

A DFT study of the Karplus-type dependence of vicinal ${}^3J(\text{Sn-C-X-C})$, X=N,O,S, in organotin(IV) compounds: application to conformationally flexible systems

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Table S1 Experimental (absolute values) and calculated vicinal coupling constants, $^3J(\text{Sn-C-X-C})$, in Hz, for the compounds of Scheme 1, **L5**, with several functionals.

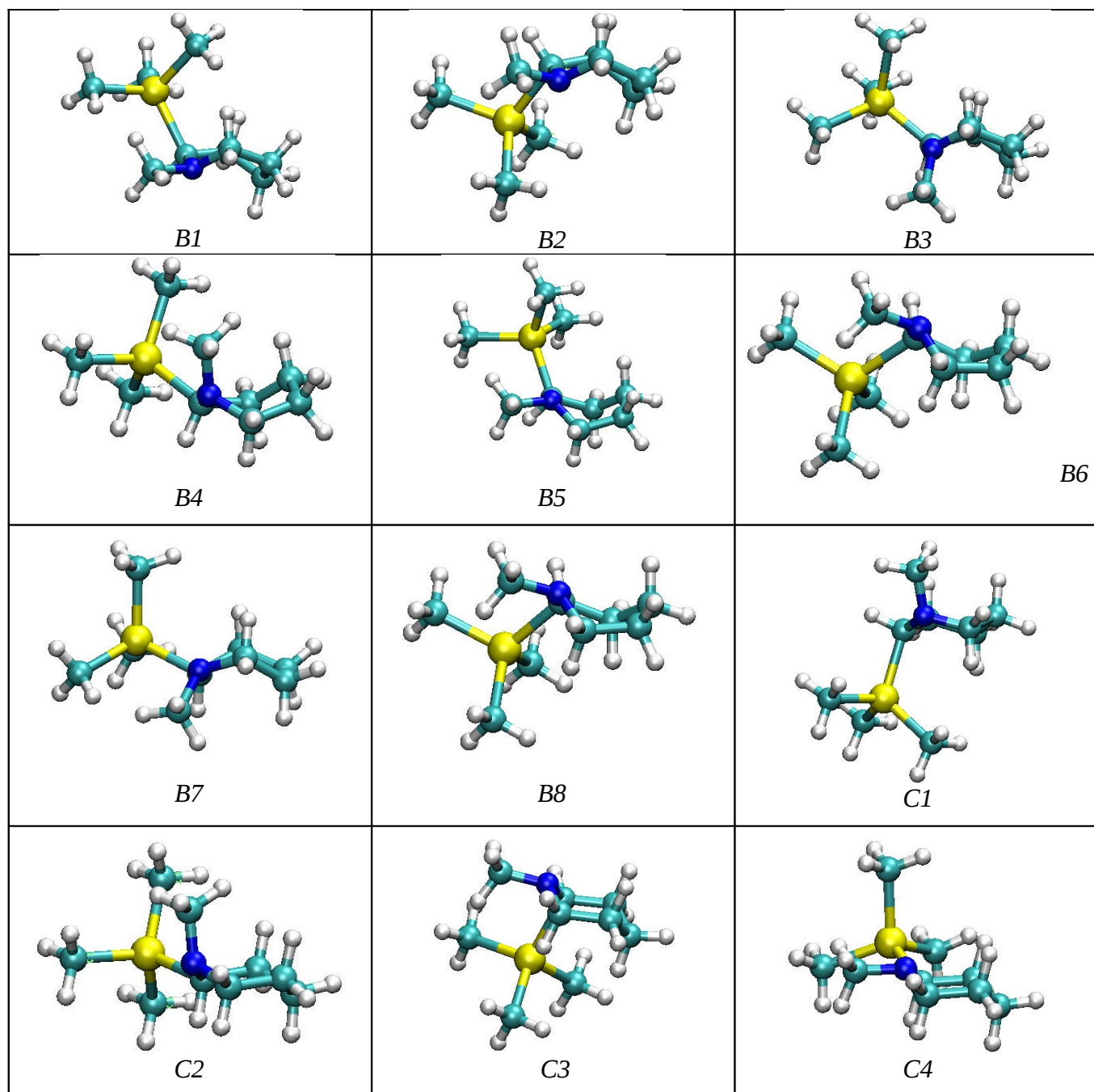
Compound	Functional								Exp.
	B3LYP	B3P86	B3PW91	MPW1PW91	O3LYP	OLYP	PBE1PBE	PBEPBE	
1									
$^3J(\text{SnCSC})$	-30.1	-29.0	-29.1	-29.4	-29.3	-29.3	-29.5	-29.0	32.4
2									
$^3J(\text{SnCOC})$	-34.7	-35.1	-35.8	-35.7	-37.3	-38.8	-36.0	-36.0	39.0
3									
$^3J(\text{SnCOC})$	-29.1	-29.8	-30.0	-29.7	-31.3	-32.8	-30.0	-32.2	34.0
$^3J(\text{SnCNC})$	-12.6	-13.2	-13.4	-13.8	-13.8	-13.4	-13.9	-12.2	14.5
4a									
$^3J(\text{SnCNC})$	-22.8	-23.1	-23.2	-23.5	-23.6	-24.0	-23.5	-23.6	30.5
$^3J(\text{SnCNMe})$	-3.3	-2.9	-2.8	-2.8	-2.9	-3.5	-3.0	-4.0	5.8
4b									
$^3J(\text{SnCNMe})$	-2.1	-2.2	-2.3	-2.5	-2.1	-1.6	-2.6	-1.3	11.8

Table S2 Experimental (absolute values) and calculated vicinal coupling constants, $^3J(\text{Sn-C-X-C})$, in Hz, for the compounds of Scheme 2, L5, with several functionals.

Compound	Functional								Exp.
	B3LYP	B3P86	B3PW91	MPW1PW91	O3LYP	OLYP	PBE1PBE	PBEPBE	
	$^3J(\text{SnCNC})$ $^3J(\text{SnCOC})$	$^3J(\text{SnCNC})$ $^3J(\text{SnCOC})$	$^3J(\text{SnCNC})$ $^3J(\text{SnCOC})$	$^3J(\text{SnCNC})$ $^3J(\text{SnCOC})$	$^3J(\text{SnCNC})$ $^3J(\text{SnCOC})$	$^3J(\text{SnCNC})$ $^3J(\text{SnCOC})$	$^3J(\text{SnCNC})$ $^3J(\text{SnCOC})$	$^3J(\text{SnCNC})$ $^3J(\text{SnCOC})$	
6cis syn	-7.15	-7.50	-7.56	-7.84	-7.63	-7.52	-8.01	-7.37	10.3
	-35.86	-36.91	-37.06	-36.97	-38.90	-40.55	-37.42	-39.70	35.5
6cis anti	1.31	1.33	1.31	1.03	1.83	2.50	1.02	2.24	10.3
	2.47	2.42	2.53	2.44	3.15	3.35	2.38	2.53	35.5
6trans syn	1.02	0.86	0.81	0.50	1.31	1.98	0.50	1.85	8.0
	2.90	2.85	2.93	2.82	3.53	3.74	2.78	3.00	27.5
6trans anti	-7.20	-8.26	-8.39	-8.72	-8.51	-8.44	-8.86	-8.03	8.0
	-32.30	-34.87	-35.03	-34.86	-36.72	-38.30	-35.24	-37.48	27.5
7cis syn	1.81	1.79	1.79	1.58	2.32	2.87	1.58	2.51	10.6
	3.59	3.62	3.74	3.63	4.54	4.86	3.58	3.86	35.1
7cis anti	-8.37	-8.73	-8.78	-9.03	-8.85	-8.85	-9.19	-8.8	10.6
	-37.56	-38.69	-38.83	-38.74	-40.67	-42.48	-39.22	-41.81	35.1
7trans syn	-7.47	-8.13	-8.3	-8.69	-8.41	-8.2	-8.83	-7.65	7.0
	-36.74	-37.91	-38.01	-37.83	-39.5	-41.16	-38.22	-40.78	28.6
7trans anti	2.41	2.32	2.34	2.20	2.81	3.19	2.18	2.18	7.0
	3.38	3.44	3.57	3.46	4.31	4.60	3.41	3.41	28.6
8cis syn	-5.48	-5.78	-5.84	-6.14	-5.75	-5.51	-6.26	-5.42	7.0
	-30.61	-32.05	-32.27	-32.39	-33.35	-34.43	-32.66	-33.78	19.1
8cis trans	2.07	2.03	2.04	1.83	2.61	3.16	1.82	2.66	7.0
	2.36	2.35	2.45	2.40	2.98	3.05	2.34	2.28	19.1
8trans syn	-10.79	-10.24	-10.43	-10.75	-10.76	-9.49	-10.92	-10.15	10.7
	-35.10	-32.61	-32.73	-32.74	-33.94	-31.38	-33.10	-34.55	38.5
8trans anti^a	-	-	-	-	-	-	-	-	10.7
	-	-	-	-	-	-	-	-	38.5
9cis anti^a	-	-	-	-	-	-	-	-	7.0
	-	-	-	-	-	-	-	-	10.0
9cis syn	-5.31	-5.60	-5.64	-5.77	-5.80	-5.99	-5.92	-5.99	7.0
	-28.94	-30.06	-30.22	-30.41	-31.36	-32.22	-30.76	-31.49	10.0
9trans syn	-3.94	-4.37	-4.46	-4.74	-4.43	-4.31	-4.90	-4.19	7.0
	-29.56	-30.84	-31.08	-31.24	-32.14	-32.91	-31.44	-31.92	28.2
9trans anti	1.57	1.45	1.40	1.12	1.92	2.52	1.11	2.27	7.0
	1.20	1.14	1.22	1.12	1.60	1.65	1.06	1.10	28.2
10cis syn	-33.3	-34.1	-34.3	-34.6	-35.6	-36.3	-34.9	-35.3	41.2
	-9.8	-10.0	-10.0	-10.0	-10.0	-10.2	-10.2	-10.6	14.0
10cis anti	3.13	3.00	3.09	3.13	3.56	3.53	3.09	2.68	41.2
	-1.32	-1.43	-1.19	-1.08	0.12	0.01	-1.18	-2.39	14.0
10trans syn	-11.6	-12.3	-12.5	-12.9	-12.6	-12.4	-13.0	-11.8	10.3
	-46.8	-48.0	-48.0	-47.9	-49.6	-51.3	-48.2	-50.8	34.7
10trans anti		3.38	3.47	3.45	3.96	4.11	3.39	3.30	10.30
		3.40	3.60	3.58	4.70	4.83	3.52	3.10	34.70

^a Optimization not converged. See text .

Scheme S1 Optimized conformers of *N*-methyl-2-(trimethylstannyl)piperidine, Xn: X= B(oat), C(hair), T(wist); n = 1,2,3,...,11 and cartesian coordinates of the studied models.



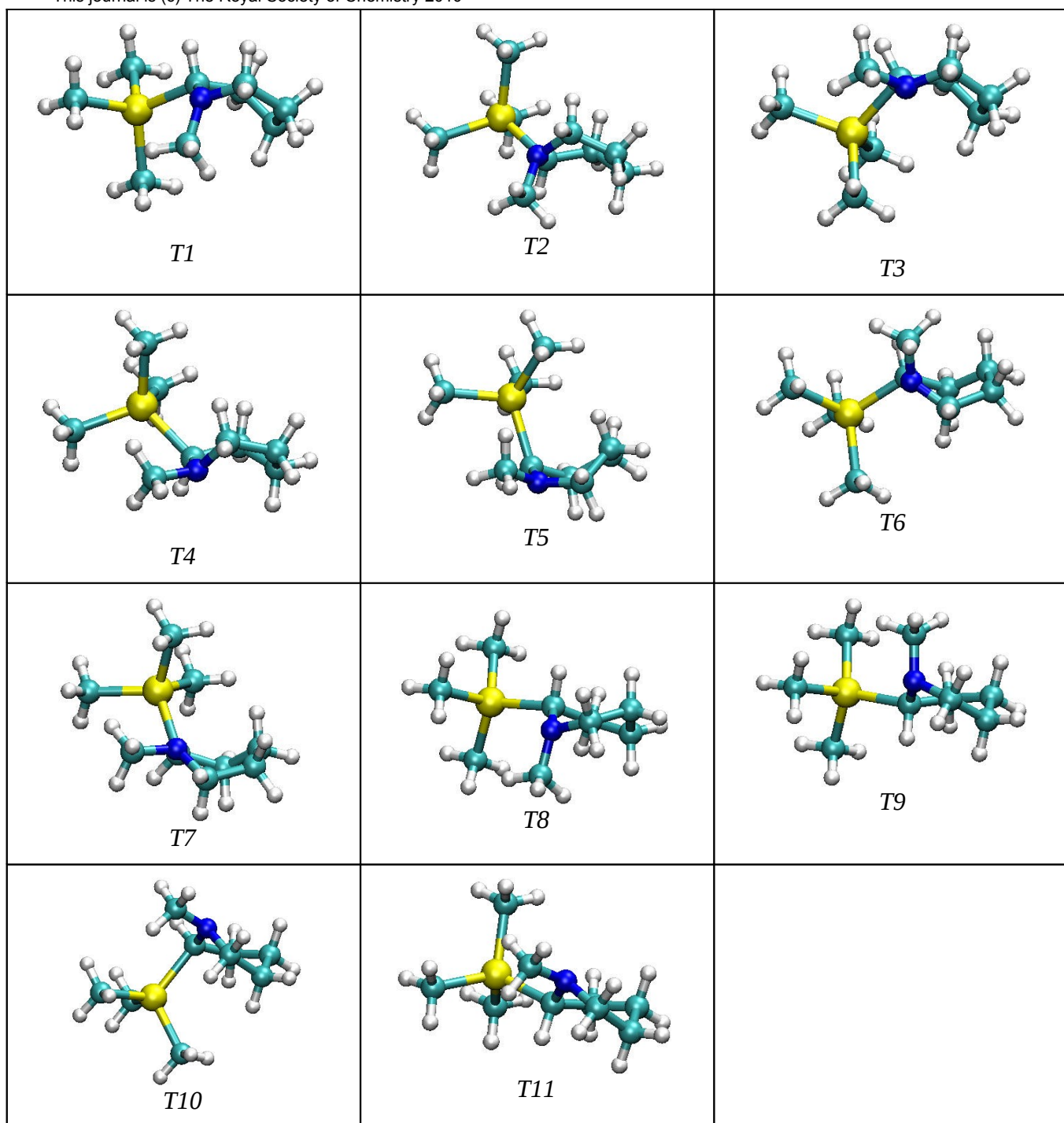


Table S3 Energy differences, including ZPE correction at 298.15 K, and calculated 3J of the conformers of *N*-methyl-2-(trimethylstannyl)piperidine. In parenthesis calculated dihedral angles.

Model	ΔE (kcal/mol)	$^3J(\text{calc})$		
		ϕ		
		SnCCC	SnCNC	SnCNMe
C4	0.0000	-46.9 (179.2°)	-43.1 (-178°)	-9.4 (56.7°)
C3	0.2290	-16.1 (-78.6)	-13.1 (72.6°)	-10.5 (-58.6)
C2	3.0371	-38.7 (-173.2°)	-37.7 (172.5)	-10.8 (-57.0°)
C1	3.2316	-11.3 (-77.9°)	0.2 (81.7°)	-52.3 (-146.8°)
T3	6.0296	-4.6 (-89.0°)	-42.6 (153.7)	-0.1 (-77.5)
T7	6.0296	-4.6 (89.0°)	-42.6 (-153.8°)	1.4 (77.5°)
B5	6.0491	-4.6 (89.0°)	-42.7 (-153.8°)	1.4 (77.5°)
B4	6.0516	-32.6 (147.8°)	-6.5 (-80.4°)	-21.7 (56.1°)
T4	6.0541	-33.1 (157.8°)	-4.2 (-88.0°)	-31.1 (46.6°)
B6	6.0554	-33.1 (-157.8°)	-4.2 (88.0°)	-31.1 (-46.6°)
B8	6.0566	-33.1 (-157.8°)	-4.2 (88.0°)	-31.1 (-46.6°)
B2	6.1426	-4.5 (-89.4°)	-43.2 (154.3°)	1.3 (-77.0°)
T11	6.6559	-29.2 (157.4°)	-42.0 (168.4°)	-18.5 (41.2°)
T10	6.6942	0.2 (-114.8°)	-25.3 (63.9°)	-0.3 (-68.3°)
B7	7.0305	-56.1 (178.4°)	-27.5 (-137.4°)	-4.2 (92.7°)
T6	7.2075	-46.1 (-165.4°)	-0.8 (109.5°)	-29.0 (-117.5°)
T2	7.2087	-46.2 (165.4°)	-0.8 (-109.5°)	-28.9 (117.4°)
B3	7.2100	-46.3 (165.4°)	-0.9 (-109.6°)	-28.8 (117.4°)
T8	8.7574	-32.2 (-167.3°)	-41.3 (-163.4°)	-6.9 (64.1°)
T9	8.7618	-32.2 (167.0°)	-41.2 (163.7°)	-7.1 (-63.8°)
T5	9.0849	-18.3 (69.5°)	11.0 (-95.9°)	-28.4 (44.3°)
T10	11.0101	-1.2 (-116.2°)	-35.5 (172.4°)	-28.0 (38.5°)
B4	11.0120	-1.0 (114.4°)	-35.0 (-171.8°)	-28.5 (-40.0°)

B1

32

N -1.801228 -1.049182 -0.036106
 C -0.861036 -0.382050 0.855295
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 C -2.866890 1.112042 1.173318
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 H -1.230703 -3.052881 0.223109
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 H 1.816343 1.693087 2.070775
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 H 1.389696 -2.412680 -1.150273

B3

32

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 H 2.396823 1.914104 1.491047
 H 2.707784 0.334815 2.285815
 H 2.909635 -2.076852 -1.006196
 H 2.034204 -2.638640 0.425277
 H 1.217330 -2.579204 -1.146587

B5

32

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B2

32

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B4

32

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B6

32

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 H -1.954998 2.105638 1.325713
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B7			C4			C2					
32			32			32					
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C	2.417810	-1.724783	-0.536821	C	-1.282080	0.110396	-0.473482	C	-1.429115	0.020572	-0.327362
N	1.376397	-1.160933	0.371197	N	0.109098	0.097522	-0.011672	C	0.015371	0.181436	0.168643
C	0.066921	-0.953636	-0.292507	C	0.214771	-0.094471	1.438506	N	0.736630	1.299850	-0.448430
C	0.157600	-0.939902	-1.801143	C	-0.591192	0.972263	2.189571	C	0.005967	2.558167	-0.259583
C	0.728355	-2.244948	-2.344647	C	-2.048874	1.029135	1.726501	C	-1.440510	2.508714	-0.784747
H	1.559199	-3.671720	-0.935343	H	-0.182593	-1.089570	1.719360	C	1.171290	1.018837	-1.806054
H	-0.687289	-1.699573	0.041951	Sn	2.301948	-0.048777	2.181250	Sn	1.111320	4.352161	-0.913454
H	2.844417	-0.867334	-1.094999	H	-0.547669	0.773416	3.262181	C	0.909344	4.724429	-3.046880
C	1.257693	-1.904618	1.648921	H	-0.134347	1.954306	2.029243	C	0.233009	6.033220	0.148884
Sn	-0.720928	1.014509	0.371408	H	-2.557208	0.102270	2.012441	C	3.209988	4.197448	-0.384801
H	-0.849541	-0.763621	-2.231654	H	-2.575837	1.845331	2.226561	H	-0.050435	2.710440	0.825616
H	0.779738	-0.085346	-2.143220	H	-3.135895	1.146608	-0.150131	H	-1.954130	3.447155	-0.557851
H	-0.069946	-3.010985	-2.399484	H	-1.708671	2.172969	-0.069482	H	-1.447178	2.410847	-1.874750
H	1.055410	-2.089134	-3.390987	H	-1.759178	-0.872998	-0.298832	H	-2.346406	1.529923	0.907613
H	3.246041	-2.141111	0.070453	H	-1.274933	0.271285	-1.553634	H	-3.203306	1.246204	-0.596448
H	2.706183	-3.124642	-2.154772	C	0.874224	-0.870848	-0.773495	H	-1.918230	-0.788517	-0.221308
H	0.574297	-1.354313	2.319825	C	2.221356	0.344555	4.318449	H	-1.427838	-0.275309	-1.380577
H	0.880786	-2.932446	1.531710	C	3.323815	-1.951991	1.925690	H	0.002822	0.354397	1.249981
H	2.241235	-1.952515	2.134314	C	3.429498	1.537326	1.220147	H	0.586103	-0.734277	-0.000464
C	-2.690719	1.261832	-0.453201	H	4.438477	1.569089	1.629492	H	1.372769	5.678123	-3.297178
C	-0.813859	0.968276	2.520047	H	3.488718	1.370816	0.146234	H	1.393483	3.938073	-3.623687
C	0.554862	2.597862	-0.318704	H	2.948269	2.497831	1.396663	H	-0.142556	4.765540	-3.326472
H	-2.905797	2.318271	-0.615357	H	4.253136	-1.944589	2.494292	H	3.732788	5.108926	-0.671956
H	-2.763898	0.740776	-1.408923	H	2.698638	-2.792304	2.292242	H	3.312570	4.055975	0.689883
H	-3.441135	0.854033	0.224358	H	3.556334	-2.135734	0.878277	H	3.670387	3.351327	-0.891425
H	-0.021624	3.508537	-0.481675	H	3.225422	0.282093	4.736795	H	0.744451	6.955672	-0.123643
H	1.333986	2.802113	0.415978	H	1.824000	1.339069	4.514491	H	-0.822114	6.135137	-0.102142
H	1.028568	2.308811	-1.258069	H	1.591538	-0.389595	4.819529	H	0.323554	5.890299	1.224994
H	-0.314137	1.836650	2.948414	H	1.938575	-0.783989	-0.553739	H	1.847303	1.803032	-2.150440
H	-1.848282	0.953630	2.862145	H	0.571919	-1.913733	-0.572626	H	1.730245	0.081793	-1.816016
H	-0.310226	0.061640	2.875628	H	0.743739	-0.685117	-1.840218	H	0.365137	0.931159	-2.550140
B8			C3			C1					
32			32			32					
C	2.422019	1.069225	-2.471344	C	-2.336222	0.860018	1.340696	N	-2.523656	-0.212009	1.886688
C	2.418612	-0.011573	-1.371648	C	-2.205769	0.934177	-0.180983	C	-2.325854	1.197486	1.549000
N	2.040860	0.576458	-0.095990	C	-1.080195	0.016482	-0.658547	C	-2.365417	1.505182	0.044498
C	0.648432	1.001973	-0.046097	C	0.233804	0.299664	0.072866	C	-1.367734	0.617245	-0.704069
C	0.221328	1.616907	-1.395774	N	0.039426	0.217810	1.508665	C	-1.616909	-0.856611	-0.373480
C	1.426187	2.194442	-2.141048	C	-0.991950	1.110871	2.019047	C	-1.625725	-1.104251	-1.144349
H	2.167074	0.607546	-3.428356	H	-1.366434	-1.022931	-0.460686	Sn	0.376376	-1.184851	2.102686
Sn	-0.914927	-0.502407	0.597759	Sn	1.259921	2.143065	-0.776686	C	0.122107	-2.339894	3.923579
H	3.412470	-0.447543	-1.267930	C	0.750645	4.104204	0.028993	C	-3.920436	-0.628332	1.868128
C	2.487462	-0.152604	1.064506	C	3.418580	1.903216	-0.590268	C	1.753563	-2.235159	0.781308
H	0.576503	0.767642	0.732022	C	0.824544	2.197111	-2.912468	C	1.281333	0.719165	2.637949
H	-0.248827	0.870003	-2.042894	C	1.264814	0.289481	2.272208	H	-2.585322	-1.149537	-0.797432
H	-0.536966	2.380563	-1.217668	H	-1.079098	0.945158	3.094668	H	-3.076024	1.784308	2.082047
H	1.105139	2.697819	-3.055098	H	-0.703030	2.169190	1.882593	H	-1.351304	1.506249	1.938083
H	1.910145	2.946707	-1.516093	H	-2.694545	-0.131992	1.627478	H	-3.372846	1.335530	-0.346859
H	1.745359	-0.841431	-1.648890	H	-3.066931	1.586002	1.703972	H	-2.141420	2.562744	-0.116647
H	3.424664	1.486026	-2.579485	H	-3.148520	0.661712	-0.659863	H	-1.433496	0.783881	-1.781273
H	2.265625	0.415594	1.969620	H	-1.992432	1.966756	-0.477763	H	-0.349073	0.892574	-0.408365
H	2.009161	-1.143686	1.168988	H	0.961650	-0.469341	-0.197862	H	-1.969683	-2.124737	1.329508
H	3.566275	-0.305830	1.017544	H	3.927187	2.610112	-1.245394	H	1.058296	-2.384217	4.478687
C	-2.850069	0.396906	0.152656	H	3.737700	2.085451	0.434950	H	-0.637145	-1.874700	4.550386
C	-0.835246	-2.414465	-0.446676	H	3.715879	0.893689	-0.872808	H	-0.192140	-3.355881	3.687792
C	-0.881266	-0.889393	2.742249	H	1.301185	4.870236	-0.517219	H	2.249984	0.532068	3.101074
H	-2.954990	1.355145	0.660407	H	-0.315773	4.296361	-0.077284	H	1.429769	1.342890	1.758157
H	-2.964799	0.555626	-0.918645	H	1.014949	4.167271	1.083195	H	0.653108	1.253144	3.348971
H	-3.646518	-0.264225	0.493335	H	1.411925	2.985894	-3.381992	H	2.708551	-2.381910	1.284921
H	-1.711816	-3.007623	-0.186723	H	1.081896	1.248224	-3.381925	H	1.352509	-3.210213	0.507017
H	-0.825879	-2.261033	-1.524847	H	-0.231216	2.398434	-3.088904	H	1.925808	-1.660484	-0.127838
H	0.059163	-2.967695	-0.164613	H	-0.939355	0.105814	-1.736956	H	-4.503182	0.032088	2.512559
H	-0.818105	0.045923	3.297353	H	1.062296	0.068099	3.320757	H	-4.391463	-0.626760	0.873352
H	-1.794767	-1.405724	3.036162	H	1.979567	-0.445699	1.900414	H	-4.000679	-1.639290	2.270140
H	-0.026973	-1.510507	3.006553	H	1.747183	1.282447	2.226048	H	-0.870904	-1.493191	-0.855503

T3 32			T2 32			T5 32					
C	-0.999292	0.800667	-1.028118	C	0.253266	-1.314826	-0.199904	C	0.079843	-1.434837	-0.093787
N	0.138730	-0.089534	-1.315750	C	1.112665	-0.608108	0.869364	N	0.817048	-0.748494	0.952124
C	0.328015	-1.124726	-0.302703	C	0.518249	0.772055	1.227609	C	0.605020	0.702124	1.053822
C	0.758468	-0.500739	1.033073	C	-0.969150	0.833718	0.863937	C	-0.745328	1.162637	0.500764
C	0.085087	0.868385	1.252794	C	-1.169199	0.629611	-0.647820	C	-0.923900	0.730411	-0.969381
C	-1.235303	0.927854	0.488482	N	-0.298165	-0.425625	-1.215433	C	-0.073511	-0.510276	-1.298456
Sn	-0.659034	2.780243	-1.982882	H	-0.584123	-1.820548	0.287469	Sn	-1.897774	-2.446226	0.410593
C	1.463833	3.171777	-2.202519	H	-1.508142	0.077867	1.443120	H	-1.541511	0.740753	1.115154
C	-1.615335	2.863501	-3.937370	H	2.139848	-0.492588	0.518807	H	0.693793	0.993335	2.101474
C	-1.547481	4.348902	-0.762321	H	0.664735	0.989842	2.287305	H	1.406635	1.226857	0.520346
H	-1.918078	0.400267	-1.488095	H	1.042865	1.557801	0.677531	H	-0.825810	2.247085	0.597691
H	-0.585915	-1.730058	-0.170177	H	-1.398621	1.796009	1.150252	H	-1.978873	0.520189	-1.160582
H	-1.875642	0.109180	0.833770	Sn	-3.262042	0.190272	-1.215000	H	-0.648577	1.545291	-1.641630
H	1.843272	-0.386395	1.052236	H	-0.915463	1.571300	-1.140382	H	-0.499462	-1.053207	-2.142622
H	-0.077439	1.048619	2.316649	C	0.671840	0.058453	-2.180891	H	0.928303	-0.193248	-1.608264
H	0.744214	1.664541	0.898696	H	1.162788	-1.247147	1.754722	C	0.906258	-1.459350	2.202895
H	-1.779093	1.845405	0.176701	H	0.828585	-2.095543	-0.700565	H	0.659364	-2.316627	-0.385156
C	0.085638	-0.627770	-2.657886	H	1.217674	-0.786087	-2.605229	H	1.275123	-2.472444	2.029342
H	0.498072	-1.186689	1.842666	H	0.155304	0.560212	-3.000928	H	1.609564	-0.962432	2.871397
H	1.098744	-1.810191	-0.658091	H	1.408407	0.769124	-1.770469	H	-0.061050	-1.546973	2.731810
H	1.621144	4.010327	-2.879598	C	-3.802047	-1.781189	-0.476614	C	-2.889111	-2.903684	-1.478797
H	1.900814	3.413654	-1.234905	C	-4.660821	1.654574	-0.404349	C	-1.499218	-4.360759	1.374160
H	1.965880	2.291854	-2.599769	C	-3.410773	0.192823	-3.382165	C	-3.340255	-1.376117	1.650229
H	-1.596652	3.885674	-4.314053	H	-4.401559	-0.139364	-3.689830	H	-3.758167	-3.534194	-1.292172
H	-1.098810	2.221227	-4.649240	H	-3.242036	1.194527	-3.775483	H	-3.221513	-1.991499	-1.972770
H	-2.652698	2.538780	-3.864584	H	-2.667945	-0.482141	-3.804167	H	-2.213429	-3.436055	-2.147466
H	-1.417331	5.309515	-1.259722	H	-5.676978	1.405761	-0.708813	H	-2.411444	-4.956212	1.403687
H	-2.613459	4.173534	-0.622155	H	-4.616240	1.662311	0.683992	H	-0.742338	-4.915015	0.819797
H	-1.068607	4.396332	0.214683	H	-4.422758	2.652396	-0.771008	H	-1.145422	-4.212199	2.393274
H	0.059607	0.180793	-3.391054	H	-4.793591	-2.052742	-0.837043	H	-2.892121	-1.067010	2.593282
H	0.973971	-1.228379	-2.855902	H	-3.085393	-2.518626	-0.834280	H	-3.716769	-0.494699	1.133265
H	-0.803367	-1.259380	-2.834414	H	-3.813172	-1.797536	0.612386	H	-4.179051	-2.038459	1.863852

T1 32			T4 32			T6 32					
N	0.048497	-0.037607	-1.405799	N	0.323291	-1.389315	-0.221707	C	0.079843	-1.434837	-0.093787
C	0.044255	-1.180544	-0.498018	C	0.921932	-0.786058	0.958754	N	0.817048	-0.748494	0.952124
C	0.767471	-0.914668	0.845582	C	0.397405	0.652401	1.140666	C	0.605020	0.702124	1.053822
C	0.744625	0.582981	1.201736	C	-1.011297	0.805098	0.541338	C	-0.745328	1.162637	0.500764
C	-0.532081	1.264275	0.700867	C	-1.786095	-0.504515	0.700360	C	-0.923900	0.730411	-0.969381
C	-0.733267	1.069774	-0.838508	C	-1.102840	-1.649474	-0.077009	C	-0.073511	-0.510276	-1.298456
H	-1.784614	0.799034	-0.989364	Sn	-1.751798	-3.625801	0.814441	Sn	-1.897774	-2.446226	0.410593
C	1.351247	0.244334	-1.980071	C	-1.513598	-5.293885	-0.567778	H	-1.541511	0.740753	1.115154
H	-1.002390	-1.430730	-0.304908	C	-0.780984	-4.147916	2.695421	H	0.693793	0.993335	2.101474
H	-1.387760	0.835635	1.233240	C	-3.886323	-3.444562	1.217648	H	1.406635	1.226857	0.520346
H	1.800719	-1.264848	0.802251	H	0.723148	-1.386174	1.863819	H	-0.825810	2.247085	0.597691
H	0.837302	0.714935	2.281345	H	-1.849397	-0.730933	1.769194	H	-1.978873	0.520189	-1.160582
H	1.611915	1.081269	0.763672	H	1.078230	1.359156	0.663499	H	-0.648577	1.545291	-1.641630
H	-0.514469	2.320451	0.980867	H	-1.543506	1.625650	1.026510	H	-0.499462	-1.053207	-2.142622
Sn	-0.624967	2.971808	-1.947468	H	-0.938676	1.054791	-0.518410	H	0.928303	-0.193248	-1.608264
H	0.280613	-1.495863	1.633128	H	-2.815062	-0.400081	0.353624	C	0.906258	-1.459350	2.202895
H	0.482199	-2.041957	-1.006844	H	-1.522987	-1.694196	-1.086154	H	0.659364	-2.316627	-0.385156
H	1.753869	-0.677030	-2.406016	C	1.076228	-2.475866	-0.796340	H	1.275123	-2.472444	2.029342
H	1.254765	0.955934	-2.801189	H	0.383838	0.896926	2.205579	H	1.609564	-0.962432	2.871397
H	2.104041	0.642008	-1.283274	H	2.004450	-0.779476	0.829561	H	-0.061050	-1.546973	2.731810
C	-0.942385	2.689804	-4.077418	H	-2.071344	-6.155729	-0.202260	C	-2.889111	-2.903684	-1.478797
C	-2.255677	4.175750	-1.164204	H	-1.892935	-5.028709	-1.554047	C	-1.499218	-4.360759	1.374160
C	1.237249	4.039928	-1.604276	H	-0.464118	-5.568794	-0.659807	C	-3.340255	-1.376117	1.650229
H	1.177160	5.030630	-2.053410	H	-4.266675	-4.391007	1.601139	H	-3.758167	-3.534194	-1.292172
H	1.419100	4.153737	-0.536390	H	-4.074760	-2.668763	1.958371	H	-3.221513	-1.991499	-1.972770
H	2.074686	3.503693	-2.047105	H	-4.430372	-3.196665	0.306827	H	-2.213429	-3.436055	-2.147466
H	-1.052046	3.658290	-4.564047	H	-1.265891	-5.024955	3.123734	H	-2.411444	-4.956212	1.403687
H	-0.104298	2.163019	-4.530017	H	0.271890	-4.373113	2.533133	H	-0.742338	-4.915015	0.819797
H	-1.848647	2.109312	-4.243292	H	-0.857181	-3.326089	3.405966	H	-1.145422	-4.212199	2.393274
H	-2.248633	5.159542	-1.632035	H	0.620144	-2.788554	-1.737354	H	-2.892121	-1.067010	2.593282
H	-3.211949	3.698076	-1.373623	H	2.096897	-2.153736	-1.006071	H	-3.716769	-0.494699	1.133265
H	-2.157982	4.303397	-0.087009	H	1.129788	-3.364974	-0.141699	H	-4.179051	-2.038459	1.863852

T7			T9			T11					
32			32			32					
C	-0.011429	-1.173078	-0.239878	C	-0.390961	-0.332685	-1.442323	C	-0.106663	-0.403801	-1.520783
N	0.329036	-0.337829	0.924923	N	0.255474	-1.293834	-0.551075	N	0.170413	-1.333836	-0.425123
C	0.869527	0.968190	0.556328	C	1.077206	-0.612147	0.468988	C	1.003667	-0.711061	0.614359
C	-0.206103	1.823903	-0.129091	C	0.583475	0.805933	0.827835	C	0.622119	0.756075	0.868696
C	-1.144912	0.956324	-0.990542	C	-0.938856	0.904601	0.718610	C	-0.834313	1.001497	0.491730
C	-0.415562	-0.305195	-1.446291	C	-1.410771	0.577679	-0.719021	C	-1.045027	0.714017	-1.007584
Sn	-1.610519	-2.615116	0.316596	C	-0.606963	-2.336412	-0.025455	C	0.725281	-2.615966	-0.799304
H	-0.785403	2.358833	0.624898	H	0.412446	0.305272	-1.823188	H	0.834161	0.055102	-1.876919
C	1.167032	-1.038961	1.873605	H	-1.392601	0.205066	1.425249	H	-1.474495	0.345170	1.083947
H	1.213185	1.462140	1.466327	H	2.113250	-0.556408	0.117581	H	2.072070	-0.768322	0.341087
H	1.756320	0.867816	-0.093899	H	0.920293	1.065198	1.833523	H	0.808964	1.005577	1.914386
H	0.285294	2.579990	-0.746048	H	1.038574	1.539146	0.156628	H	1.261090	1.415591	0.276259
H	-2.025014	0.674743	-0.407589	H	-1.281214	1.898100	1.013647	H	-1.129531	2.026408	0.725148
H	-1.508363	1.522593	-1.849570	H	-2.401666	0.119584	-0.676482	H	-2.095194	0.453708	-1.164225
H	-1.025109	-0.879346	-2.145201	H	-1.526828	1.498913	-1.297076	H	-0.860685	1.618847	-1.592160
H	0.478254	-0.008794	-2.005515	Sn	-1.158055	-1.227696	-3.307823	Sn	-0.999326	-1.285575	-3.340420
H	0.857009	-1.786889	-0.531619	H	1.085894	-1.233606	1.366205	H	0.880519	-1.298386	1.528845
H	0.676077	-1.953885	2.211037	H	-1.052855	-2.898298	-0.848397	H	0.038910	-3.162504	-1.446679
H	2.146437	-1.328397	1.452395	H	-0.013391	-3.040280	0.559096	H	1.698731	-2.537947	-1.315202
H	1.345009	-0.414117	2.749375	H	-1.430797	-1.983433	0.615360	H	0.878262	-3.220251	0.097033
C	-2.819100	-1.833510	1.940336	C	-1.218691	0.347051	-4.806539	C	-1.665067	0.386640	-4.557812
C	-2.891848	-2.993070	-1.402471	C	0.170860	-2.801637	-3.987312	C	0.422047	-2.429312	-4.522532
C	-0.747798	-4.523929	0.911154	C	-3.176703	-2.007993	-3.085007	C	-2.715943	-2.514535	-2.830441
H	-1.535779	-5.269386	1.013383	H	-1.588317	-0.050430	-5.751123	H	-2.105896	0.015647	-5.482326
H	-0.038768	-4.868399	0.159141	H	-1.879556	1.151696	-4.486810	H	-2.410998	0.976259	-4.027558
H	-0.228186	-4.434415	1.864072	H	-0.222185	0.756348	-4.967975	H	-0.823329	1.030883	-4.808763
H	-3.645883	-3.732364	-1.134138	H	-0.187009	-3.207190	-4.932835	H	-0.014109	-2.657172	-5.494533
H	-3.396811	-2.080516	-1.716092	H	1.174108	-2.403875	-4.131287	H	1.332241	-1.851270	-4.676914
H	-2.312107	-3.378652	-2.240288	H	0.217710	-3.603472	-3.252915	H	0.680943	-3.362958	-4.026665
H	-3.431408	-2.627401	2.365976	H	-3.516238	-2.410566	-4.038781	H	-3.195685	-2.873658	-3.740062
H	-2.178346	-1.420350	2.716761	H	-3.209126	-2.801478	-2.340319	H	-2.410281	-3.370558	-2.231525
H	-3.472303	-1.043745	1.572482	H	-3.859191	-1.215444	-2.781026	H	-3.437748	-1.931677	-2.260592
T8			T10								
32			32								
C	0.208828	-0.252256	-1.601483	N	0.273730	-1.214503	-0.428709				
C	0.547856	-1.382561	-0.601979	C	0.946966	-0.909884	0.825365				
N	1.127838	-0.891910	0.646599	C	0.445766	0.416475	1.430397				
C	0.164803	-0.059445	1.394942	C	-0.892567	0.818696	0.813758				
C	-0.870583	0.658557	0.502724	C	-0.746808	1.004323	-0.704332				
C	-0.272452	1.017656	-0.858398	C	0.166021	-0.086378	-1.330761				
H	-0.391100	-1.869427	-0.320687	H	-1.634204	0.045822	1.020408				
C	2.455605	-0.315533	0.535505	H	2.044037	-0.867659	0.686350				
H	-1.741597	0.015190	0.352199	H	0.362067	0.319091	2.513708				
H	-0.359233	-0.684939	2.125776	H	1.173986	1.209158	1.248735				
H	0.729615	0.679570	1.966021	H	-1.259182	1.741574	1.267237				
H	-1.237094	1.550153	1.015375	H	-1.734616	0.966419	-1.169795				
H	-0.999199	1.560119	-1.465754	H	-0.357377	2.005117	-0.905928				
H	0.567992	1.700235	-0.709137	H	-0.301137	-0.455815	-2.244412				
H	-0.569581	-0.610120	-2.281299	Sn	2.058708	0.841620	-2.171375				
H	1.066072	0.002201	-2.229309	H	0.753848	-1.739247	1.509987				
Sn	1.653505	-3.068860	-1.497748	C	0.754912	-2.434684	-1.033155				
H	3.145305	-1.050931	0.117500	H	0.155317	-2.679087	-1.911025				
H	2.522101	0.588896	-0.090216	H	1.811094	-2.376075	-1.347069				
H	2.824689	-0.056721	1.528607	H	0.666120	-3.257160	-0.321559				
C	3.372549	-2.424264	-2.665098	C	3.524235	-0.550685	-2.990816				
C	2.289599	-4.441185	0.056582	C	1.366772	2.076275	-3.829965				
C	0.284678	-4.094824	-2.840804	C	3.110805	2.162290	-0.791318				
H	2.819647	-5.284802	-0.383685	H	4.257330	-0.001846	-3.581995				
H	2.948103	-3.936123	0.760644	H	4.042012	-1.075816	-2.189779				
H	1.422373	-4.814437	0.599078	H	3.036041	-1.283319	-3.631703				
H	0.772306	-4.966426	-3.275976	H	2.213383	2.585697	-4.289558				
H	-0.601284	-4.426151	-2.300441	H	0.881165	1.460216	-4.586187				
H	-0.025728	-3.432207	-3.647683	H	0.656650	2.826721	-3.484663				
H	3.766269	-3.270372	-3.227285	H	3.909967	2.674401	-1.326875				
H	3.086094	-1.643768	-3.368740	H	2.436334	2.911085	-0.378169				
H	4.158638	-2.039546	-2.017462	H	3.548011	1.593144	0.027627				

Table S4. Contributions, in Hz, to the $^3J(\text{Sn-C-O-C})$ coupling in $\text{Me}_3\text{Sn-CH}_2\text{-O-CH}_3$. Scalar ZORA BLYP/TZ2P.

$\phi / ^\circ$	DSO	PSO	SD	FC	TOT
0	-0.04	-0.43	0.315	-89.925	-90.09
15	-0.04	-0.47	0.325	-84.395	-84.59
30	-0.04	-0.42	0.325	-68.225	-68.35
45	-0.03	-0.24	0.285	-45.005	-44.99
60	-0.02	-0.09	0.196	-20.306	-20.22
75	-0.01	0	0.106	1.344	1.45
90	0.01	0.01	0.082	12.508	12.62
105	0.03	-0.02	0.141	8.239	8.39
120	0.04	-0.11	0.215	-11.825	-11.68
135	0.06	-0.26	0.141	-39.931	-39.99
150	0.07	-0.45	-0.13	-64.9	-65.41
165	0.07	-0.57	-0.412	-79.858	-80.77
180	0.07	-0.62	-0.527	-84.953	-86.02

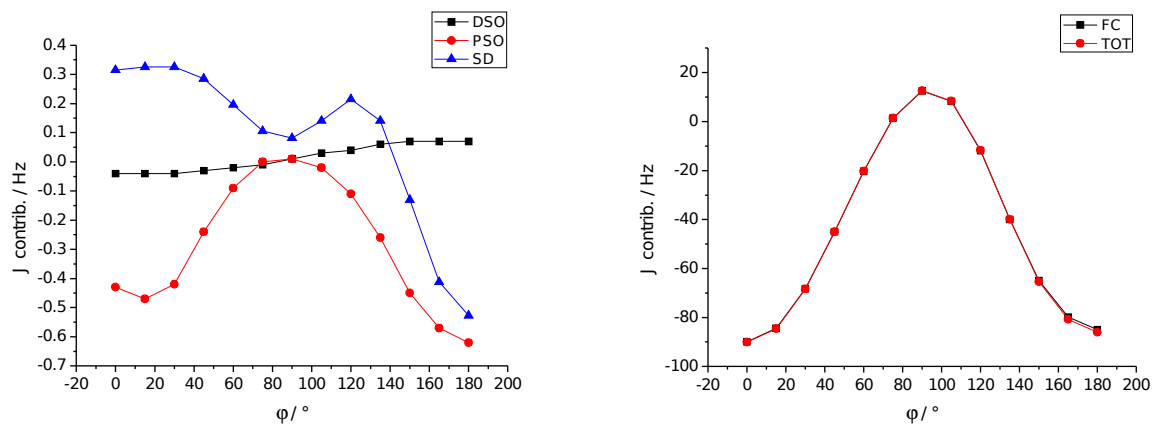


Figure S1. Graphical representation of the various contribution of Table S.