Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

^{119}Sn NMR spectroscopy in D_6-DMSO solution

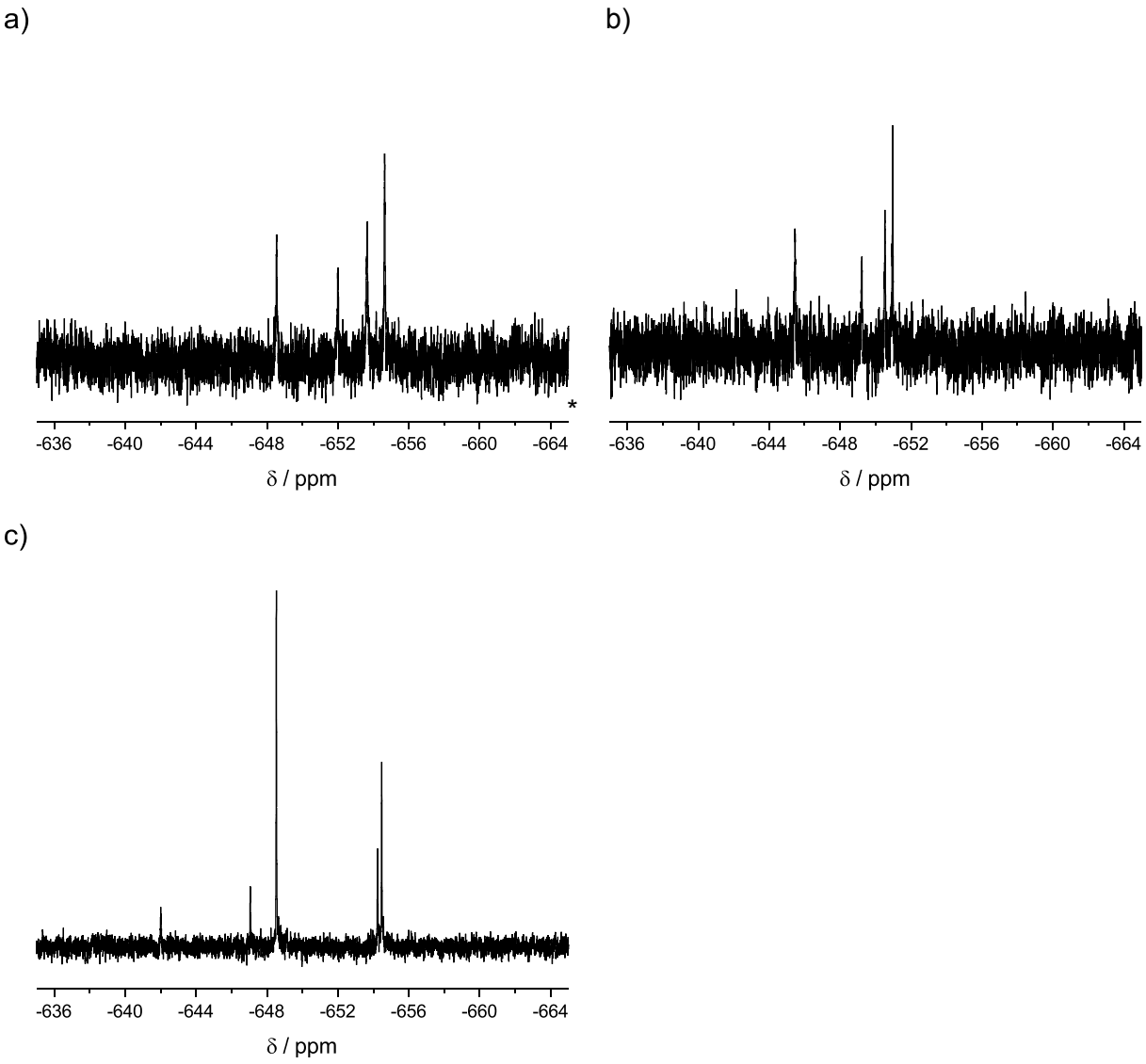

Figure S 1 ^{119}Sn NMR spectra of compound a) **1**, b) **2** and c) **3** in D_6-DMSO solutions.

Dynamic light scattering

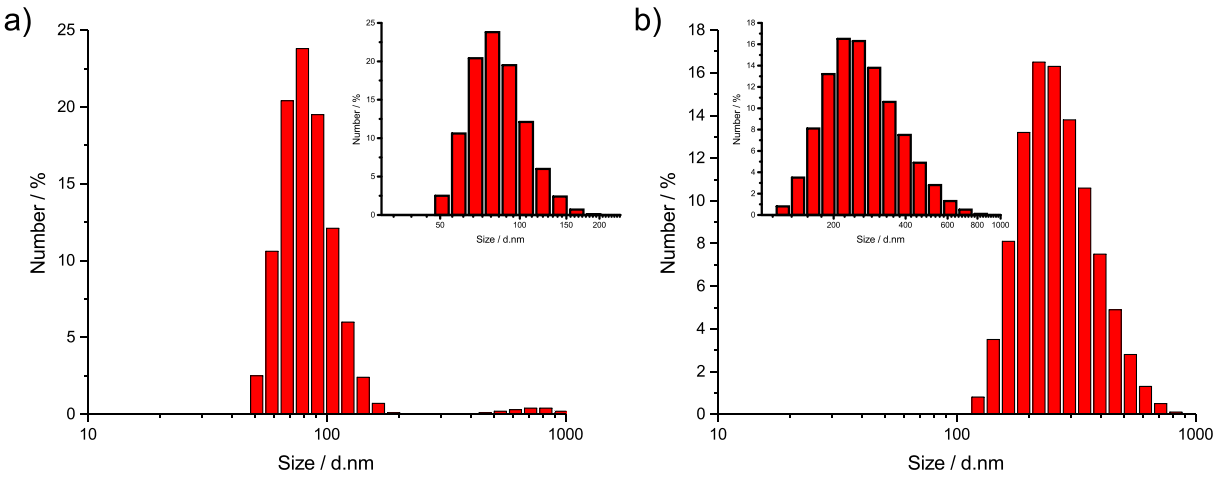

Figure S 2 Dynamic light scattering measurement of a) compound **2** in DMSO and b) **Ox-2** in ethylene glycol.

Solid state NMR spectroscopy

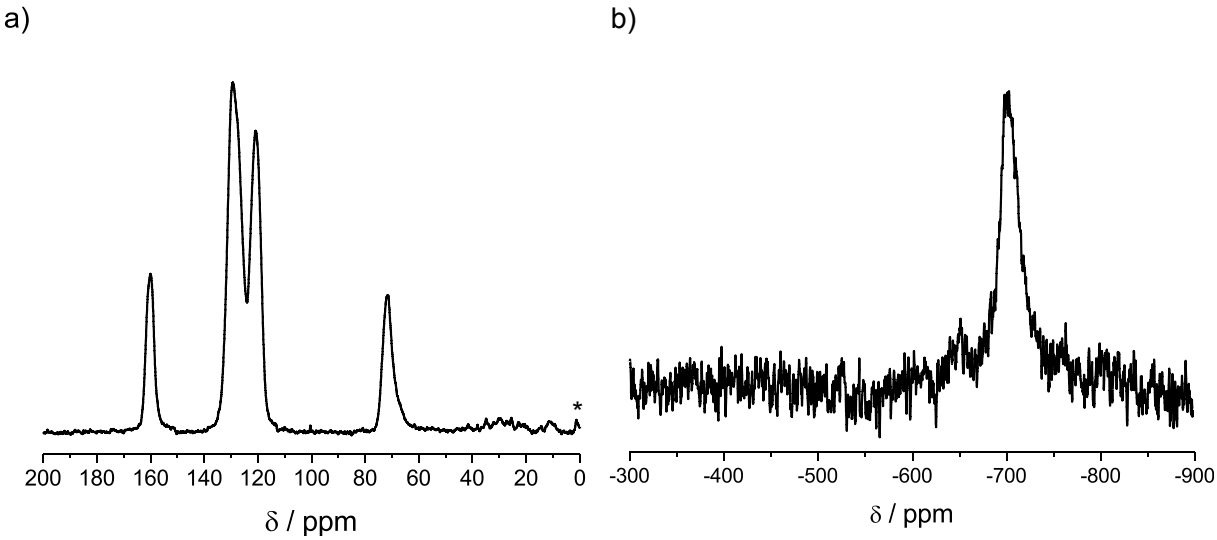

Figure S 3 a) $^{13}C\{^{1}H\}$ CP MAS NMR and b) ^{119}Sn CP MAS NMR spectra of compound **1**. The asterisk * marks spinning side bands.

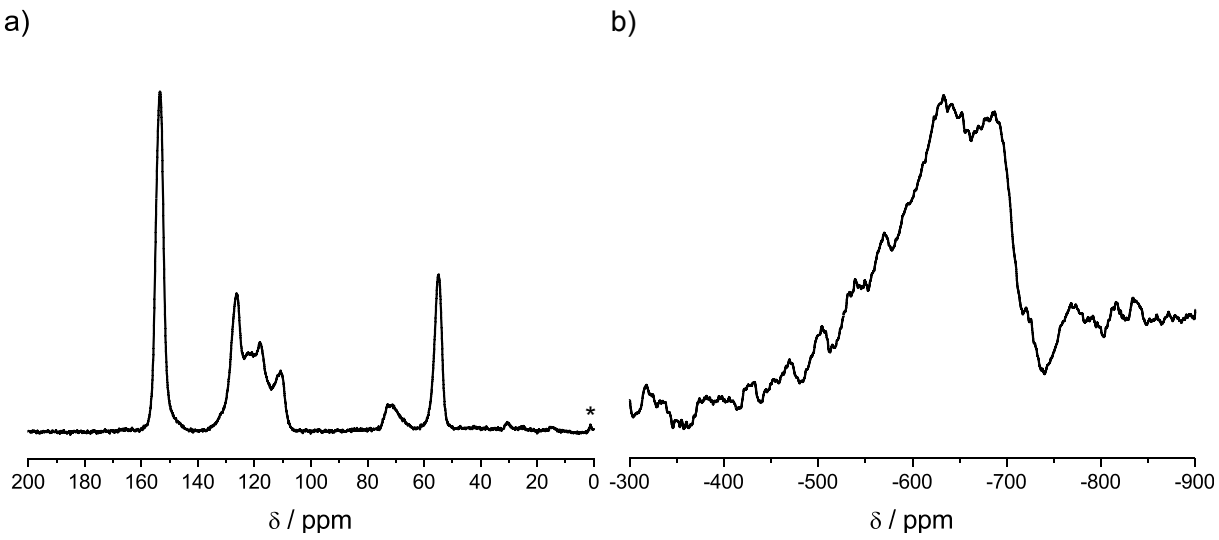

Figure S 4 a) $^{13}C\{^{1}H\}$ CP MAS NMR and b) ^{119}Sn CP MAS NMR spectra of compound **2**. The asterisk * marks spinning side bands.

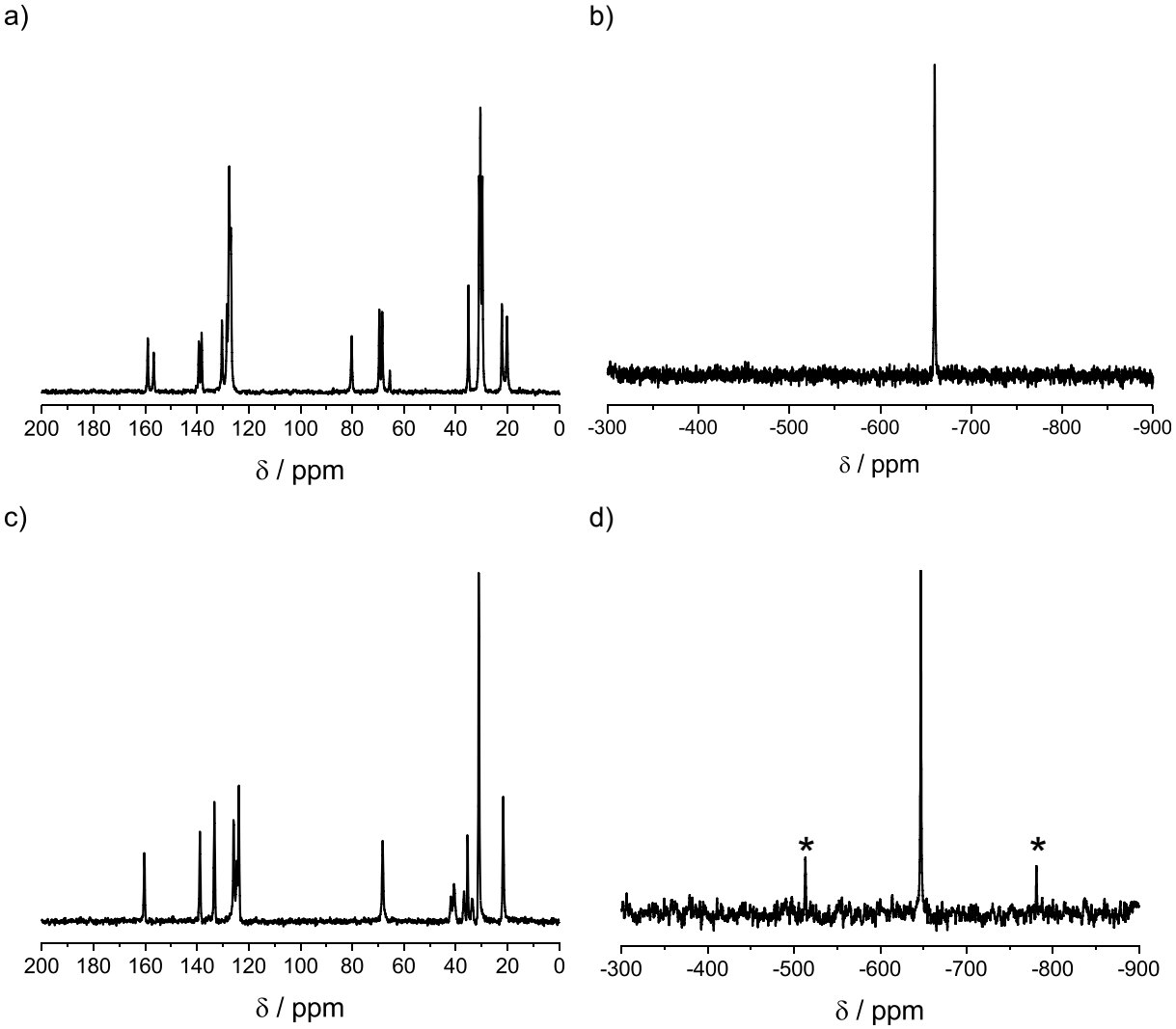

Figure S 5 a) $^{13}C\{^{1}H\}$ CP MAS NMR and b) ^{119}Sn CP MAS NMR spectra of compound **3** and c) $^{13}C\{^{1}H\}$ CP MAS NMR and d) ^{119}Sn CP MAS NMR spectra of crystals of **3**$(dmso)_2 \cdot 2$ DMSO. The asterisks in d) indicate rotational sidebands.

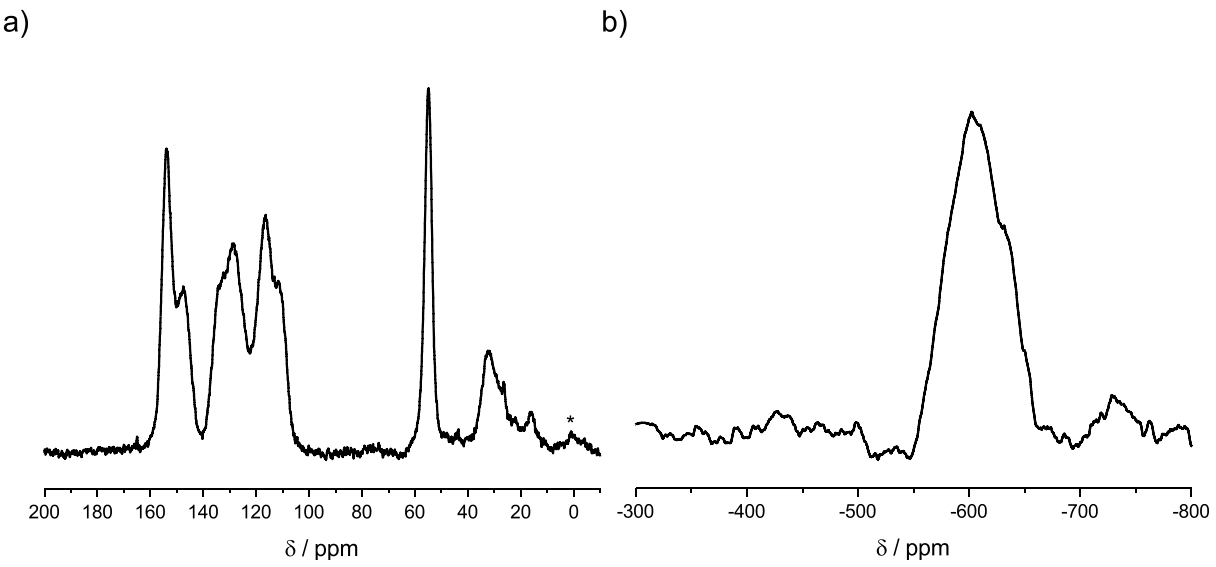

Figure S 6 a) $^{13}C\{^{1}H\}$ CP MAS NMR and b) ^{119}Sn CP MAS NMR spectra of compound **HM-2**. The asterisk * marks spinning side bands.

Thermal analysis

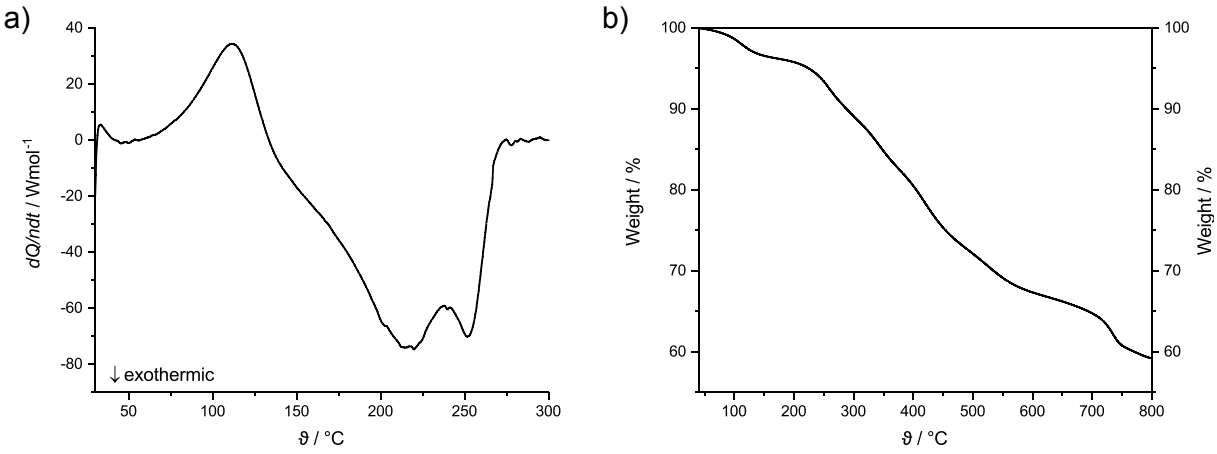

Figure S 7 a) Differential scanning calorimetry (DSC) and b) thermal gravimetric analysis (TGA) of compound **2**; heating rate 10 K min^{-1}, N_2 atmosphere for DSC and Ar atmosphere TGA measurement, inert gas volume flow 50 mL min^{-1} (DSC) / 60 mL min^{-1} (TGA).

Powder X-ray diffraction

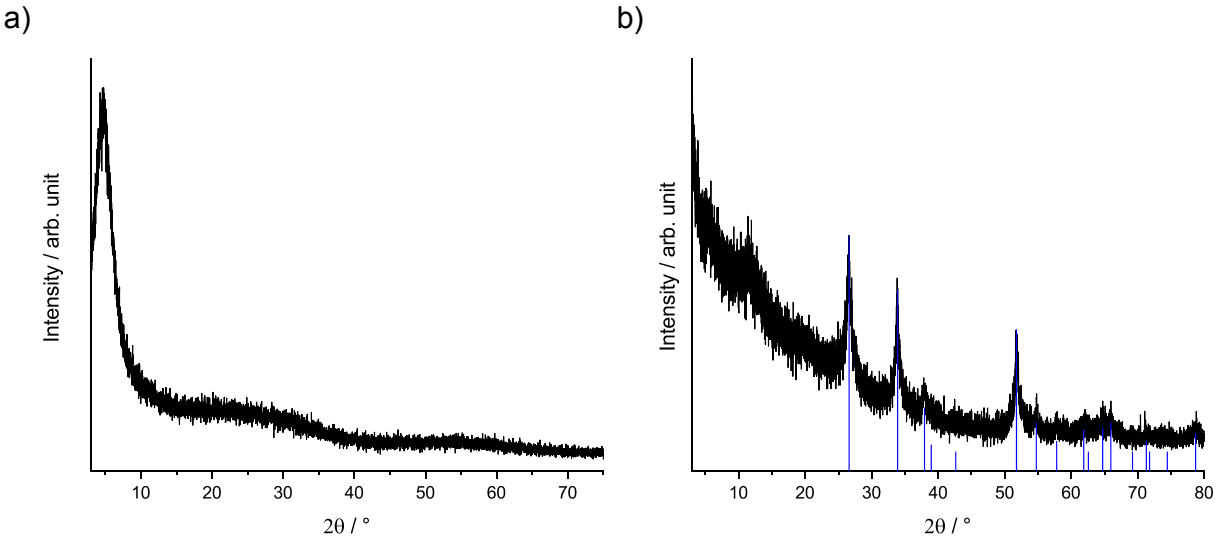

Figure S 8 Powder X-ray diffraction pattern of a) **HM-2** and b) ***Ox-2***. The blue bars in b) display the diffraction pattern of tetragonal SnO_2 (ICDD no. 00-041-1445).

ATR-FT-IR spectroscopy

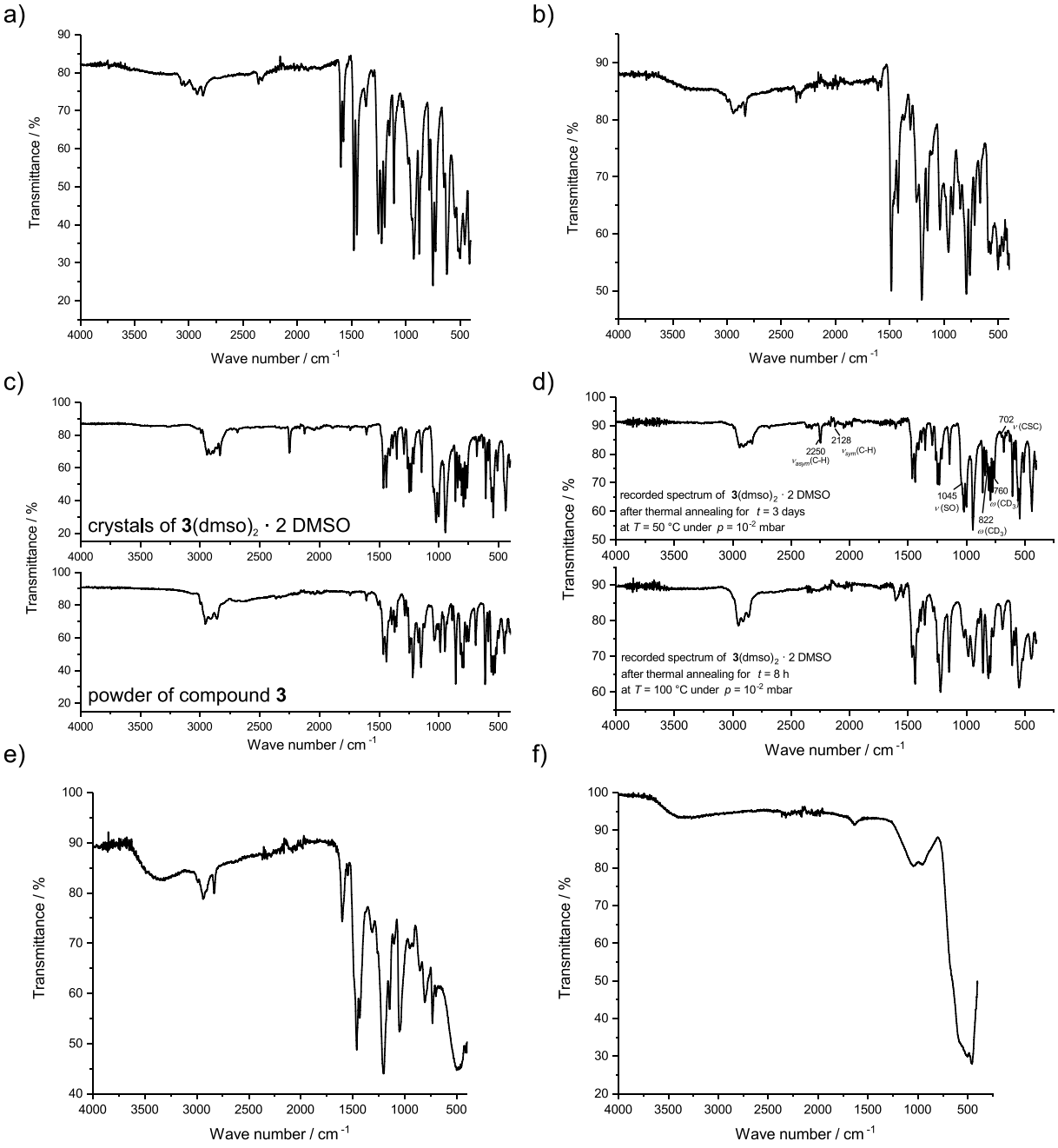

Figure S 9 ATR-FT-IR spectra of compound a) **1**, b) **2**, c) **3**$(dmso)_2 \cdot$ 2 DMSO (top) and **3** (bottom), d) **3**$(dmso)_2 \cdot$ 2 DMSO after thermal annealing (spectra depicted for two setups of parameters) e) **HM-2** and f) **Ox-2**.

Scanning electron microscopy

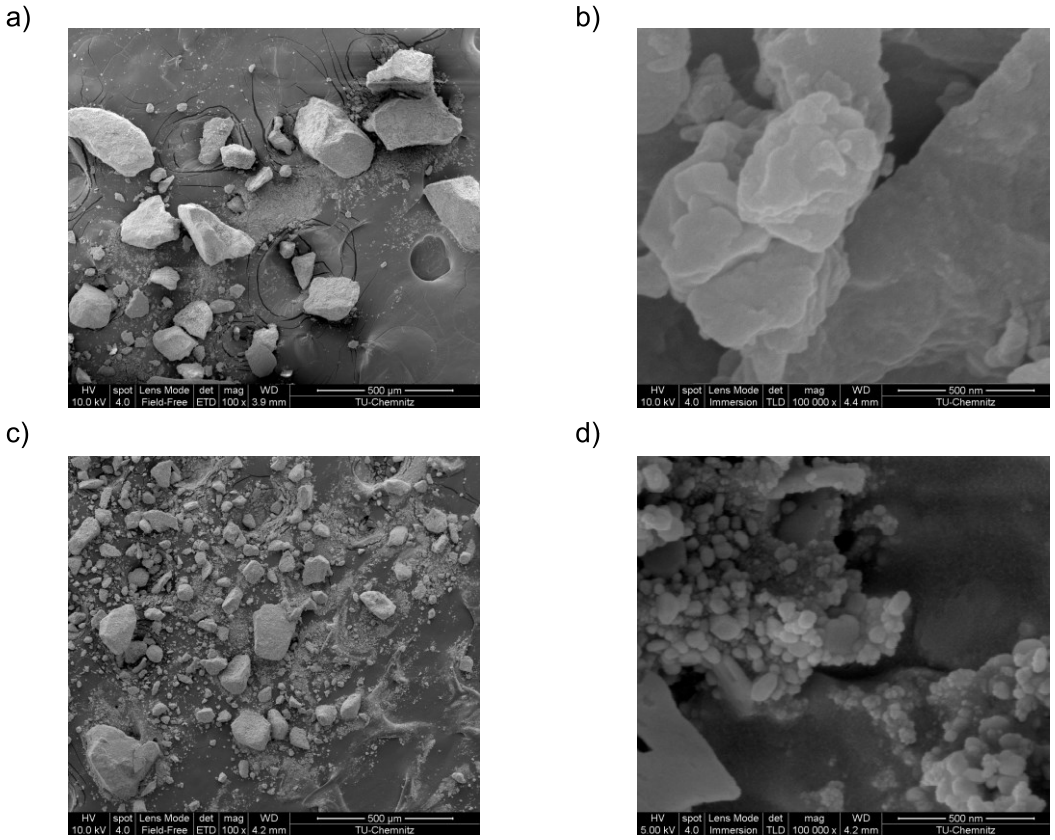

Figure S 10 Scanning electron microscopy images of **HM-2** in picture a) and b) and of **Ox-2** in picture c) and d).

Computational studies

Table S1 xyz data of the optimized geometries of $(\mathbf{1})_4$ and $(\mathbf{2})_4$.

$(\mathbf{1})_4$		$(\mathbf{2})_4$	
124		156	
Energy = -4223.680227108279		Energy = -5139.820604834179	
H -0.191609 -5.389533 -2.186867	H -1.385131 3.486902 -3.073956	H -0.762875 -5.429555 -2.296970	C -4.387464 0.074406 -2.231709
H 0.856409 -5.094620 -0.160344	H 2.334560 7.485171 -3.233001	H 0.452518 -5.098134 -0.346537	O -2.570418 0.977519 2.110197
H 3.305517 -5.364473 6.875100	C -2.823697 1.960299 -2.646351	H 3.340219 -5.442380 6.550071	C -3.717458 1.245044 -1.911452
H 1.578407 -6.925674 7.736426	C 0.518648 5.657731 -2.384529	C 2.300123 -5.301055 6.290121	H -5.101307 -0.321985 -1.522411
H -2.159005 -5.235938 -3.666194	C -1.985331 3.139943 -2.237076	C -1.620860 -4.933276 -1.862568	C -1.976278 1.489691 3.330933
C 2.275767 -5.267388 6.556531	O -4.357173 -0.929634 1.370463	C 1.345449 -6.150373 6.849453	H 0.262504 6.384686 -3.152669
C -1.085880 -4.884919 -1.842194	C -4.494798 0.281558 -2.109477	C -0.198858 -4.361156 0.129142	H -2.390787 0.906183 4.149473
C 1.309892 -6.142882 7.040057	O -2.336179 0.946425 2.211092	O -0.266044 -4.704554 1.497171	C -4.701825 -0.860073 3.908469
C 0.182044 -4.346506 0.263546	C -3.713913 1.369055 -1.732373	H 0.290793 -3.389483 -0.006656	O -3.931795 1.843183 -0.694150
O 0.023644 -4.677993 1.626520	H -5.139753 -0.169441 -1.368246	H 2.651037 -3.659032 4.952468	O -0.507723 5.656590 -1.421664
H 0.691677 -3.381925 0.155125	C -1.695136 1.428298 3.422697	C -2.807432 -4.899273 -2.596594	C -5.048537 -0.329312 2.651885
H 2.670631 -3.592346 5.255505	H 0.250608 6.461923 -3.071931	C 1.915049 -4.310404 5.404252	H -2.624313 3.822362 -2.180142
C -2.192521 -4.799160 -2.677714	H -2.047487 0.794602 4.233575	C -1.524689 -4.355239 -0.603353	O -0.184027 5.516366 1.647626
C 1.929138 -4.272796 5.652040	C -4.710251 -1.054285 3.749785	H 3.858604 -0.849039 1.826276	H -2.334102 2.514801 3.434032
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H 4.080525 -1.106925 1.982543	C -4.962737 -0.455277 2.502394	C 2.845170 -0.089040 0.105219	H -4.786911 -0.546984 6.032632
C -0.005776 -6.006881 6.612797	H -2.608935 3.966937 -1.895657	C 2.909939 -0.786569 1.312381	C -5.063894 -0.169778 5.057035
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H 5.697705 6.097718 -0.976231	Sn -0.982799 -3.551051 2.884914	C 2.292244 1.569473 3.507460	H 0.152799 -7.486656 8.891677
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H 4.723227 7.680080 -2.623550		H -4.325396 -2.929372 3.433099	O 2.295890 0.277623 5.463156
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C 2.768992 6.794149 -2.520226		C -2.449612 1.059058 -3.952537	C -6.534580 6.558356 4.768861
O -0.115736 2.409445 1.170592		C -3.867911 -2.110514 3.988499	H -6.804557 7.087730 5.679108
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C -3.808277 -2.253194 3.849550		H -1.294565 3.279966 -3.212149	H 3.703106 0.775869 -2.361948
H -3.753260 -2.603321 4.876703		H 2.310431 7.451931 -3.180197	H 3.172330 2.129083 -1.319485
C -0.194561 1.429811 3.372967		C -2.741093 1.755199 -2.787177	Sn -1.147401 -3.536432 2.818852
O -1.055993 2.785355 -1.168393		C 0.498104 5.597776 -2.433607	Sn -2.604216 -1.084231 1.546646
H -5.007467 -1.070560 -3.687278		C -1.962629 2.986251 -2.406347	Sn -2.215944 1.947863 0.326588
C -4.403058 -0.219906 -3.401079		O -4.597317 -0.928905 1.501532	Sn -0.255485 4.363341 0.050360

Table S2 xyz data of the optimized geometries of $(\mathbf{3})_3$ and $\mathbf{3}(dmso)_2$.

$(\mathbf{3})_3$		$\mathbf{3}(dmso)_2$
183		81
Energy = -4346.914748093323		Energy = -2555.2512102650
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Sn 3.478992 1.406942 -2.387865	O 4.537351 4.245919 -6.033398	H 0.887623 1.633276 10.967827
O 2.914088 0.093616 -3.773757	O 1.559897 1.729983 -1.885979	H 0.189080 2.238873 12.470401
C 2.724637 0.323321 -5.092663	C 0.963655 1.425241 -0.719626	C 2.062271 1.229224 12.701980
C 2.726871 -0.794008 -5.961659	C -0.116929 2.212194 -0.263997	C 1.684801 0.664882 13.914767
C 2.982906 -2.213468 -5.432469	C -0.650827 3.385222 -1.102662	H 0.704582 0.895220 14.319137
C 1.830595 -2.617078 -4.490824	C -1.861516 4.063791 -0.446930	C 2.532580 -0.195528 14.603789
C 3.051156 -3.247111 -6.566206	H -1.612687 4.496640 0.522874	C 3.778065 -0.473321 14.038314
H 2.111831 -3.330930 -7.114278	H -2.692853 3.369579 -0.316878	H 4.425762 -1.150097 14.577090
H 3.272723 -4.224932 -6.136672	H -2.206330 4.875286 -1.088968	C 4.220045 0.081618 12.835444
H 3.845862 -3.012671 -7.276086	C -1.118708 2.878690 -2.484196	C 3.332726 0.953574 12.159313
C 4.330409 -2.291147 -4.691853	H -1.956578 2.187838 -2.377783	C 2.138687 -0.793622 15.930734
H 4.493564 -3.307578 -4.326469	H -1.455337 3.722399 -3.090898	H 2.515924 -1.812246 16.037037
H 5.147450 -2.038921 -5.366047	H -0.326158 2.358292 -3.012764	H 1.054604 -0.824360 16.046253
H 4.370447 -1.619314 -3.843301	C 0.442749 4.457436 -1.264196	H 2.537717 -0.215231 16.769900
H 2.022122 -3.602617 -4.059924	H 1.346525 4.050737 -1.705927	C 5.610546 -0.238616 12.262963
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H 0.887122 -2.659877 -5.037482	H 0.081999 5.264150 -1.906187	H 6.458261 -1.109213 10.459280
C 2.421555 -0.559764 -7.296923	C -0.685753 1.857568 0.958126	H 4.976814 -0.183467 10.176033
H 2.388963 -1.395239 -7.980774	H -1.503148 2.450373 1.341803	H 4.890448 -1.791928 10.909908
C 2.168295 0.708241 -7.824305	C -0.256424 0.777019 1.732734	C 6.379808 -1.236629 13.143222
H 2.772310 0.668182 -9.893023	C -0.914388 0.460751 3.051632	H 7.351926 -1.439209 12.690935
C 1.881391 0.869490 -9.292838	H -1.748683 -0.234573 2.927734	H 5.854700 -2.188667 13.237331
H 1.109402 0.171975 -9.622549	H -0.206816 0.001535 3.741922	H 6.560791 -0.844000 14.145635
H 1.540136 1.878712 -9.523848	H -1.309795 1.362464 3.521023	C 6.455420 1.049953 12.171225
C 2.214262 1.787148 -6.960200	C 0.776412 -0.002902 1.236734	H 7.456777 0.811090 11.803656
H 2.043182 2.789702 -7.332087	H 1.139010 -0.854338 1.796992	H 6.561569 1.507990 13.157168
C 2.463746 1.614735 -5.595886	C 1.372430 0.289653 0.008941	H 6.014145 1.780782 11.500241
C 2.308899 2.807430 -4.693894	C 2.360979 -0.667870 -0.585918	C 4.301978 3.033958 15.147718
H 1.429338 2.725295 -4.060120	O 3.663847 -0.031702 -0.853523	H 3.973665 2.040607 14.847582
H 2.252178 3.721299 -5.276067	H 4.737416 4.274408 5.115435	H 3.927355 3.269119 16.143748
O 3.438129 2.967431 -3.771717	H 2.556351 -1.495648 0.089570	H 5.386903 3.110902 15.100291
O 6.467486 1.788787 -5.799482	H 2.021020 -1.056685 -1.545557	C 4.316788 5.721449 14.576612
C 6.870224 0.512669 -5.550820	O 6.311420 0.526018 0.759706	H 4.025796 6.496304 13.870198
C 7.205966 -0.300313 -6.655879	C 6.957195 0.187353 1.928377	H 5.399958 5.614093 14.597731
C 7.073693 0.214792 -8.095007	C 8.375126 0.199322 1.911242	H 3.919966 5.945391 15.566050
C 7.384796 -0.876389 -9.131034	C 9.157250 0.425188 0.609640	O 1.636398 3.428540 11.684729
H 8.412764 -1.236564 -9.070063	C 8.772043 -0.665973 -0.409770	O 3.680142 1.517768 10.989075
H 6.714799 -1.730925 -9.025747	H 9.290807 -0.501168 -1.355766	O 4.365166 3.929709 12.687298
H 7.241113 -0.460926 -10.129334	H 7.702956 -0.682868 -0.594243	S 3.578520 4.190097 13.977631
H 4.940810 -0.145164 -8.306752	H 9.062585 -1.648279 -0.032911	Sn 3.397091 3.535959 10.752953
C 5.636034 0.690974 -8.378576	C 8.874005 1.832170 0.056376	O 5.158983 3.643866 9.823288
H 5.573692 1.102659 -9.388854	H 7.816671 1.994769 -0.116766	O 3.112799 5.553676 10.515170
H 8.031576 1.739324 -9.320803	H 9.217808 2.584976 0.767140	O 2.431385 3.142084 8.817615
C 8.084300 1.362477 -8.296509	C 10.675470 0.331360 0.813885	C 5.667338 4.948650 9.589433
H 9.099759 1.003740 -8.117750	H 11.172408 0.489693 -0.144108	C 3.463172 6.118174 9.345967
H 7.889754 2.186766 -7.615536	H 11.042429 1.094682 1.500537	S 3.220775 2.880508 7.529123
H 5.310666 1.457488 -7.685924	C 9.041288 0.001361 3.114524	H 5.905135 5.438591 10.544238
C 7.738189 -1.557342 -6.383379	H 10.120425 0.040951 3.130620	H 6.608411 4.834690 9.043147
H 8.029251 -2.193364 -7.206232	C 8.379873 -0.229918 4.320362	C 4.735377 5.843602 8.806829
C 7.925931 -2.048265 -5.092178	C 9.147986 -0.396349 5.605263	C 2.577020 6.989346 8.667229
H 10.977379 -0.6466301.189902	H 9.518449 -1.418069 5.726992	C 2.501261 4.036902 6.356871
C 8.480871 -3.434364 -4.891176	H 10.015003 0.264400 5.634861	C 2.482513 1.349610 6.929090
H 9.349004 -3.606811 -5.529423	H 8.522516 -0.164642 6.467848	C 5.116063 6.408755 7.595428
H 7.738428 -4.193437 -5.150851	C 7.001339 -0.326296 4.282272	C 3.022113 7.544948 7.465821
H 8.785046 -3.603532 -3.858238	H 6.459045 -0.547366 5.195682	C 1.184429 7.308158 9.235503
C 7.551353 -1.238302 -4.030825	C 6.269994 -0.144596 3.106304	H 2.829711 5.030076 6.657432
H 7.672542 -1.592860 -3.015021	C 4.759867 -0.306117 3.281797	H 2.878221 3.800979 5.361908
C 7.024345 0.035064 -4.242110	H 4.592637 -1.235124 3.832474	H 1.416160 3.960953 6.401554
C 6.714448 0.898462 -3.051471	H 4.400823 0.507579 3.919123	H 2.770929 0.574921 7.636747
H 6.687208 0.305867 -2.142701	O 3.947866 -0.401063 2.114232	H 1.399507 1.457934 6.904999
H 7.474996 1.670904 -2.915486	C 4.559070 3.807212 -0.445231	H 2.881794 1.124725 5.940858
O 5.448293 1.596893 -3.167056	H 4.416867 4.365379 -1.368701	H 6.097706 6.179358 7.193974
Sn 5.338310 3.000676 -4.730805	H 5.620279 3.809617 -0.207653	C 4.269628 7.268623 6.904118
O 6.729552 4.248723 -4.053895	C 3.761630 4.412881 0.668706	H 2.375431 8.221246 6.925265
C 6.577550 5.606676 -4.111924	C 3.196326 5.672328 0.502595	C 1.319332 7.938080 10.638752
C 7.258611 6.413849 -3.180023	H 3.281231 6.164546 -0.459197	C 0.416683 8.305074 8.352667
C 8.344908 5.839177 -2.260363	C 2.526499 6.297927 1.545103	C 0.340591 6.018747 9.325104
C 9.407800 5.104346 -3.101485	C 1.939331 7.676366 1.395711	C 4.667161 7.867855 5.578771
H10.168069 4.680011 -2.441579	H 2.662978 8.444501 1.682515	H 0.330383 8.178369 11.036368
H 8.970550 4.298239 -3.683341	H 1.066038 7.802277 2.035749	H 1.811823 7.254141 11.324405
H 9.901111 5.795942 -3.786937	H 1.636341 7.877073 0.367432	H 1.898911 8.862486 10.590362
C 7.738447 4.866843 -1.241668	C 2.419927 5.613208 2.754414	H -0.557102 8.506510 8.801859
H 7.259895 4.026218 -1.734525	H 1.878549 6.096768 3.554090	H 0.940882 9.257754 8.260047
H 7.004092 5.383086 -0.621632	C 2.963341 4.348568 2.975895	H 0.239357 7.912043 7.349757
H 8.518604 4.479662 -0.587055	C 2.809829 3.636294 4.328164	H -0.662144 6.256732 9.689459
C 9.069207 6.937300 -1.472430	C 2.015449 2.332463 4.130385	H 0.237991 5.560207 8.339034
H 9.853069 6.479156 -0.868082	H 2.502778 1.654419 3.437625	H 0.780606 5.288693 9.997751
H 8.395624 7.467064 -0.795460	H 1.024534 2.555519 3.735333	H 4.290393 8.886647 5.472387
H 9.540100 7.665193 -2.134391	H 1.894071 1.816790 5.085313	H 5.751555 7.898521 5.466208
C 6.941571 7.772203 -3.174422	C 4.194778 3.343723 4.941616	H 4.270283 7.290319 4.738018
H 7.414573 8.413904 -2.446407	H 4.799186 2.715660 4.294050	
C 6.039430 8.352604 -4.064258	H 4.076974 2.840190 5.903743	
C 5.649310 9.800272 -3.926754	C 2.036498 4.492906 5.341998	
H 4.841993 9.922740 -3.199285	H 1.029879 4.730204 4.995320	
H 6.485830 10.408553 -3.578955	H 1.942307 3.939396 6.276564	
H 5.295203 10.210445 -4.873018	H 2.553127 5.427794 5.562862	
C 5.520135 7.550201 -5.072449	C 3.655112 3.752987 1.900573	
H 4.891621 7.985648 -5.841158	O 4.260376 2.550678 2.085315	
C 5.799915 6.187791 -5.126525	H 9.407568 1.986448 -0.883680	
C 5.370590 5.374091 -6.323119	O 4.199353 2.426196 -0.707215	
H 6.264744 5.040176 -6.864647		

Table S3 Calculated chemical shifts of tin atoms of the optimized geometries of (**1**)$_4$, (**2**)$_4$, (**3**)$_3$ and **3**(dmso)$_2$ being referenced on the chemical shift of tetracyclohexylstannane (δ = -97.3 ppm).

	(RI) TPSS/def2-TZVPP (Sapporo-DZP-2012/Autoaux for Sn)				(RI) M06L/def2-QZVPP (Sapporo-DZP-2012/Autoaux for Sn)			
	Sn1	Sn2	Sn3	Sn4	Sn1	Sn2	Sn3	Sn4
(**1**)$_4$	-594	-651	-649	-595	-751	-798	-796	-749
(**2**)$_4$	-598	-657	-656	-599	-752	-810	-807	-754
(**3**)$_3$	-545	-689	-534		-698	-834	-691	
3(dmso)$_2$	-650				-801			