\H,0.684106441,3.0688434509,0.4576437133\H,3.6597320405,-2.3793952781,1.8321931088\H,3.6692265115,-0.6245907377,2.0794895882\H,4.520999142,-1.3329935565,0.6905451835

HF=-623.0528709

MP2=-625.122337

ZeroPoint=0.3185232

Thermal=0.3447962

Dimethyltin dimethoxide dimer (2d)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,-1.7493261487,0.1197691872,-0.2204624837\O,0.0051187176,1.1992525262,-0.2454607499\O,-2.2078265338,-1.1078121863,1.254421785\C,-2.9853046051,1.8054516677,0.2986296791\C,-2.2801351596,-0.5544041442,-2.1650026724\C,0.1268005774,2.6017428196,-0.0046641828\C,-3.2567619083,-0.9135319235,2.1802063305\Sn,1.7493260799,-0.1197692152,-0.220462444\O,-0.005118791,-1.1992525792,-0.2454608277\O,2.2078267613,1.1078125409,1.2544214251\C,2.9853042611,-1.8054517524,0.2986301549\C,2.2801350908,0.5544035092,-2.1650028417\C,-0.1268005028,-2.6017427879,-0.0046637414\C,3.2567624904,0.913532532,2.1802056214\H,-2.6163059404,2.3464102975,1.1728626705\H,-3.9991282887,1.4619447815,0.5205892787\H,-3.052793739,2.5128235276,-0.5322256077\H,-1.6995943816,-0.0099003587,-2.9146913837\H,-2.0629565311,-1.617766551,-2.2778529083\H,-3.3408178977,-0.3887506421,-2.3682376719\H,1.0788668122,2.9486572842,-0.4092373663\H,0.1187460886,2.8094835673,1.0663257463\H,-0.6850384597,3.1386360984,-0.50063851\H,-3.1695975689,-1.681697111,2.9536205061\H,-4.2471994677,-1.0143481828,1.7156305995\H,-3.2099459234,0.067255355,2.6702760625\H,2.6163056388,-2.3464099217,1.1728634431\H,3.9991281035,-1.4619450884,0.520589384\H,3.0527929664,-2.5128239721,-0.5322248616\H,2.0629559702,1.6177657466,-2.2778536703\H,3.3408179559,0.3887504368,-2.3682375396\H,1.6995947626,0.009899044,-2.9146914101\H,0.6850369833,-3.1386364318,-0.5006402415\H,-1.0788680081,-2.9486569191,-0.40923417\H,-0.1187431247,-2.8094834985,1.0663261855\H,3.1695988972,1.6816983916,2.9536192096\H,4.247199891,1.0143479235,1.7156293559\H,3.2099462515,-0.0672543268,2.6702761683

HF=-623.0531791

MP2=-625.1224162

ZeroPoint=0.3184812

Thermal=0.3447324

Dimethyltin dimethoxide dimer (2e)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,1.7427291611,-0.1381522297,0.0080222067\O,-0.0033446055,0.9961847149,-0.0466549365\C,2.2845381045,-1.0528320555,-1.8325948707\O,2.7293883211,1.5994675767,-0.1132970271\C,2.4307715269,-0.8030485702,1.9086801708\C,-0.0330034837,2.4524217435,-0.0250965671\C,4.1347336314,1.6577485773,-0.0434244852\Sn,-1.7469307064,-0.1527400436,-0.0058857703\O,-0.0021826375,-1.3982118322,0.1552324592\C,-2.4741319793,-0.8474094057,1.8708992465\O,-2.6770420323,1.6123562221,-0.1064305681\C,-2.2804069927,-1.0386983197,-1.8626534273\C,0.0015658451,-2.8075665435,0.0589341339\C,-4.0763110705,1.7245882043,-0.0023938979\H,2.3874364063,-2.135228321,-1.728174433\H,3.2215632788,-0.6460113495,-2.2166973588\H,1.501899333,-0.8606385342,-2.570879739\H,2.4310799314,0.040828296,2.6029061522\H,1.7824956217,-1.584269983,2.3072453102\H,3.453392173,-1.1860865603,1.8567380834\H,-0.6333327822,2.8011207682,-0.8616982275\H,0.9938740838,2.7994688252,-0.0937412516\H,-0.5012569335,2.7814034561,0.9016161545\H,4.4435413626,2.7068157434,-0.0794064581\H,4.6199249157,1.1412145291,-

0.8856429088\H,4.5288144279,1.2258936035,0.8887225402\H,-1.8073013008,-1.6020796906,2.2897066047\H,-3.476650141,-1.2748033626,1.7830113631\H,-2.5346032867,-0.0074335676,2.567125449\H,-2.3474635929,-2.1261021308,-1.7854049745\H,-3.2348255391,-0.6524029688,-2.2251338194\H,-1.5145136846,-0.801539849,-2.6055063015\H,0.8807859933,-3.221271718,0.5662892314\H,0.0143682437,-3.1393545252,-0.9853500127\H,-0.8873884792,-3.2250358984,0.5458423797\H,-4.3433605921,2.7857461224,-0.002224809\H,-4.4686254259,1.2825959733,0.9261465609\H,-4.6008625398,1.2521895832,-0.8472125941

HF=-623.0589159

MP2=-625.1255156

ZeroPoint=0.3174132

Thermal=0.3445056

Dimethyltin dimethoxide trimer (3a)

MP2/6-31G-LANL2DZ(Sn)*

Sn,2.9208381368,-0.5162670397,-0.10630409\O,3.3773611877,-1.840154855,1.3006883198\O,1.1248290384,-0.2862499339,0.8286380137\C,4.3535999806,1.013020763,0.2706909445\C,3.0787785413,-1.7457517101,-1.8431775311\C,4.5879281259,-2.565654765,1.2064952953\C,0.675852499,-1.0164189485,1.9865905872\Sn,-2.920838957,-0.5162667984,0.1063020834\O,-1.6416393489,0.8992128063,1.1971945402\C,-3.0788730523,-1.7456974219,1.8432056569\C,-4.3535527568,1.0130420835,-0.2707889185\O,-3.3773555678,-1.8401792025,-1.3006701002\C,-2.0988494358,1.7029814968,2.2809332594\C,-4.5879409849,-2.5656500394,-1.2064878127\Sn,-0.0000038104,1.3808520257,-0.000007147\C,-0.9430228159,2.6986786807,-1.4183398387\O,-1.1247855506,-0.2863218602,-0.8285747294\O,1.6416396134,0.8992107795,-1.1971984191\C,0.9429699563,2.698779743,1.4182626265\C,-0.6757577657,-1.0165647209,-1.9864613409\C,2.0988526849,1.7029783799,-2.2809369848\H,4.0130730712,1.6132294015,1.1186747127\H,4.4827774183,1.6771349737,-0.5863521069\H,5.3248546016,0.5867239861,0.5336471364\H,4.1232949051,-2.0043477158,-2.0404596522\H,2.5392059431,-2.6824532397,-1.6784892705\H,2.6658590785,-1.2557189729,-2.7258534332\H,4.6811480517,-3.209150152,2.0877823824\H,5.4749225903,-1.9123651703,1.1805132553\H,4.6242422133,-3.2123286444,0.3164642385\H,1.4745800674,-1.6786428907,2.3136337809\H,-0.2137602014,-1.5897020346,1.720029946\H,0.4210236,-0.3079175313,2.7799544737\H,-2.6659560926,-1.2556568793,2.7258782675\H,-2.5393358031,-2.6824260664,1.678555714\H,-4.1234051539,-2.0042449496,2.0404691192\H,-4.0130098822,1.6131838711,-1.1188140239\H,-4.4827086941,1.6772170968,0.586209864\H,-5.3248208401,0.5867576736,-0.5337159506\H,-1.3119446175,1.8092270455,3.0334152961\H,-2.9629131648,1.2207059259,2.7496452405\H,-2.3996776351,2.701349364,1.941387127\H,-5.4749208969,-1.9123401032,-1.1805170125\H,-4.624278827,-3.2123198124,-0.3164548583\H,-4.6811671603,-3.2091459292,-2.0877738785\H,-1.8654828585,3.1013177649,-0.9880375502\H,-1.2062595045,2.1838005603,-2.3460405349\H,-0.2982109761,3.5478006044,-1.6646497202\H,1.8654036459,3.1014482442,0.9879315137\H,1.2062444389,2.1839503121,2.345979706\H,0.2981204133,3.5478799333,1.6645486949\H,0.2138535271,-1.5898183637,-1.7198292661\H,-0.4209078192,-0.3081123437,-2.779862455\H,-1.4744641406,-1.6788207048,-2.313490612\H,2.3996865835,2.7013445009,-1.9413906566\H,1.3119473587,1.8092286806,-3.0334177567\H,2.9629133182,1.220699126,-2.7496507334

HF=-934.3720977

MP2=-937.2235141

ZeroPoint=0.4856142

Thermal=0.5249656

Dimethyltin dimethoxide trimer (3g)

MP2/6-31G-LANL2DZ(Sn)*

Sn,-2.9641789249,-0.458210696,0.0859420083\O,-3.3299808618,-2.1579511532,-0.8723386053\O,-1.0809157652,-0.5362948481,-0.674809533\C,-4.3094873664,0.8738327001,-0.8887813688\C,-3.3167788483,-1.0818517474,2.0965403975\C,-4.570684913,-2.8104802091,-0.6849980993\C,-0.5763890706,-1.5412308946,-1.5743889004\Sn,2.8873137287,-0.5713914311,0.3194501548\O,1.8270535439,0.4961667038,-1.0899674366\C,3.8696604702,0.578108288,1.8168702218\C,2.4500981475,-2.6384218806,0.6337388993\O,4.3056052324,-0.731411629,-1.0641647347\C,2.3284347404,0.8959575674,-2.3850596915\C,5.4456443795,-1.5213929089,-0.7836130662\Sn,0.0220513697,1.3210215518,-0.2613574068\C,0.8451530311,3.0645229994,0.6990094682\O,0.9721720185,0.0491410566,1.1059640349\O,-1.7618480267,1.2402819054,0.8142059489\C,-0.7082604807,2.0688483849,-2.1432156212\C,0.4106189463,-0.4029093139,2.3303372065\C,-2.3096457215,2.3429961414,1.5312009122\H,-3.8717496619,1.1809854031,-1.8424490658\H,-4.5020425115,1.7715518243,-0.2979191989\H,-5.2625205587,0.3840364098,-1.1032496892\H,-4.3848998282,-1.2402783175,2.2721202257\H,-2.8149819778,-2.03683364,2.2753239228\H,-2.9473325261,-0.3515275283,2.8175977325\H,-4.5948921826,-3.7067678402,-1.3139358955\H,-5.4292857657,-2.1827966582,-0.9728838412\H,-4.7266609641,-3.1305962085,0.3567682078\H,-1.3405528423,-2.3019542525,-1.7202536397\H,0.3233595218,-1.9817004871,-1.1407677871\H,-0.3227493889,-1.0755109344,-2.5317297433\H,3.4115047489,0.4253146684,2.7965662564\H,3.7713345612,1.6371973507,1.5634854263\H,4.9345748744,0.3435071682,1.8821442357\H,2.4791898444,-3.170181172,-0.3210112561\H,1.4677712025,-2.7832217249,1.085833282\H,3.202353654,-3.0963320266,1.2835253619\H,1.5930781641,0.6283851129,-3.146978249\H,3.2697781965,0.3814949707,-2.5623539904\H,2.4846780736,1.9788427396,-2.399059699\H,5.1939645295,-2.5783433496,-0.6061947493\H,6.0067314497,-1.1602748571,0.0929703822\H,6.1210717746,-1.481633063,-1.6447277752\H,1.8286256924,3.2895804151,0.2735452094\H,0.9773983049,2.9104626651,1.7732254848\H,0.2133504563,3.945301198,0.5480204678\H,-1.66801815,2.5667249518,-1.9701048439\H,-0.87197759,1.2787380174,-2.8795077987\H,-0.0275429931,2.8093158605,-2.5728043512\H,-0.3876363071,-1.1287433304,2.1482787623\H,-0.0013032992,0.4392469205,2.8955532877\H,1.1894673888,-0.8792378219,2.9358558843\H,-2.5666823372,3.1706993741,0.8594619616\H,-1.5949998817,2.7046313475,2.2765018024\H,-3.2185814499,2.0216146093,2.0504562648

HF=-934.3711674

MP2=-937.2225141

ZeroPoint=0.4854411

Thermal=0.5248858

Dimethyltin dimethoxide trimer (3m)

MP2/6-31G-LANL2DZ(Sn)*

Sn,2.8220067682,-0.6423844589,0.2533431127\O,4.379906094,-0.3125600204,-0.9367689255\O,0.7731375853,-0.4152496766,0.9066405281\C,2.4770065122,-2.7035798777,-0.1885826155\C,3.5894357538,-0.0579919709,2.1532512606\C,5.5094905622,-1.1582948771,-0.8333344984\C,0.3405340136,-0.9414707444,2.1580239998\Sn,-2.8494225715,-0.6020569645,-0.306763988\O,-1.931752514,0.878127968,0.8030048285\C,-3.8687591703,0.0090390767,-2.0715670698\C,-2.1630692123,-2.6059317441,-0.0259624579\O,-4.3052767192,-0.4994879787,1.0454352483\C,-2.5063578182,1.5733241218,1.9316987126\C,-5.4053210762,-1.3810507741,0.9264993634\Sn,-0.0077387052,1.3652722496,0.0201375161\C,-0.5145921023,2.9025335373,-1.3987451264\O,-0.9746639087,-0.0447044421,-1.2180178168\O,1.895480221,0.8664571393,-0.8130397005\C,0.6430402206,2.5400615644,1.7095798021\C,-0.3312353276,-0.8284717621,-2.2140387355\C,2.5274733276,1.6997288561,-1.81179537\H,2.5073617256,-2.8603580979,-1.2703061078\H,1.5081137678,-3.0363964317,0.1869093985\H,3.2585770972,-3.3313643162,0.2498279039\H,4.6789865956,-0.1325389661,2.1760784889\H,3.3156585113,0.9822962368,2.347605767\H,3.1812038645,-0.6703166492,2.9606062802\H,6.2852250317,-0.7928908761,-1.5145660361\H,5.2837159686,-2.1988649336,-1.1116530339\H,5.9411192439,-1.1706308868,0.1805751288\H,0.8098132542,-1.9172522383,2.3275556924\H,-0.7433284828,-1.0792092057,2.1493539604\H,0.6061761593,-0.2783399121,2.9893977538\H,-3.3512186905,-0.3389673369,-2.9679628277\H,-3.8840868146,1.1022289064,-2.0987501145\H,-4.9020643964,-0.3439341566,-2.0972159981\H,-2.6077175267,-3.0506105337,0.8672685214\H,-1.0766227357,-2.5997924735,0.0808347534\H,-2.4192542707,-3.2368629931,-0.8824691949\H,-1.8536301198,1.4508058183,2.7994424351\H,-3.4869063362,1.1481862536,2.1320548611\H,-2.5928316395,2.6374383994,1.6935703553\H,-5.1025492355,-2.440364499,0.9152494581\H,-5.9986054574,-1.1952260169,0.0177880845\H,-6.0667405156,-1.2372072429,1.7874642623\H,-1.5203511389,3.2712198234,-1.1704190413\H,-0.5281959238,2.525853241,-2.4239694037\H,0.1698418328,3.7541867113,-1.3430926865\H,1.6491810554,2.9198728911,1.5010514905\H,0.6844406059,1.9879145145,2.6508468714\H,-0.0071535245,3.408961047,1.8494962457\H,0.3735085488,-1.5371300782,-1.7686508696\H,0.2093701198,-0.1794037088,-2.9103096747\H,-1.0822275743,-1.3895367603,-2.7813867764\H,2.6729861694,2.7064225277,-1.4091678642\H,1.8784293746,1.7543070292,-2.6886495343\H,3.4869807649,1.2579273935,-2.0684374417

HF=-934.3679917

MP2=-937.2214546

ZeroPoint=0.4855091

Thermal=0.5248326

Dimethyltin dimethoxide trimer (3s)

MP2/6-31G-LANL2DZ(Sn)*

Sn,3.5152909465,0.1590130271,0.0080435253\O,4.7919513772,-1.3458688507,0.2084360474\C,-0.048281732,-0.5816199291,2.0722730187\C,3.9742984738,1.3267959441,1.7263828295\C,3.9883189922,0.8162489327,-1.9688294315\C,6.180887532,-1.0951821234,0.1297207212\Sn,-3.5152891526,0.1590142135,-0.0080327552\O,-1.5499016167,1.2761246546,0.0087204156\C,-3.9882870511,0.8161975814,1.9688646059\C,-3.9743300657,1.3268343095,-1.7263375742\O,-4.7919533299,-1.3458630139,-0.2084357622\C,-1.5159637043,2.5877717793,0.566469284\C,-6.1808872674,-1.0951808375,-0.1296672786\Sn,0.0000006406,-0.1157531153,-

0.0000163485\C,0.0482783987,-0.5815776372,-2.0723149083\O,-2.0103696254,-1.1728799587,-0.104193227\O,2.0103689692,-1.1728829856,0.1041406236\O,1.5499016008,1.2761248028,-0.0087206847\C,-2.1592278356,-2.6005878639,-0.0510272973\C,2.1592237292,-2.6005918645,0.0509868472\C,1.515961524,2.5877793677,-0.5664530171\H,0.084290914,-1.6546295328,2.2297192775\H,-1.003208013,-0.2857779761,2.5117615801\H,0.7620543602,-0.0621804773,2.5892557139\H,5.0339244027,1.2758195205,1.9867880655\H,3.4008088287,0.9371750796,2.5721084409\H,3.6897480512,2.3709079001,1.5815964315\H,4.7322936215,1.618417693,-1.9612357809\H,3.1074009374,1.1707940533,-2.5062688582\H,4.4150019255,-0.0264323127,-2.5191229801\H,6.5385721128,-0.4314654067,0.9327499728\H,6.4774120865,-0.6438645993,-0.8308603145\H,6.7172299055,-2.0452792553,0.2260397935\H,-4.4148307367,-0.0265386371,2.5191824649\H,-4.7323715693,1.6182649301,1.9613045528\H,-3.1073912905,1.1708639523,2.5062598199\H,-3.4008486016,0.9372356439,-2.5720789763\H,-3.6897867341,2.3709457892,-1.5815340945\H,-5.0339592173,1.275854298,-1.9867289247\H,-0.8619009764,2.6319513292,1.4455483051\H,-2.5229582025,2.8813491607,0.8796585284\H,-1.1669132899,3.3124934019,-0.1742808659\H,-6.5385928036,-0.431403566,-0.9326375491\H,-6.4773859451,-0.6439351439,0.8309552119\H,-6.7172330277,-2.0452701853,-0.2260444582\H,1.0032023826,-0.2857242456,-2.5118010249\H,-0.7620618322,-0.0621302129,-2.5892829877\H,-0.0842921205,-1.6545843886,-2.2297821014\H,-1.4692484695,-3.0509849689,-0.7723618326\H,-3.1841725856,-2.8738228321,-0.2961936701\H,-1.9138923546,-2.9610611239,0.9539261788\H,1.913812216,-2.9610765706,-0.9539439275\H,1.4693002283,-3.0509818627,0.7723793061\H,3.1841872703,-2.8738208371,0.2960818009\H,1.1669235983,3.3124927986,0.1743111513\H,0.8618862547,2.6319719618,-1.4455220103\H,2.5229519635,2.8813572783,-0.8796534112

HF=-934.3628271

MP2=-937.2117713

ZeroPoint=0.4851527

Thermal=0.5250055

Dimethyltin dimethoxide trimer (3w)

MP2/6-31G-LANL2DZ(Sn)*

Sn,-3.4584925681,0.0018091199,-0.0141474698\O,-4.0733288236,-1.8878125068,-0.092338343\C,0.1780476546,0.9811137851,-2.0409628839\C,-4.3291777698,0.7839764574,-1.7959580963\C,-4.1246731842,0.5424408234,1.9369587023\C,-5.454735591,-2.1828065062,-0.0671907986\Sn,3.3940560036,-0.4440034548,0.0375847407\O,2.1942805074,1.1775491803,0.0513452255\C,3.9246241807,-1.1815252115,1.9661974417\C,3.4518858013,-1.7065332019,-1.6774107015\O,4.8968272989,0.7970015565,-0.3340093687\C,2.6397178832,2.5077294931,-0.2544412719\C,6.1967792527,0.2980261134,-0.5712431556\Sn,0.0005560936,0.526859092,0.0250386532\C,0.0020715446,1.1220320669,2.0660015967\O,1.2522114647,-1.1224203931,0.2672863215\O,-1.5805319493,-0.8805867952,-0.1851571022\O,-1.9664844092,1.5355044141,-0.0479799354\C,0.9277155713,-2.1514779507,1.2091474045\C,-1.431314613,-2.0423582077,-1.0399633813\C,-2.2209749787,2.8895774536,0.2910182831\H,0.9996981976,0.4232510614,-2.4958780986\H,0.3761141783,2.0475271895,-2.1773650775\H,-0.7538069588,0.7420025975,-2.5569846833\H,-5.3424020649,0.4118352284,-1.962228782\H,-3.7163721208,0.4743988702,-2.6478196444\H,-4.3492998231,1.8754128635,-1.7805433336\H,-5.128025181,0.1562542321,2.1316491145\H,-4.1297636308,1.6235620786,2.0880164428\H,-3.4533225544,0.0984633184,2.6777262161\H,-5.9994070551,-1.7498023818,-0.9212833483\H,-

5.9495186621,-1.8324673866,0.8529251308\H,-5.583577541,-3.2698730197,-0.1134865477\H,4.9977274487,-1.0499874158,2.1239413521\H,3.681315115,-2.2374554302,2.09814726\H,3.4016452567,-0.6096570658,2.7377790872\H,3.0117527973,-1.1820482555,-2.5303254234\H,2.8707380835,-2.6138206491,-1.502236477\H,4.4738751284,-1.9806240824,-1.9497803432\H,2.8087296221,2.6271772723,-1.328247128\H,3.5683906673,2.7268000042,0.2700689575\H,1.858345729,3.2053003085,0.0679230147\H,6.2607769918,-0.2917634519,-1.4987222747\H,6.570282369,-0.3355554255,0.2502124147\H,6.8867703983,1.1433631738,-0.6694803958\H,0.0596995744,2.2114722684,2.1386384341\H,0.8680773476,0.7043562906,2.5823531\H,-0.9129169614,0.8004278572,2.5697283764\H,1.198126162,-1.8567712945,2.2284257726\H,1.4746246877,-3.0639349142,0.9491195511\H,-0.1429092788,-2.3640496577,1.1822035531\H,-1.9148364226,-2.8942486966,-0.5670996134\H,-0.3651222014,-2.2192983865,-1.1858590723\H,-1.9055740964,-1.8601512076,-2.0082652094\H,-1.4656868211,3.5381486873,-0.1699188286\H,-2.2026138472,3.0511675774,1.3757929116\H,-3.2010982446,3.2022956615,-0.0890158325

HF=-934.3579395

MP2=-937.2094787

ZeroPoint=0.4854051

Thermal=0.5249556

Trimethyltin methoxide monomer (4)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,-0.3021629915,-0.0200427958,-0.0013480896\O,1.4378873042,0.8898629792,0.0162128623\C,-0.4411445271,-1.2213950982,1.7586098223\C,-1.6801160726,1.5932304132,-0.0135192919\C,-0.3965806169,-1.2314443058,-1.7570238712\C,2.6846437024,0.2284338149,0.0175617308\H,-1.3811363283,-1.7788566821,1.7779456022\H,-0.3989835902,-0.6003135415,2.6558716227\H,0.3755034179,-1.9451016859,1.8099852193\H,-1.2919335033,2.4058329441,0.6035946291\H,-2.6527804714,1.2954061512,0.3846832304\H,-1.8292882077,1.9777982487,-1.0241104546\H,0.3168773475,-2.0572545361,-1.7105749665\H,-1.3938886499,-1.6601714256,-1.884118433\H,-0.1696346277,-0.6374804424,-2.6450359029\H,3.4738766182,0.9844156389,0.0091993718\H,2.8195551641,-0.408965374,-0.8678071542\H,2.8243348186,-0.3940898056,0.912640023

HF=-236.619948

MP2=-237.4468012

ZeroPoint=0.1514559

Thermal=0.1636077

Trimethyltin methoxide dimer (5a)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,1.8216082364,-0.1230189697,-
0.0063500208\O,0.2580575541,1.183064498,0.0279101446\C,2.0775635419,-1.162060047,-
1.8526340972\C,3.3685857785,1.3940591881,-0.0198222298\C,2.1407948048,-
1.1367857921,1.849947782\C,0.3732458965,2.595472329,-0.0188986672\H,1.9402346637,-
2.2386495292,-1.7329942478\H,3.0663134546,-0.9837215915,-2.2822332732\H,1.3237452058,-
0.8126035368,-2.5631749559\H,3.4393975155,1.922541047,-
0.9745560518\H,4.3357033821,0.9104110162,0.1546233551\H,3.230787663,2.1381681914,0.7692
126991\H,2.5716437651,-0.4459467649,2.5792479939\H,1.2090342876,-
1.5340604588,2.2544808708\H,2.8446165947,-1.9664198919,1.7312000566\H,-
0.5860270333,3.0200721298,-0.330116358\H,1.1336181902,2.9127172828,-
0.7383088242\H,0.629124765,3.007405379,0.9636579382\Sn,-
1.8216163381,0.123015874,0.0063547385\O,-0.258057706,-1.1830575975,-0.0279466268\C,-
2.140803187,1.1368365719,-1.8499136871\C,-3.3685712579,-1.394082927,0.0198561095\C,-
2.077540311,1.1620358477,1.852654153\C,-0.3732388145,-2.5954675664,0.0188140421\H,-
1.2089475607,1.5337009464,-2.2546340412\H,-2.8442329518,1.966785474,-1.7310483468\H,-
2.5720953279,0.4461653336,-2.5791093072\H,-3.2307860067,-2.1381821035,-0.7691902196\H,-
4.3357039324,-0.9104515142,-0.154552077\H,-3.4393394542,-1.9225744804,0.9745877177\H,-
1.9400662372,2.2386104442,1.733050076\H,-3.0663376116,0.9838098742,2.282191865\H,-
1.323810448,0.8124613522,2.5632314032\H,0.5860702353,-3.0200808083,0.3299020857\H,-
0.6292269703,-3.007359367,-0.9637309223\H,-1.1335286164,-2.9127444402,0.7382981137

HF=-473.2526544

MP2=-474.9306139

ZeroPoint=0.3061282

Thermal=0.3303189

Trimethyltin methoxide dimer (5b)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,-1.7855134188,0.0046965204,0.0139263389\O,-0.0000866946,-1.2082474857,-
0.1667186029\C,-2.0856138142,-0.704977042,2.0095432464\C,-
3.0016874711,1.8038683854,0.0164099119\C,-2.5775231832,-1.0796373683,-1.6520881804\C,-
0.0001156238,-2.6177835514,-
0.1480444113\Sn,1.785527315,0.0046286929,0.0137650804\O,0.0000910494,1.1661184023,-
0.1958723353\C,2.5767350848,-1.0789641543,-
1.6530768951\C,3.0020226731,1.803599394,0.017307484\C,2.0860683245,-
0.7059519028,2.009019525\C,0.0000318459,2.5714281359,-0.4601086122\H,-1.5630743349,-
1.6415892622,2.2077400979\H,-3.1500906418,-0.8442954835,2.2194627119\H,-
1.7128053965,0.0442006072,2.7146313733\H,-2.6422880016,2.5699687499,0.7077889997\H,-
3.9995250816,1.50228015,0.3543104411\H,-3.1234427857,2.261063449,-0.9692481027\H,-
1.9337561112,-0.9245381321,-2.5224513883\H,-2.6056837293,-2.1537694362,-1.4561800944\H,-
3.5860581533,-0.7460323931,-1.9076093278\H,-0.0004411078,-3.0260920497,-1.1652742376\H,-
0.8837106923,-3.0015100009,0.3761142021\H,0.8838068067,-
3.0015242623,0.3755473522\H,2.6048164555,-2.153193194,-1.4576870535\H,3.5852060298,-
0.7453916336,-1.9088885025\H,1.9325855554,-0.9233562783,-
2.5230643819\H,3.1242123152,2.2612167887,-
0.9681013704\H,3.9996880206,1.5017019393,0.3554406773\H,2.6425000747,2.5694488809,0.708
9090615\H,1.5625771835,-1.6419965752,2.2073662395\H,3.1505292926,-
0.8465512707,2.2181835213\H,1.7146400168,0.0435154832,2.7145284747\H,-

0.0011764109,3.1432455335,0.4728145888\H,-0.8849680596,2.8370181233,-1.0370013278\H,0.8862221355,2.837460907,-1.0349478186

HF=-473.2434079

MP2=-474.9236019

ZeroPoint=0.3063075

Thermal=0.3303675

Trimethyltin methoxide dimer (5c)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,1.8252973847,-0.0635902594,-0.0163724222\O,3.6681566686,-0.8320452058,0.0882243644\C,1.9388647139,0.9859663348,-1.8756657202\C,0.8383983274,-1.9481680408,-0.013217531\C,1.7537488425,1.1000467013,1.7770649301\C,4.8378916214,-0.0558422002,0.0980170177\H,0.9469364888,1.2018433249,-2.2740235068\H,2.4778353095,0.3616205823,-2.5932816306\H,2.4907060423,1.925630156,-1.7824792225\H,1.6249880101,-2.7001271446,0.0836100598\H,0.30213865,-2.136011535,-0.9448030844\H,0.148841947,-2.0708188344,0.8242769108\H,2.4999453493,0.7216835633,2.4800645267\H,1.9730115031,2.1550220092,1.5930722796\H,0.7698163156,1.0388737684,2.2453754773\H,5.705424615,-0.7185966028,0.181299303\H,4.8744478127,0.6436643428,0.9487732629\H,4.9596504233,0.5343470685,-0.824020334\Sn,-2.3381213133,-0.1652981098,0.0124422765\O,-0.6423459718,0.872384088,-0.1607732198\C,-3.906185657,1.2759631339,-0.1164958753\C,-2.3620329686,-1.496773151,-1.644771771\C,-2.2639579001,-1.0811276689,1.9343997865\C,-0.6614839249,2.2938623709,-0.0834712613\H,-4.8732907931,0.7883068733,0.0337506813\H,-3.9287603567,1.7597336674,-1.0954600949\H,-3.8050963687,2.0516603017,0.6455451391\H,-1.6119151793,-1.1854636869,-2.3749247838\H,-3.3388752829,-1.486356721,-2.1342799507\H,-2.1405100387,-2.5216371486,-1.3428905832\H,-3.1362772804,-0.8094570862,2.5334668628\H,-2.2301866627,-2.16989318,1.8581375507\H,-1.3691179973,-0.7504335017,2.4660169039\H,0.3063775791,2.6745600853,-0.4159180036\H,-0.8316141645,2.6422260085,0.9422800733\H,-1.4312234622,2.7277662183,-0.7318471207

HF=-473.2405879

MP2=-474.9125922

ZeroPoint=0.305676

Thermal=0.3304623

Dimethylsilicon dimethoxide monomer (6)

MP2/6-311+G-LANL2DZ(Si)*

Si,-0.5269249819,-0.0699609248,0.0210525091\O,-0.0366250901,1.4987519086,-0.4375969555\O,0.4717502732,-1.2617456187,-0.6838252521\C,1.754497189,-1.6327834042,-0.2132679438\C,-0.4483534348,-0.227957946,1.887635407\C,-2.2106156839,-0.2996947594,-0.7149850424\C,1.2245582513,2.067054363,-0.1370354859\H,2.0492707279,-2.5399855005,-

0.7423764612\H,1.7517469387,-1.8445331826,0.862550515\H,2.5000768552,-0.8563811078,-0.4176478818\H,0.5468606702,-0.0265641211,2.2903414639\H,-0.7339461444,-1.234812716,2.2033017299\H,-1.1390601375,0.4782829341,2.3551651481\H,-2.1580153371,-0.2146560026,-1.8016664208\H,-2.6133575291,-1.2843340717,-0.4688899429\H,-2.9034033406,0.4597663277,-0.346828694\H,1.166347319,3.1351939753,-0.3506446935\H,2.0134443249,1.6312234904,-0.759480781\H,1.4954660198,1.9404930663,0.918736974

HF=-312.0592047

MP2=-313.079443

ZeroPoint=0.1620593

Thermal=0.1736837

Dimethylsilicon dimethoxide dimer (7)

MP2/6-311+G-LANL2DZ(Si)*

Si,-2.1054449788,0.1765028419,-0.035669527\O,-1.1183626728,-1.1370312774,-0.4910985271\C,-1.8129096584,1.5474604587,-1.258119416\O,-3.6895044868,-0.4559328765,-0.2130356589\C,-1.8327328325,0.6721958421,1.7426082388\C,-1.470650588,-2.4789449201,-0.1783711777\C,-4.851518379,0.2784339173,0.1215977108\Si,2.0981590924,-0.1684745928,0.0378725389\O,1.1278718973,1.1823763665,0.4136308537\C,1.8806433939,-0.7235396206,-1.7304780948\O,3.6902225009,0.4347823001,0.2463114536\C,1.7337999413,-1.4814968157,1.304578312\C,1.5105996889,2.5000768763,0.0386294566\C,4.8440107462,-0.3427080673,-0.0100658912\H,-0.7592443075,1.8241731371,-1.2686106134\H,-2.3946114565,2.4387408933,-1.0058144013\H,-2.1016349294,1.2274505699,-2.2618233898\H,-2.0363674931,-0.1559645314,2.4269313355\H,-0.7953428293,0.9885804384,1.8698151688\H,-2.4830310942,1.5043976473,2.0283458334\H,-0.7247107215,-3.1278679084,-0.6419384366\H,-2.4612614159,-2.7291913772,-0.5656207377\H,-1.4639600312,-2.6576201598,0.9042345551\H,-5.7148842926,-0.3573566449,-0.0794029533\H,-4.9464919928,1.188837652,-0.4836137547\H,-4.86631465,0.5575732648,1.1823174903\H,0.8376820014,-1.0029558231,-1.8926081541\H,2.5089323711,-1.5905431618,-1.9555779717\H,2.1477033985,0.0694373447,-2.4343279629\H,0.6686784753,-1.7098026121,1.3161407388\H,2.2758742935,-2.4071324508,1.0908575603\H,2.0289040889,-1.1377756181,2.2986376714\H,0.7901917919,3.1882983263,0.4853089665\H,1.489800511,2.6312892333,-1.0505994093\H,2.513687875,2.7397802132,0.3997232257\H,5.7159108964,0.2803395669,0.1940315871\H,4.890484565,-0.6716943885,-1.0555216516\H,4.8927355367,-1.2258112053,0.6395333473

HF=-624.1211645

MP2=-626.1748026

ZeroPoint=0.3248735

Thermal=0.3499475

Trimethylsilicon methoxide monomer (8)

MP2/6-311+G-LANL2DZ(Si)*

Si,-0.3929191467,0.0000155413,0.0076335692\O,1.0917929868,-0.0016267333,-0.869898458\C,-0.497063021,1.5389550199,1.0848054452\C,-1.7151628227,-0.0028644404,-1.3128415464\C,-0.4967360318,-1.5344761857,1.09116479\C,2.3458450886,-0.0004032161,-0.2152185027\H,-1.4655044561,1.5840073841,1.5915806349\H,-0.3924856622,2.4478289404,0.4869748783\H,0.2752002333,1.5554374029,1.8581526693\H,-1.6299806277,0.8786684008,-1.9518852673\H,-2.7143192857,-0.0026447638,-0.8683513344\H,-1.6290331571,-0.8864681342,-1.9488922833\H,0.2756449459,-1.547668891,1.8644578052\H,-1.4650960583,-1.5775177612,1.5982706202\H,-0.3921613718,-2.4458189507,0.4971040799\H,3.1206739612,-0.0014578367,-0.9834267446\H,2.4812793853,-0.8908315125,0.4118067354\H,2.4810069966,0.8919949668,0.4090647841

HF=-237.1602145

MP2=-237.9878875

ZeroPoint=0.1561901

Thermal=0.1665748

Trimethylsilicon methoxide dimer (9)

MP2/6-311+G-LANL2DZ(Si)*

Si,-2.1833048588,0.3886491279,0.019505426\O,-1.4532227134,-1.0737946222,-0.555550723\C,-1.5591211801,1.7049682979,-1.1505376049\C,-4.0557978336,0.2206153085,-0.0871832357\C,-1.6529440769,0.7044657404,1.7904616702\C,-1.9165974238,-2.3406486372,-0.129490092\H,-1.9077454586,2.697477078,-0.8499381001\H,-1.9063327036,1.5208515765,-2.1701517412\H,-0.4691447825,1.7151991031,-1.1527606572\H,-4.37414636,-0.0624697785,-1.0941823383\H,-4.5318511536,1.1763927217,0.1517944441\H,-4.4510697339,-0.5210572571,0.6117469189\H,-1.9224260938,-0.1208416685,2.4561780444\H,-0.5712295505,0.8504670657,1.8310927694\H,-2.1372109416,1.6056792969,2.1799767046\H,-1.2804288074,-3.1007434754,-0.5883275148\H,-2.9522498154,-2.5225590759,-0.4418783299\H,-1.8586490904,-2.4591939152,0.9611210944\Si,2.1820152222,-0.3887733407,-0.0185895418\O,1.4564819688,1.0771831608,0.5534180383\C,1.6507911988,-0.7066194016,-1.7888967133\C,4.0550222662,-0.226297934,0.0876974769\C,1.5543938073,-1.700373177,1.154994801\C,1.9233379296,2.3414712484,0.1234442075\H,0.5685426267,-0.8485745375,-1.8291648393\H,2.1317975752,-1.6104386902,-2.1764125638\H,1.9235041019,0.1163243621,-2.4562243315\H,4.4526836238,0.5123606382,-0.6130677664\H,4.528084285,-1.1841626889,-0.1488612032\H,4.3741860694,0.0582798618,1.0940215743\H,1.8928960476,-2.6956625717,0.8520586243\H,1.9093182103,-1.5193845809,2.1725185075\H,0.4644374157,-1.7017800687,1.1640033603\H,1.2907973945,3.1048220505,0.5818673935\H,1.863443944,2.4575866294,-0.9673212362\H,2.9602659134,2.5205698934,0.4332072316

HF=-474.3209104

MP2=-475.9901357

ZeroPoint=0.313356

Thermal=0.3359146

Distannoxane monomer (10)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,1.7545386462,-0.0842969769,-0.4967197228\Cl,2.2237401191,1.3960068508,1.289524688\Sn,-1.7557472561,-0.1760997404,0.4673976577\O,-0.0033939339,-0.7130433788,-0.0803160865\Cl,-2.2090333047,1.6688508274,-0.9442707525\C,3.1093726784,-1.6922888226,-0.3354418102\C,1.7282326192,1.0847778754,-2.2541938546\C,-1.720263267,0.5724028553,2.4408788692\C,-3.1255474896,-1.6950384291,-0.046115902\H,2.9240908686,-2.4349446987,-1.1136175444\H,2.9922792215,-2.171060603,0.6375446493\H,4.139227905,-1.3423081113,-0.4261788351\H,0.8685401572,1.7557417142,-2.2218105133\H,1.6413271641,0.4527281796,-3.1403097518\H,2.6377322863,1.6818396854,-2.340044018\H,-0.8542330677,1.2256002998,2.5576567585\H,-1.6402795679,-0.241729391,3.164088419\H,-2.6241695916,1.1439738401,2.6583706294\H,-2.9481224384,-2.5939172215,0.5471478172\H,-3.0119488246,-1.9464433727,-1.1013537157\H,-4.1521446161,-1.3642951232,0.1213018365

HF=-1159.0486843

MP2=-1160.2036281

ZeroPoint=0.1533366

Thermal=0.1711158

Distannoxane dimer (11)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,0.0944233192,1.657548035,0.00002772\Sn,3.2461706699,-0.0259993857,-0.0000662823\O,1.255689249,-0.0144319272,0.0000132999\Cl,2.4714580627,2.7496670056,0.0002534238\Cl,3.2271860353,-2.4490571607,-0.0002799024\Sn,-0.0944164801,-1.657542775,0.0000596949\Sn,-3.2461743529,0.0259948973,-0.0000351905\O,-1.2556849257,0.0144360612,-0.0000162814\Cl,-2.4714479713,-2.7496658043,0.0002268724\Cl,-3.2272181405,2.4490566103,-0.0001860432\C,-0.2921482685,2.3421541675,-1.9509420354\C,-0.2924107182,2.3420542006,1.9509811469\C,4.046174963,0.3673546413,-1.9049940652\C,4.0463126285,0.3670213072,1.9048727672\C,0.2922364003,-2.3422017511,-1.9508730942\C,0.2923493955,-2.3419966632,1.9510437697\C,-4.0462242347,-0.3673132829,-1.9049536572\C,-4.0462707123,-0.3670813593,1.9049111696\H,0.5522671044,2.0822680384,-2.5925293629\H,-1.2068227025,1.892425244,-2.3360069117\H,-0.4016748196,3.4280007794,-1.9573352528\H,-1.2073719726,1.8926496257,2.3357394443\H,-0.4014660672,3.4279472743,1.9574986997\H,0.5517249306,2.0817244094,2.5927598725\H,3.2189317176,0.4595725843,-2.6119798321\H,4.6960942809,-0.4470456617,-2.2274628923\H,4.5959429698,1.3085447863,-1.904164744\H,3.2190888673,0.4594952287,2.6118479188\H,4.6959647807,-0.4476028017,2.2273121827\H,4.5963842189,1.308034633,1.904091363\H,-0.5521520189,-2.0823354715,-2.5925030734\H,1.2069265694,-1.89248203,-2.3359129668\H,0.4017670171,-3.4280482308,-1.9572283008\H,1.2072834148,-1.8925624755,2.3358324049\H,0.4014272054,-3.4278875831,1.9575918455\H,-0.5518224156,-2.0816711424,2.5927763352\H,-3.2189974414,-0.459477932,-2.6119659095\H,-4.696174139,0.4470824364,-2.2273727523\H,-4.5959665817,-1.3085182586,-1.9041481596\H,-3.2190310918,-0.4595901498,2.6118629474\H,-4.6959082063,0.4475362937,2.2273964277\H,-4.5963506902,-1.3080898473,1.904107487

HF=-2318.1416891

MP2=-2320.4940672

ZeroPoint=0.3098103

Thermal=0.3457496

Distannoxane monomer (12)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,1.8924205138,0.1915150351,0.0089438215\Sn,-1.7583005638,-0.3722865672,0.1825963675\O,0.0499711595,-0.2190122177,-0.3892894246\O,2.5463503221,-1.2153016334,1.1923781835\Cl,-2.0780497274,1.5009204396,1.5966192104\C,2.9047749571,0.1231719827,-1.8520771817\C,2.0210195432,1.9333206827,1.1968935375\C,-3.0478611356,-0.107534842,-1.4670318653\C,-2.0313447456,-2.0774107796,1.4015292961\H,2.6028234504,-2.1338100795,0.9237483804\H,2.6834583896,-0.8151016062,-2.3638440353\H,2.5842580072,0.9434049683,-2.4973507162\H,3.9854250121,0.1953105511,-1.7138094908\H,2.443444575,2.7740389641,0.6436501053\H,2.654714207,1.7310524071,2.0620864084\H,1.0269972571,2.2133448374,1.5487994712\H,-2.7933452055,0.8178094503,-1.9854387075\H,-4.0873566286,-0.0445059837,-1.140058467\H,-2.9541605746,-0.9369078689,-2.1705921343\H,-1.2904311472,-2.0748868711,2.2025274525\H,-3.0261004597,-2.0803379552,1.8507849565\H,-1.9101573662,-2.9938236378,0.820272269

HF=-774.9743614

MP2=-776.1998403

ZeroPoint=0.1650367

Thermal=0.1831516

Distannoxane dimer (13a)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,-0.0981976857,1.6612785438,-0.0027255588\Sn,-3.1915603757,0.26582252,0.0118831323\O,-1.2255132257,-0.0369900217,0.0197970785\O,-2.1915827567,2.2137975842,-0.0019069359\Cl,-3.3837672058,-2.2185950677,-0.0245385866\Sn,0.0981970121,-1.6612549372,0.0026439222\Sn,3.191573748,-0.2658062303,-0.0118298696\O,1.2255314029,0.0370228525,-0.0198515785\O,2.1915502229,-2.2137790365,0.0017841213\Cl,3.3838461379,2.2185938135,0.0245962287\C,0.3119307197,2.4494218643,1.9078955809\C,0.2905683242,2.456047925,-1.9171236112\C,-4.0349259891,0.5978033164,1.9171896049\C,-4.1019259356,0.5911155855,-1.8680795046\C,-0.2905803778,-2.4560198574,1.9170478436\C,-0.3119775926,-2.4494043909,-1.9079667446\C,4.1015391018,-0.5913301351,1.8682844496\C,4.035197801,-0.5978360672,-1.9170126956\H,-2.5589124811,3.051243181,-0.2931304362\H,2.5588740364,-3.0513199752,0.2927406115\H,-0.6114486376,2.4919986529,2.4883310156\H,1.0428570546,1.8204511269,2.4172346606\H,0.7317828098,3.454672258,1.8350923754\H,1.3234033255,2.261108736,-

2.2029576219\H,0.1249498304,3.5356685078,-1.9394906829\H,-0.3859628995,1.9927908507,-2.6396197155\H,-3.2301895817,0.5536485532,2.6549983513\H,-4.7736734483,-0.1649190702,2.1645042351\H,-4.4929042985,1.5868495525,1.9732353768\H,-3.3701714263,0.3664672846,-2.647982631\H,-4.955101706,-0.0737764576,-2.007581867\H,-4.4243269223,1.6272513328,-1.9856341311\H,0.386633837,-1.9935453886,2.6394023401\H,-1.3231391444,-2.2601941008,2.2032760913\H,-0.1259888582,-3.5358044005,1.9391414207\H,-1.0432531173,-1.8206966545,-2.417123163\H,-0.7314043475,-3.4548341121,-1.8351611155\H,0.6113103848,-2.4915825238,-2.4885779191\H,3.3690802681,-0.3683470448,2.6480056661\H,4.9537655547,0.0745709833,2.0087356797\H,4.4252608777,-1.6271365331,1.9851445152\H,3.2305238841,-0.55398765,-2.6549061739\H,4.7737903118,0.1650271885,-2.1643523559\H,4.4934262736,-1.5867782935,-1.9728767323

HF=-1550.0295749

MP2=-1552.5163222

ZeroPoint=0.3337501

Thermal=0.3700804

Distannoxane dimer (13b)

MP2/6-311+G-LANL2DZ(Sn)*

Sn,0.0366083028,1.6435747245,-0.0056516635\Sn,3.17635005,-0.2697367544,-0.003824175\O,1.2168904048,0.0223989434,-0.0026286067\Cl,3.0535668192,2.339962342,0.0238480819\O,2.3111908872,-2.1805307425,0.0274728495\Sn,-0.0176002284,-1.6706038263,-0.0040868721\Sn,-3.1733096253,-0.2498267842,0.0100294095\O,-1.2107733808,0.0545871929,-0.0229135647\O,-2.2571088072,-2.1714912793,-0.0266915691\Cl,-3.2007242539,2.3030010126,-0.0324134162\C,0.0019535192,2.5354986863,-1.906048636\C,-0.0329043985,2.5091256584,1.906548899\C,4.0681962227,-0.3460678329,-1.9140699147\C,4.1771504443,-0.3486109528,1.8556521112\C,0.0981781194,-2.3999031334,-1.9793517711\C,-0.0337200179,-2.3597184904,1.988509262\C,-4.185441577,-0.448846628,-1.8353672724\C,-4.0085029645,-0.413350593,1.9410298425\H,2.722368034,-2.9584189527,0.4115386262\H,-2.6473828192,-2.9462559998,-0.4378971943\H,0.5563196069,1.9016275615,-2.6011284026\H,-1.0287726751,2.6450420462,-2.243298097\H,0.4834126483,3.513509482,-1.8779987779\H,-1.0694368955,2.6714988428,2.2021903626\H,0.5051431125,3.4574181955,1.9183804705\H,0.4522209931,1.8319015268,2.6127356982\H,3.3719294694,0.080229508,-2.6397960903\H,4.2886603061,-1.3759720858,-2.1986871354\H,4.9816409749,0.2499924992,-1.9432212182\H,3.4645350681,-0.0940330341,2.6436604068\H,4.5768968343,-1.3446202941,2.056527282\H,4.9866609139,0.3813821215,1.8897456123\H,-0.7653214156,-2.0707556295,-2.5602018161\H,1.0191138575,-2.0418210188,-2.4407645993\H,0.1268449532,-3.4926494117,-1.9866819655\H,0.8123316403,-1.9436868677,2.5380317041\H,0.0341585414,-3.4502510194,2.0225851521\H,-0.9712660512,-2.0691151748,2.4644767813\H,-3.4825509273,-0.2206316114,-2.6402759111\H,-5.0114636031,0.2600494327,-1.9022531231\H,-4.5642171292,-1.4623803261,-1.9816362238\H,-3.323397855,0.0495687495,2.6551405306\H,-4.9590755146,0.1189128266,2.0037979165\H,-4.1511497085,-1.4597595813,2.2139777637

HF=-1550.0158184

MP2=-1552.503739

ZeroPoint=0.334148

Thermal=0.3702566

Diethyltin dimethoxide monomer

B3LYP/6-311+G-LANL2DZ(Sn)*

Sn,0.0541097942,-0.1324077472,-0.1418802433\O,0.9025933745,1.4481636544,-0.9207859406\O,-0.2351427256,0.1784459228,1.7686431009\C,-1.0762391751,1.1189067467,2.3972707732\C,-1.8619338513,-0.4410191014,-1.0877131269\C,1.5621591865,-1.6392608959,-0.2143543993\C,0.3801555443,2.7450515747,-1.1031454335\C,-2.6671407949,-1.6179844876,-0.5179457484\C,2.8837655001,-1.2071064481,0.4377578898\H,-1.1453846354,0.8676757685,3.4602117067\H,-2.0972462264,1.1179883165,1.987408263\H,-0.6794080731,2.1397944268,2.3180200169\H,-2.4295210691,0.490518821,-0.9996164151\H,-1.6762913005,-0.5794286894,-2.1574105691\H,1.1610981933,-2.5318431845,0.2747843264\H,1.7150469239,-1.9030130086,-1.2652522385\H,1.0809092126,3.3175587543,-1.7185138239\H,0.2588441985,3.2763571821,-0.1496607785\H,-0.5913582021,2.7426515023,-1.6186522099\H,-2.8708422314,-1.4952089649,0.5491859323\H,-2.1424398356,-2.5704500763,-0.6388194241\H,-3.6329800583,-1.7182885683,-1.0239618275\H,2.751001726,-0.9742856702,1.4969591036\H,3.2982917591,-0.3191934956,-0.0450625396\H,3.6318344628,-2.0037118511,0.3662632586

HF=-392.2203205

ZeroPoint=0.2125493

Thermal=0.228547

MP2/6-311+G-LANL2DZ(Sn)*

Sn,0.0887828032,-0.1447727213,-0.265368166\O,0.7015618539,1.5937288154,-0.9097292121\O,-0.2073061154,-0.029427439,1.6638682992\C,-1.2241700214,0.7080675897,2.3110299375\C,-1.800008502,-0.6242485856,-1.1482527256\C,1.7623589613,-1.4245712205,-0.4663660423\C,0.0113193949,2.8232114425,-0.8048045281\C,-2.4572351397,-1.860826286,-0.5154406288\C,2.9444938674,-0.9484721367,0.3927831365\H,-1.3592235048,0.3012963958,3.3167060718\H,-2.1914503595,0.6467690213,1.7910871937\H,-0.9527990714,1.7667155734,2.4050590133\H,-2.4567080239,0.2470447462,-1.0496881087\H,-1.6539254129,-0.7715495744,-2.2235104315\H,1.46192589,-2.4381536901,-0.1812830108\H,2.0444246386,-1.4671640642,-1.5232544793\H,0.5027049265,3.548284827,-1.4582805561\H,0.0389509265,3.213619081,0.219901768\H,-1.0396021498,2.745981266,-1.1173379304\H,-2.60852484,-1.7331125707,0.5594336773\H,-1.8476011023,-2.7585545258,-0.653191537\H,-3.434005098,-2.0609071532,-0.965301193\H,2.6742509365,-0.9054299432,1.4502799626\H,3.2743947313,0.0490353571,0.0932648801\H,3.796373421,-1.6270619069,0.2906155847

HF=-389.5896372

MP2=-390.8914359

Diethyltin dimethoxide dimer

B3LYP/6-311+G-LANL2DZ(Sn)*

Sn,-1.7497107706,0.0011000022,0.3323936235\O,-0.3718690991,-0.0132436634,-1.1662776846\C,-2.1252811124,1.9241758712,1.2291783017\O,-3.1787846303,0.0119829631,-1.0830666006\C,-2.163771023,-1.9088857879,1.2390218815\C,-0.660726413,-0.0370299084,-2.5677047975\C,-4.5609997371,0.015688086,-0.8441230035\C,-2.2139163792,3.0626105847,0.2025095029\C,-2.2267164879,-3.0587278793,0.2232708224\Sn,1.7497111992,0.0010999679,-0.3323934652\O,0.371869523,-0.013242776,1.166277891\C,2.1252810065,1.9241751779,-1.2291796564\O,3.1787850589,0.0119838918,1.0830667382\C,2.1637717691,-1.908886153,-1.2390208073\C,0.6607266829,-0.0370255737,2.5677050938\C,4.5610001763,0.0156890493,0.844123157\C,2.2139130295,3.0626112197,-0.2025120546\C,2.226715456,-3.0587282126,-0.2232696053\H,-3.0681891814,1.8446105747,1.7811888557\H,-1.3501758081,2.1288266632,1.970614341\H,-1.414540558,-2.1085489577,2.0078481966\H,-3.1233678966,-1.8173125927,1.7593921258\H,-0.1191175657,0.7722845304,-3.0672065047\H,-1.7302387268,0.0876737798,-2.7244675975\H,-0.3435389332,-0.9920617312,-2.998152234\H,-5.0923691731,0.0213005924,-1.8031635002\H,-4.894716702,0.9025861999,-0.2810721038\H,-4.9001793772,-0.8737396337,-0.2885532878\H,-2.4724083274,4.0111721132,0.6854740995\H,-2.9706817878,2.8614730531,-0.5592938315\H,-1.2646980518,3.2147932237,-0.3190533132\H,-2.5015843593,-4.0012181523,0.7090710161\H,-1.2638284602,-3.2195113783,-0.2699617859\H,-2.9617283211,-2.8642572185,-0.5613938766\H,3.0681902028,1.8446103419,-1.7811883371\H,1.3501767977,2.1288241549,-1.9706173467\H,3.1233693518,-1.8173133918,-1.7593898133\H,1.4145422249,-2.1085490318,-2.0078481066\H,0.3435308034,-0.9920529046,2.9981562875\H,0.1191249832,0.7722956008,3.0672036418\H,1.7302400762,0.0876697126,2.7244672377\H,5.0923695912,0.0213017096,1.8031636589\H,4.8947170566,0.9025871206,0.2810721593\H,4.9001798746,-0.8737387235,0.2885535614\H,2.4724045279,4.011172526,-0.6854773275\H,2.9706774856,2.8614756196,0.559292752\H,1.2646936332,3.2147932396,0.3190489908\H,1.2638268091,-3.2195111666,0.2699619664\H,2.9617265643,-2.8642579011,0.5613958716\H,2.5015833645,-4.0012186656,-0.7090694286

HF=-784.4732313

ZeroPoint=0.4290227

Thermal=0.4610423

MP2/6-311+G-LANL2DZ(Sn)*

Sn,1.7401095493,0.0104624692,-0.2735142965\O,0.3196011564,-0.0389008389,1.169894249\C,2.0482216152,1.9522713528,-1.1048512417\O,3.108399007,0.0559978897,1.1970307258\C,2.1744084595,-1.9042117344,-1.1087199708\C,0.5585955148,-0.1363089486,2.575491627\C,4.4883088048,0.0701145127,0.922152834\C,2.0708046645,3.0210379308,0.0004093851\C,2.1328671433,-2.9877647089,-0.0182053205\Sn,-1.7400086578,0.0100372331,0.2736475682\O,-0.3195063053,-0.0361360001,-1.1698726458\C,-2.0478838815,1.949941389,1.1095068084\O,-3.1082935632,0.0591655877,-1.1967860904\C,-2.1745408543,-1.9065245599,1.1043907834\C,-0.5585123552,-0.1302401671,-2.5756931535\C,-4.4882013891,0.0728107956,-0.9218744212\C,-2.0703347581,3.0212832437,0.0067395478\C,-2.1331356692,-2.987538978,0.0113544777\H,2.9963600989,1.9650838843,-1.6551856291\H,1.2574364368,2.1582034376,-1.8316295488\H,1.4599020192,-2.1241687941,-1.9067036453\H,3.1679597604,-1.8787089825,-1.5708615835\H,-0.276207155,0.3308846741,3.1086482917\H,1.4901702328,0.3656095902,2.8330043276\H,0.6313010547,-1.1856871484,2.8780852295\H,5.0386541244,0.1220129957,1.8671513153\H,4.7910582064,0.9390379863,0.3158949318\H,4.8225952942,-0.8371246949,0.3945257142\H,2.2595392489,4.0158744,-

0.4152531352\H,2.8472508176,2.8110346034,0.7399369326\H,1.1182364705,3.0659359786,0.536
5496455\H,2.3920318729,-3.9704124198,-0.4246794348\H,1.137302024,-
3.0719894515,0.4276881516\H,2.8327499988,-2.7633714451,0.7908753532\H,-
2.9960214999,1.9615875816,1.6598686049\H,-1.2570744002,2.1540825837,1.8367637645\H,-
3.1680876911,-1.8819766418,1.5665937121\H,-1.4600591242,-2.1284278964,1.9018575941\H,-
0.6313317513,-1.178902125,-2.8807326559\H,0.2763403672,0.3381049353,-3.1077600426\H,-
1.4900329762,0.3723784828,-2.8320333055\H,-5.0385412613,0.1269732014,-1.866749018\H,-
4.790844422,0.940359169,-0.313597507\H,-4.8225977714,-0.8356120474,-0.3963576841\H,-
2.258948101,4.0151715636,0.4247188397\H,-2.8468057217,2.8130987059,-0.7332760463\H,-
1.1177604235,3.0673138527,-0.5292937463\H,-1.1375820875,-3.0708470363,-0.434736931\H,-
2.8329929729,-2.761175249,-0.797199215\H,-2.3924201494,-3.9710991622,0.4155388545

HF=-779.2091303

MP2=-781.8432557

Dibutyltin dimethoxide monomer

B3LYP/6-311+G-LANL2DZ(Sn)*

Sn,-0.0002009741,-0.506124911,0.0004198304\O,0.4777040071,0.6518973503,-1.505125769\O,-
0.4774574608,0.6526593912,1.5055847751\C,0.3520760073,1.5920906841,2.1566588365\C,-
1.8334754064,-1.5519128037,-0.3763617454\C,1.8324877807,-1.5528150342,0.3775452301\C,-
0.3513034948,1.5915788378,-2.1565086271\C,-2.3672054737,-
2.3518740795,0.8220700971\C,2.365769859,-2.3534686869,-0.8206236489\C,-3.7071284838,-
3.0420775118,0.5332788088\C,3.7053063187,-3.0443271546,-0.5316054659\C,-4.2437977867,-
3.8377059679,1.7254348479\C,4.241530049,-3.8406475702,-1.7234999712\H,-
0.2282566455,2.0729939286,2.9499334816\H,0.7069025272,2.3755421264,1.4739901851\H,1.230
1393454,1.1216466795,2.6214330845\H,-2.5631777905,-0.7951112657,-0.6823301937\H,-
1.6832236957,-2.2033313031,-1.2439114129\H,2.562613723,-
0.7963216026,0.6832650768\H,1.6818715006,-
2.2038642348,1.2453088715\H,0.2292981938,2.0718963618,-2.9499412558\H,-
0.7056912842,2.3754531361,-1.4740975426\H,-1.2296301153,1.1214737288,-2.6211282809\H,-
2.483138399,-1.6876481595,1.6858989232\H,-1.6371395578,-
3.1146343065,1.1238931172\H,2.4820745157,-1.6895916341,-1.6846706627\H,1.6352770502,-
3.115919244,-1.1221961037\H,-3.5924847153,-3.7072428546,-0.3318383897\H,-4.4427594619,-
2.2847336573,0.2358001735\H,3.5902902955,-3.7091439292,0.3337302288\H,4.4413611574,-
2.2872975117,-0.2343756177\H,-5.1987753095,-4.316324569,1.4905024005\H,-4.4037324515,-
3.1926475881,2.5952029495\H,-3.5462225482,-4.626204892,2.0262042823\H,5.1962395292,-
4.3197234456,-1.4884101948\H,4.4018256854,-3.1959646364,-2.5934799627\H,3.5435135085,-
4.6288546706,-2.0240103655

HF=-549.5112977

ZeroPoint=0.326532

Thermal=0.347913

MP2/6-311+G-LANL2DZ(Sn)*

Sn,-0.0001956959,-0.4859723643,0.0004164935\O,0.551218036,0.6785056003,-1.4713369841\O,-
0.5509561423,0.6792978867,1.4717874703\C,0.2697922971,1.6706464241,2.0639951862\C,-
1.7764660566,-1.577397228,-0.4209401866\C,1.7754621459,-1.578254921,0.4221321978\C,-
0.2689750779,1.6701183163,-2.0638716336\C,-2.2949364188,-
2.3379392594,0.8073849143\C,2.2935079454,-2.3394895743,-0.8059430439\C,-3.5869710416,-

3.1051586907,0.5243071165\C,3.5851132708,-3.1073383337,-0.5226125212\C,-4.0990991276,-3.8645004416,1.747311789\C,4.0968178026,-3.867366978,-1.7453677738\H,-0.3229994185,2.1963733605,2.8164788736\H,0.623298963,2.4056335127,1.3298528776\H,1.1449598616,1.2351188543,2.5641286271\H,-2.5352770448,-0.8708056796,-0.7762976937\H,-1.5813996456,-2.271457405,-1.247385813\H,2.5346686107,-0.8719722145,0.7772589433\H,1.5800062615,-2.271934846,1.2488050127\H,0.3241113328,2.1952659402,-2.8165276054\H,-0.6220711207,2.4055445487,-1.3299715333\H,-1.144385746,1.2349159627,-2.5638627015\H,-2.4663587632,-1.6362364824,1.6326269407\H,-1.5359892411,-3.0503916468,1.1600642075\H,2.4653232176,-1.6381533802,-1.6314149611\H,1.5341627273,-3.0516330796,-1.1583892644\H,-3.4147758267,-3.804241244,-0.3033224775\H,-4.3504466427,-2.397237561,0.1796763947\H,3.412526684,-3.8060532265,0.3052459977\H,4.348984174,-2.3997311365,-0.1782131195\H,-5.0252616586,-4.4023560732,1.5271349519\H,-4.2992688889,-3.1797195518,2.5765316031\H,-3.3621104833,-4.5965775807,2.0909619643\H,5.0226793833,-4.4056679891,-1.5250137283\H,4.2973709712,-3.182969861,-2.5748117535\H,3.3594203742,-4.5991446578,-2.0887787505

HF=-545.7585299

MP2=-547.6204436

Dibutyltin dimethoxide dimer

B3LYP/6-311+G-LANL2DZ(Sn)*

Sn,0.0006462698,1.7603261395,0.2606188141\O,0.0126695666,0.3216986272,-1.1804306613\C,1.9104250268,2.2175005811,1.1453127208\O,-0.0140667739,3.1318565816,-1.2131723687\C,-1.9160175197,2.1824829037,1.1490140137\C,0.0356624491,0.5542115607,-2.5925578485\C,-0.0208288293,4.5203500532,-1.0157605409\Sn,0.0008020592,-1.760444109,-0.2605260192\O,0.0136420581,-0.3218109032,1.1805196742\C,1.9105523256,-2.2170565008,-1.1455523058\O,-0.0134332444,-3.1319771864,1.2132656732\C,-1.9158391023,-2.1831012314,-1.148722961\C,0.0361745594,-0.5542573187,2.5926663722\C,-0.0213604244,-4.5204683349,1.0158673289\C,3.0609003951,2.2463129254,0.1274749376\C,-3.0637817386,2.2271813013,0.1287589755\C,3.0610341235,-2.2462366074,-0.1277323432\C,-3.0637768172,-2.2270564102,-0.1286342098\C,4.39890082,2.6823476688,0.7395489139\C,-4.4064754361,2.6383631578,0.7477614849\C,4.3990973299,-2.6817914083,-0.7400087531\C,-4.4063725164,-2.6385904023,-0.7476218456\C,5.5479766681,-2.6991576655,0.2711927648\C,-5.5533029425,-2.6696111354,0.2654710214\C,5.5478083368,2.6993153285,-0.2716261477\C,-5.5531872643,2.6701532616,-0.2655575149\H,1.8154271079,3.1984913748,1.6261340968\H,2.1167655504,1.5015162245,1.944880755\H,-2.119418411,1.4447826968,1.9293505099\H,-1.8306197379,3.1518833619,1.6545786259\H,0.9836416699,0.2039463693,-3.0127222235\H,-0.0722970607,1.6186233841,-2.7908991866\H,-0.7845200653,0.0076818466,-3.0683522368\H,-0.0302374435,5.0237059167,-1.9898309721\H,0.868989665,4.8780921873,-0.4723259217\H,-0.9071079291,4.8683012659,-0.4601691136\H,1.8156351804,-3.1978366132,-1.6268209424\H,2.1167971899,-1.5006919146,-1.9448082524\H,-1.8304224606,-3.1528468983,-1.6536204659\H,-2.1190880457,-1.4459066745,-1.9295734522\H,-0.7860755764,-0.0103240071,3.0678738342\H,0.9827326281,-0.2009945284,3.0135140684\H,-0.0686980577,-1.6190005975,2.7908896349\H,-0.0314308441,-5.0238026556,1.9899418876\H,0.8682855206,-4.8789600009,0.4726463009\H,-0.9078026594,-4.8676762177,0.4600734003\H,2.806517455,2.9179069713,-0.7002571728\H,3.1844208862,1.2538307046,-0.3242589532\H,-3.1785477706,1.2449165822,-0.3468754404\H,-2.812419125,2.9199170192,-0.682147808\H,2.8067184259,-2.9182872698,0.6996483386\H,3.1844161553,-1.2539751859,0.3245237254\H,-3.1786015826,-1.244466644,0.3463119799\H,-2.8126121424,-

2.9192753124,0.6827797356\H,4.6518809325,2.0142574322,1.5724753162\H,4.2828926661,3.680
5014309,1.1803109773\H,-4.2992825543,3.6267561722,1.2121710278\H,-
4.6561187264,1.9489399199,1.5641391453\H,4.6520236039,-2.0132321354,-
1.5725752884\H,4.2832199675,-3.6797263398,-1.181300888\H,-4.2991366707,-3.6273103742,-
1.2113240638\H,-4.6557992939,-1.9497161223,-1.5645285615\H,6.4866110385,-3.0154104913,-
0.1930411754\H,5.3416470349,-3.3865974202,1.0978263002\H,5.7133713749,-
1.7073494842,0.7043547084\H,-6.4951673048,-2.9690197427,-0.2033730952\H,-5.7105703341,-
1.6862329587,0.7203138728\H,-5.350203407,-
3.3761783549,1.0766470937\H,6.4863901599,3.0159178665,0.1924755971\H,5.3414286964,3.386
301081,-1.0986241248\H,5.7133329037,1.7072991118,-0.7042615467\H,-
6.4951396288,2.969283109,0.2032879226\H,-5.7104032729,1.6871022593,-0.7211243765\H,-
5.3498718246,3.3772748841,-1.0761962824

HF=-1099.0520374

ZeroPoint=0.6559221

Thermal=0.699072

MP2/6-311+G-LANL2DZ(Sn)*

Sn,1.7147622058,-0.0073393551,-
0.4053530308\O,0.404660982,0.0192710128,1.1396924751\C,2.0332951358,1.9294885436,-
1.2423054953\O,3.1781781809,-0.0439601773,0.9696617608\C,1.9646155035,-1.945445291,-
1.2625853488\C,0.7537804981,0.1037805467,2.5217693122\C,4.5361990448,-
0.042318818,0.6018670103\Sn,-1.7171937515,-0.0061946317,0.4049108796\O,-
0.4070519293,0.0221481381,-1.1400838952\C,-2.0333310623,1.9291380278,1.2461926416\O,-
3.1806798792,-0.0379629501,-0.9701431678\C,-1.9692842065,-1.9459165863,1.2577978531\C,-
0.7560463022,0.110478281,-2.5219549151\C,-4.538696886,-0.0355362339,-
0.6023324075\C,1.977408448,2.9875288899,-0.130232288\C,1.9588678378,-3.0142000951,-
0.1596643418\C,-1.9758151726,2.9895891844,0.1365027147\C,-1.9649001569,-
3.0121701869,0.1524547025\C,2.1386453284,4.4143554467,-0.6551247885\C,2.0851968502,-
4.4350482068,-0.7100573177\C,-2.1350166561,4.4154675246,0.6645824212\C,-2.0927887319,-
4.4341186287,0.699637559\C,-2.0536154019,5.4602594122,-0.4476313035\C,-2.0666356446,-
5.4887547944,-0.4059312885\C,2.0588102203,5.4567661111,0.4594340621\C,2.0576653138,-
5.4921594885,0.3931109048\H,3.0083689842,1.9691035729,-
1.7439725799\H,1.2706977344,2.1252232277,-2.0038848875\H,1.1574985986,-2.1252121912,-
1.9808864465\H,2.9094107396,-1.9920208936,-
1.8191307654\H,1.0473840348,1.1246965097,2.7840582118\H,1.5870201103,-
0.5618868215,2.7457048302\H,-0.1176251019,-0.1813035916,3.1214957452\H,5.151071901,-
0.0779070488,1.5071899943\H,4.8220841519,0.8643085318,0.044464759\H,4.8089243375,-
0.9132838004,-0.0162078958\H,-3.008437181,1.9689384032,1.7477810587\H,-
1.270591773,2.1221306545,2.0083283953\H,-2.9140839096,-1.9926350265,1.8143227405\H,-
1.1623167081,-2.1282634266,1.9756163461\H,0.1148377346,-0.1747642815,-3.1223626213\H,-
1.0478429866,1.1325205222,-2.7818756408\H,-1.5904692628,-0.5531951867,-2.7473875707\H,-
5.1536157455,-0.0683751435,-1.5077276489\H,-4.8235017561,0.8701815763,-0.0429045798\H,-
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980099,0.4112864677\H,1.0352144243,-2.9446586128,0.4306803641\H,2.778300628,-
2.8217695891,0.5442400167\H,-2.7583706631,2.7877799394,-0.6061936143\H,-
1.0228548946,2.9199988009,-0.4050937693\H,-1.0412490767,-2.9423453085,-0.4378594359\H,-
2.7842052314,-2.8172004439,-0.5508991129\H,1.3633686972,4.6104428875,-
1.4069022322\H,3.1003878307,4.4963667183,-1.1771599837\H,3.0185496953,-4.5143997369,-
1.2818100205\H,1.2715703388,-4.6180941227,-1.4235723298\H,-
1.3594950773,4.6087448837,1.4168349562\H,-3.0966659974,4.49770045,1.1867540049\H,-

3.0261509953,-4.5136944929,1.2713434709\H,-1.2792721372,-4.6197212116,1.4126178534\H,-2.1802768614,6.4749601797,-0.0594627798\H,-2.830541702,5.2903555032,-1.1992861512\H,-1.0848520422,5.4158251976,-0.9548092665\H,-2.1692565661,-6.5001699194,-0.0023145022\H,-1.1261765107,-5.4461719588,-0.9638068935\H,-2.8825582145,-5.3282041908,-1.1172167316\H,2.1869493877,6.4721482188,0.0735392417\H,2.8355090808,5.2840355135,1.2106796283\H,1.089997878,5.4126151166,0.9665434637\H,2.1591856532,-6.5027723931,-0.0127868531\H,1.1171718908,-5.4497639343,0.9509438346\H,2.8736657314,-5.334160666,1.1048781581

HF=-1091.5412941

MP2=-1095.3066161

Complete reference 11

Gaussian 03, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.