

Supplementary Material

Extending NMR quantum computation systems by employing compounds with several heavy metals as qubits

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Table S1: Coordinates of calculated geometries for the studied complexes.

Complex 1				Complex 2				Complex 3				Complex 4			
Hg	-0.731604	1.473029	1.107749	Hg	-0.480384	1.282650	0.778948	Cd	-0.604672	1.202860	0.749525	Cd	-0.491199	1.019556	1.148343
Te	1.594544	2.715626	0.152548	Se	1.829430	1.979525	-0.366544	Te	1.829632	2.295218	-0.358331	Se	1.490394	2.643129	0.190500
Te	-3.109501	1.901512	2.369876	Se	-2.551830	2.346838	1.866491	Te	-2.849904	2.466373	1.881376	Se	-2.982897	2.002018	1.157723
P	-3.191378	-0.479735	2.808217	P	-3.062306	0.474964	2.854749	P	-3.271545	0.364652	2.982946	P	-3.625876	0.380991	2.428089
Si	3.544174	1.091190	2.409617	Si	3.640481	0.747870	1.996486	Si	3.801233	0.752547	1.926946	Si	3.730322	0.700936	1.540854
F	-0.913622	0.252289	-0.695063	F	-0.859093	-0.216964	-0.738980	F	-1.021240	0.001542	-0.910776	F	-0.095816	-0.325802	-0.399933
F	0.288971	-0.090711	2.339916	F	0.362933	-0.055697	2.342673	F	0.155903	-0.029351	2.307520	F	-0.246224	0.339617	3.115564
N	-3.172760	-1.525030	1.548766	N	-3.297543	-0.861230	1.945702	N	-3.431396	-0.993944	2.076837	N	-3.315720	-1.150350	1.937617
C	2.748493	0.989033	0.692074	C	2.770640	0.421301	0.334466	C	2.868944	0.527478	0.293489	C	2.776940	1.191268	-0.032142
C	3.799979	-0.670722	2.978621	C	5.379509	1.340826	1.606905	C	5.419627	1.625263	1.554369	C	5.391985	0.067529	0.942007
C	2.441637	2.001451	3.613256	C	3.670491	-0.882827	2.905665	C	4.125316	-0.966356	2.594825	C	2.816308	-0.640868	2.455902
C	5.184665	1.988264	2.233298	C	2.742112	2.042991	3.000320	C	2.777726	1.734014	3.140888	C	3.979153	2.204406	2.632096
C	1.192975	2.120018	-1.868760	C	1.365597	1.290663	-2.130161	C	1.284812	1.562096	-2.302758	C	0.738432	2.567579	-1.609037
C	-1.952489	-1.015560	3.977140	C	-1.937165	0.041208	4.169075	C	-2.103999	-0.004520	4.287798	C	-3.069931	0.514728	4.122052
C	-4.117967	-1.346634	0.432873	C	-4.208030	-0.820018	0.787892	C	-4.312809	-0.988038	0.896550	C	-3.602743	-1.570633	0.557878
C	-3.322262	-1.770914	-0.792640	C	-3.553960	-1.751783	-0.221222	C	-3.543073	-1.796015	-0.136448	C	-2.447737	-2.499188	0.219825
C	-2.371979	-2.821999	-0.235890	C	-2.864471	-2.781355	0.663368	C	-2.799204	-2.812704	0.718575	C	-2.156567	-3.169372	1.556442
C	-1.946679	-2.228896	1.097641	C	-2.291690	-1.941288	1.794688	C	-2.356262	-2.005643	1.931401	C	-2.321369	-2.045297	2.574132
H	3.504252	0.883893	-0.089443	H	3.503377	0.149437	-0.429267	H	3.562851	0.280612	-0.513160	H	3.478016	1.537956	-0.795320
H	2.047298	0.154447	0.658230	H	2.035125	-0.375885	0.442289	H	2.119711	-0.258876	0.385278	H	2.202650	0.345474	-0.421185
H	4.425830	-1.235959	2.283158	H	5.362800	2.261951	1.017475	H	5.253322	2.607254	1.103017	H	5.957024	0.847460	0.424705
H	2.825128	-1.160631	3.045326	H	5.940931	0.591220	1.042464	H	6.037934	1.040135	0.868147	H	5.268619	-0.772551	0.253244
H	4.275271	-0.704747	3.962773	H	5.934533	1.547789	2.526055	H	5.996273	1.777629	2.470950	H	5.997052	-0.280881	1.783569
H	1.474831	1.492866	3.654748	H	4.174110	-1.662130	2.327636	H	4.688971	-1.575484	1.883381	H	2.638046	-1.498963	1.801936
H	2.886901	1.995711	4.612295	H	4.184393	-0.792055	3.866460	H	4.697257	-0.925256	3.525887	H	3.415285	-0.984969	3.304607
H	2.284149	3.047827	3.334854	H	2.638016	-1.192803	3.086772	H	3.176054	-1.467576	2.799027	H	1.848008	-0.303652	2.841655
H	5.686617	2.072376	3.201114	H	3.262855	2.205638	3.948494	H	3.262534	1.750585	4.121294	H	4.606066	1.945025	3.489803
H	5.045732	3.001524	1.845589	H	1.730494	1.689054	3.211970	H	1.796028	1.260266	3.239753	H	3.028370	2.574528	3.025125
H	5.859329	1.459423	1.554537	H	2.686915	3.008031	2.488817	H	2.640863	2.773715	2.829094	H	4.467461	3.022530	2.096391
H	2.145736	1.903625	-2.347565	H	2.289003	0.998455	-2.627178	H	2.190774	1.237399	-2.809970	H	1.511115	2.858001	-2.318553
H	0.704713	2.959214	-2.361477	H	0.892702	2.109482	-2.671252	H	0.834633	2.394900	-2.841130	H	-0.089246	3.274680	-1.650085
H	0.529763	1.254905	-1.808581	H	0.667699	0.463342	-1.993702	H	0.561605	0.758858	-2.155208	H	0.390729	1.549135	-1.779976
H	-0.969615	-0.814255	3.512072	H	-0.951023	-0.124217	3.700234	H	-1.118753	-0.121094	3.811656	H	-1.972937	0.457142	4.107535
H	-2.059423	-0.413902	4.880170	H	-1.880079	0.885819	4.856154	H	-2.084034	0.846677	4.968632	H	-3.384252	1.488484	4.498429
H	-2.089772	-2.074334	4.204434	H	-2.295219	-0.849421	4.688525	H	-2.406511	-0.909980	4.817031	H	-3.505553	-0.282450	4.727140
H	-4.455813	-0.647418	3.406799	H	-4.313615	0.768016	3.430195	H	-4.526377	0.554401	3.594822	H	-5.028813	0.509599	2.454208
H	-4.995932	-1.982893	0.594638	H	-5.200332	-1.173991	1.091301	H	-5.271418	-1.455144	1.151429	H	-4.568147	-2.089911	0.521376
H	-4.453329	-0.306475	0.371787	H	-4.306277	0.201226	0.409397	H	-4.506155	0.037662	0.568173	H	-3.652116	-0.702469	-0.104219
H	-3.967565	-2.145113	-1.588928	H	-4.282199	-2.187194	-0.907197	H	-4.203972	-2.254026	-0.874233	H	-2.710000	-3.208895	-0.566356
H	-2.732857	-0.925891	-1.157481	H	-2.794029	-1.203554	-0.784684	H	-2.820909	-1.153713	-0.650627	H	-1.586327	-1.909007	-0.110715
H	-1.509451	-2.989773	-0.880987	H	-2.077005	-3.324409	0.140520	H	-1.944769	-3.250776	0.202178	H	-1.157407	-3.603258	1.605326
H	-2.886979	-3.776381	-0.086058	H	-3.585400	-3.506848	1.053673	H	-3.465517	-3.624561	1.026704	H	-2.881866	-3.964932	1.752452
H	-1.117098	-1.532065	0.963536	H	-1.313350	-1.534498	1.530227	H	-1.384091	-1.531928	1.772617	H	-1.382086	-1.515284	2.753594
H	-1.664314	-2.988087	1.829620	H	-2.200545	-2.500024	2.728496	H	-2.296793	-2.617052	2.834931	H	-2.698545	-2.412941	3.531804

Table S2: Vibrational frequencies for the studied complexes, cm^{-1} .

	Complex 1	Complex 2	Complex 3	Complex 4						
0	0	0	0	0	66	908.22	939.26	905.82	940.93	
1	0	0	0	0	67	938.59	942.68	939.80	942.84	
2	0	0	0	0	68	943.05	962.91	942.49	946.81	
3	0	0	0	0	69	964.52	974.81	965.50	976.26	
4	0	0	0	0	70	991.21	992.66	992.58	993.80	
5	0	0	0	0	71	1012.80	1014.78	1014.93	1019.96	
6	2.17	6.59	5.76	9.85	72	1036.33	1051.71	1027.04	1051.80	
7	14.18	20.34	11.69	16.13	73	1050.79	1074.46	1051.05	1083.88	
8	25.64	25.59	21.75	24.38	74	1105.04	1122.69	1090.55	1120.81	
9	30.29	33.42	27.06	28.90	75	1119.81	1140.77	1116.45	1148.74	
10	38.17	42.31	36.30	36.41	76	1146.04	1148.30	1146.86	1150.93	
11	47.29	51.60	48.70	54.74	77	1154.91	1156.80	1153.07	1157.83	
12	52.21	55.83	61.60	65.80	78	1205.31	1205.68	1204.13	1203.99	
13	66.42	67.89	62.61	69.77	79	1225.17	1228.08	1227.81	1232.89	
14	72.63	74.10	71.98	79.72	80	1263.04	1263.01	1268.41	1272.06	
15	81.02	85.77	76.85	86.06	81	1265.14	1266.93	1269.77	1278.46	
16	88.39	91.71	89.13	89.78	82	1267.71	1276.54	1273.04	1278.68	
17	100.75	112.52	92.04	102.24	83	1277.10	1280.81	1279.77	1286.56	
18	108.11	113.56	113.23	109.63	84	1279.40	1286.44	1280.80	1298.99	
19	112.99	124.16	116.66	126.24	85	1287.77	1309.09	1285.67	1304.44	
20	124.60	132.57	127.80	135.72	86	1325.90	1326.46	1325.07	1322.44	
21	133.27	152.60	136.47	145.02	87	1333.65	1331.89	1328.71	1328.16	
22	143.34	161.51	144.50	150.93	88	1366.79	1367.01	1366.51	1365.24	
23	147.85	163.42	147.28	156.16	89	1377.10	1381.65	1383.75	1384.48	
24	160.89	168.10	156.51	159.62	90	1386.34	1394.86	1395.36	1397.31	
25	162.49	171.57	159.95	166.56	91	1394.14	1405.95	1396.90	1419.76	
26	163.72	183.14	164.18	169.49	92	1431.92	1432.51	1433.31	1433.62	
27	181.47	184.28	170.69	174.54	93	1439.55	1439.03	1441.06	1440.20	
28	182.71	194.32	174.76	182.68	94	1439.83	1444.52	1443.08	1444.51	
29	189.01	196.83	179.28	191.47	95	1447.79	1448.38	1446.53	1448.78	
30	194.55	204.26	189.18	206.84	96	1450.78	1451.17	1450.81	1452.73	
31	196.12	204.75	197.16	211.91	97	1453.32	1452.93	1454.80	1455.81	
32	210.42	208.80	210.71	219.63	98	1459.93	1461.39	1458.39	1458.71	
33	218.23	222.88	215.15	222.87	99	1470.58	1470.68	1471.37	1470.12	
34	222.45	227.20	220.78	234.21	100	1472.69	1472.83	1472.47	1473.21	
35	231.30	237.77	231.32	245.57	101	1475.42	1477.68	1473.06	1479.28	
36	257.21	258.69	246.60	247.64	102	1477.67	1480.02	1484.00	1486.36	
37	264.59	274.08	264.11	272.77	103	1486.06	1488.84	1497.58	1501.81	
38	277.22	290.25	281.46	281.62	104	1503.55	1507.68	1510.06	1513.85	
39	295.95	298.89	286.14	299.86	105	1515.92	1521.57	1533.76	1540.26	
40	308.29	322.40	345.55	353.22	106	2442.92	2449.48	2441.85	2439.57	
41	347.54	355.71	365.59	407.71	107	2896.57	2918.71	2973.08	2995.05	
42	354.80	372.60	386.63	416.76	108	3024.27	3025.32	3023.80	3021.00	
43	364.81	405.58	421.64	426.70	109	3034.46	3038.97	3029.17	3025.20	
44	489.09	504.10	491.63	508.32	110	3040.70	3040.83	3041.74	3042.57	
45	526.09	563.53	526.80	559.18	111	3042.47	3042.01	3044.28	3043.43	
46	536.69	572.41	536.48	581.02	112	3043.14	3048.56	3048.91	3047.46	
47	570.92	599.18	577.57	600.79	113	3051.28	3051.43	3051.94	3051.19	
48	612.48	623.52	612.29	625.83	114	3067.44	3066.26	3056.16	3053.96	
49	641.21	660.04	641.02	675.40	115	3070.49	3067.50	3058.07	3058.25	
50	680.79	681.77	682.66	682.83	116	3075.98	3073.80	3078.86	3061.45	
51	698.72	698.67	698.66	699.26	117	3076.12	3086.05	3078.88	3093.66	
52	700.89	702.87	703.73	709.57	118	3106.49	3110.03	3105.30	3099.72	
53	714.00	724.22	711.94	731.41	119	3114.48	3118.08	3114.94	3107.62	
54	738.60	743.54	737.47	743.29	120	3121.23	3119.01	3115.68	3120.85	
55	752.19	757.33	754.99	763.06	121	3123.39	3122.24	3121.63	3121.41	
56	769.77	773.00	770.00	766.12	122	3124.18	3123.14	3122.96	3123.38	
57	787.18	793.68	788.65	803.96	123	3125.68	3125.58	3123.97	3123.90	
58	800.28	811.84	798.52	810.09	124	3131.43	3130.20	3124.69	3125.06	
59	857.13	862.42	855.83	865.16	125	3131.80	3135.54	3125.73	3125.77	
60	862.13	868.36	861.53	868.18	126	3134.73	3137.54	3133.40	3126.74	
61	868.18	871.85	870.59	871.16	127	3139.36	3138.22	3134.71	3128.34	
62	870.24	873.26	871.82	872.06	128	3157.45	3154.33	3157.05	3131.46	
63	879.02	880.24	877.58	880.37	129	3163.92	3165.24	3164.99	3164.26	
64	879.85	898.28	879.10	898.93	130	3166.27	3165.31	3169.39	3173.85	
65	897.51	937.68	898.72	934.86	131	3185.44	3177.28	3185.06	3176.84	

Table S3: For Complex 1: on the diagonal are the Larmor frequencies for the nuclei, on the lower triangle of the matrix are the coupling constants between the two nuclei, on the upper triangle are the differences in Larmor frequencies between the two coupled nuclei.

	Hg1	Te2	Te3	P4	Si5	F6	F7	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	H19	H20	H21	H22	H23
Hg1	-191843	96802165	96686569	158654340	13737898	535132459	535167977	50763004	50762543	50762732	50762608	50761553	50766341	50772179	50767781	50768191	50771828	576615020	576617014	576614025	576614714	576613958
Te2	3302.70	10295	115597	61852174	83064267	438330293	438365811	46039162	46039622	46039433	46039558	46040612	46035825	46029987	46034385	46033974	46030337	479812855	479814849	479811860	479812548	479811792
Te3	5102.88	19.03	125887	61967771	82948671	438445890	438481408	45923565	45924025	45923836	45923961	45925015	45920228	45914390	45918788	45918378	45914741	479928451	479930446	479927456	479928145	479927389
P4	-166.30	1.75	1411.66	-5296	144916442	376478119	376513637	107891336	107891796	107891607	107891732	107892786	107887999	107882161	107886559	107886149	107882512	417960680	417962675	417959685	417960374	417959618
Si5	0.13	38.67			-614	521394561	521430079	37025106	37024645	37024835	37024710	37023655	37028443	37034281	37029883	37030293	37033930	562877122	562879117	562876127	562876816	562876060
F6	-2621.28	49.16	83.24		0.15	-133242	35518	484369455	484369915	484369726	484369851	484370905	484366118	484360280	484364678	484364268	484360631	41482561	41484556	41481566	41482255	41481499
F7	-2405.23	34.35	100.36		0.01	1.87	-97846	484404973	484405433	484405244	484405369	484406423	484401636	484395798	484400196	484399786	484396149	41447043	41449038	41446048	41446737	41445981
C9	-15.82	195.08			-34.38	-0.11	5.16	280	460	271	396	1450	3337	9175	4777	5187	8824	525852016	525854011	525851021	525851710	525850954
C10		-7.57			-41.49	-0.03	1.01	4.90	-179	189	64	990	3797	9635	5237	5648	9285	525852477	525854471	525851482	525852170	525851414
C11		-23.39			-41.75	-0.16	5.66	2.68	3.52	10	125	1179	3608	9446	5048	5458	9096	525852287	525854282	525851293	525851981	525851225
C12		1.73			-37.53	-0.05	0.42	2.68	3.38	3.37	-114	1054	3733	9571	5173	5583	9220	525852412	525854407	525851417	525852106	525851350
C13	-24.25	164.32			-2.40	15.39	-0.14	3.90	0.10	-0.08	-0.03	-1165	4787	10625	6227	6638	10275	525853467	525855461	525852472	525853160	525852404
C14	-3.78		33.80	20.86		0.08	31.41	-0.20	0.01	0.01	0.00	0.0	3606	5838	1440	1850	5487	525848679	525850674	525847684	525848373	525847617
C15			0.11	5.81		-0.69	-0.08	0.09	0.00	-0.01	-0.01	0.0	0.28	9424	4398	3988	351	525842841	525844836	525841847	525842535	525841779
C16			-0.96	5.32		11.88	-0.03	-0.01	0.00	-0.01	-0.01	0.0	0.23	26.44	5041	410	4047	525847239	525849234	525846244	525846933	525846177
C17			0.95			-1.08	0.45	0.00	0.00	-0.01	-0.01	0.0	-0.03	0.02	23.53	5450	3637	525846829	525848823	525845834	525846523	525845767
C18			-3.18	2.84		3.57	3.47	0.01	0.01	0.01	-0.01	0.02	0.48	3.66	0.08	26.76	9075	525843192	525845186	525842197	525842886	525842130
H19		-15.77			3.22	1.24	2.18	123.68	-0.25	3.23	1.37	2.34	0.03	-0.03	-0.01	0.01	0.01	969	1994	995	306	1062
H20		0.95			4.60	1.83	2.38	135.65	1.65	-0.27	4.10	1.00	0.06	-0.01	0.02	0.04	0.09	-7.71	2956	2989.26	2301	3057
H21					4.56			0.19	112.77	5.29	0.08	-0.06	0.03	-0.01	0.00	0.01	0.02	0.31	0.36	-23	688	67
H22					6.74			0.23	117.10	0.20	5.37	-0.07	0.08	-0.01	0.00	0.02	0.04	0.30	0.58	-11.59	663	756
H23					3.68			8.07	112.22	0.10	-0.08	0.15	0.04	-0.02	-0.01	0.00	0.01	-0.22	0.62	-11.82	-11.50	-90
H24					6.92			0.35	0.13	119.40	5.80	-0.21	0.12	-0.05	-0.05	-0.02	0.01	-0.17	0.49	-0.15	0.43	0.20
H25					4.27			5.76	0.27	111.88	-0.09	-0.19	0.04	-0.04	-0.03	-0.02	-0.01	1.39	-0.17	-0.15	0.09	0.20
H26					3.74			0.13	5.32	110.67	0.19	0.05	0.03	-0.07	-0.06	-0.04	-0.04	-0.30	0.23	2.41	-0.12	-0.15
H27					3.93			6.77	-0.09	0.12	112.02	-0.02	0.00	-0.03	-0.03	-0.02	-0.02	0.35	1.87	0.04	-0.27	0.13
H28					4.59			0.25	5.20	0.07	111.68	-0.12	-0.02	-0.04	-0.04	-0.03	-0.03	0.25	-0.04	-0.29	2.14	-0.31
H29					4.64			0.22	0.22	5.04	112.20	-0.04	-0.01	-0.03	-0.02	-0.02	-0.02	0.39	-0.01	0.12	-0.18	0.04
H30		-16.98			0.32	0.53	1.15	1.44	0.02	-0.05	-0.02	132.24	-0.07	-0.02	0.01	0.00	-0.01	0.47	0.10	0.01	-0.08	-0.09
H31		-90.20			-0.86	-0.25	-0.72	3.43	0.36	-0.19	-0.06	129.49	-0.09	-0.01	0.01	0.00	-0.03	-0.46	-0.79	-0.18	-0.27	0.09
H32		0.87			0.38	-6.33	0.81	0.60	-0.04	-0.15	-0.04	151.11	-0.08	0.02	0.06	0.04	0.03	0.10	0.71	0.00	-0.04	-0.14
H33			3.54	-18.88		-0.11	-27.47	0.03	0.07	0.10	-0.02	-0.10	134.29	-0.22	-0.01	0.11	0.23	0.00	0.42	0.17	0.37	0.20
H34			-1.42	0.11		-0.38	-0.97	-0.01	0.03	0.06	-0.02	-0.10	123.44	0.82	0.20	-0.03	0.51	-0.10	0.05	0.06	0.18	0.11
H35			20.35	-10.83		-0.14	-0.53	0.01	0.03	0.03	-0.02	-0.06	121.84	-0.18	0.07	0.05	0.22	-0.05	0.12	0.07	0.18	0.09
H36			-55.07	422.22		-0.61	1.30	-0.12	-0.04	-0.05	-0.06	-0.15	3.07	-0.30	0.05	0.39	3.19	-0.16	-0.19	-0.13	-0.13	-0.11
H37			2.33	9.24		0.91	0.08	-0.03	-0.01	-0.03	-0.03	-0.01	-0.19	129.93	-1.83	0.08	0.28	-0.10	-0.04	-0.04	-0.02	-0.05
H38			3.28	22.07		0.89	-0.27	-0.06	-0.03	-0.07	-0.05	-0.01	-0.27	128.27	-1.82	6.66	3.27	-0.19	-0.16	-0.10	-0.10	-0.11
H39			-0.25	0.40		2.50	0.08	-0.01	-0.01	-0.04	-0.03	0.04	0.68	2.22	121.40	-1.23	7.90	-0.03	0.05	-0.02	-0.01	-0.04
H40			0.19	-0.36		-0.60	0.02	-0.01	-0.01	-0.06	-0.04	0.09	-0.06	-3.96	129.67	-3.68	0.73	-0.04	0.11	-0.03	-0.02	-0.07
H41			1.27	2.08		0.55	0.44	0.04	0.01	-0.02	-0.02	0.04	0.03	8.36	-1.41	126.03	2.38	0.09	0.27	0.05	0.09	0.01
H42			0.04	-0.39		1.63	1.55	0.02	0.01	-0.02	-0.02	0.02	0.00	0.63	-2.72	116.70	-3.51	0.01	0.13	0.02	0.06	0.00
H43			-1.80	15.60		3.11	3.31	0.09	0.05	0.00	-0.03	0.02	0.11	-0.05	0.14	-2.86	141.85	0.11	0.55	0.14	0.28	0.10
H44			-2.28	0.34		3.06	-0.06	0.04	0.03	0.00	-0.02	0.00	0.32	4.25	6.03	-1.31	129.44	0.04	0.26	0.08	0.17	0.07

cont. Table S3: For Complex 1: on the diagonal are the Larmor frequencies for the nuclei, on the lower triangle of the matrix are the coupling constants between the two nuclei, on the upper triangle are the differences in Larmor frequencies between the two coupled nuclei.

	H24	H25	H26	H27	H28	H29	H30	H31	H32	H33	H34	H35	H36	H37	H38	H39	H40	H41	H42	H43	H44
Hg1	576615251	576613952	576613913	576614025	576614232	576614036	576615020	576615058	576618312	576619399	576615211	576615893	576619497	576615769	576616412	576615063	576616692	576615532	576615186	576617212	576615975
Te2	479813086	479811787	479811748	479811860	479812066	479811871	479812855	479812893	479816147	479817233	479813046	479813728	479817332	479813604	479814246	479812898	479814527	479813367	479813021	479815047	479813810
Te3	479928682	479927383	479927345	479927456	479927663	479927468	479928451	479928489	479931743	479932830	479928642	479929324	479932928	479929201	479929843	479928495	479930123	479928963	479928618	479930644	479929407
P4	417960911	417959612	417959574	417959685	417959892	417959697	417960680	417960718	417963972	417965059	417960871	417961553	417965157	417961430	417962072	417960724	417962352	417961192	417960847	417962873	417961636
Si5	562877353	562876054	562876016	562876127	562876334	562876139	562877122	562877160	562880414	562881501	562877313	562877995	562881599	562877872	562878514	562877166	562878794	562877634	562877289	562879315	562878077
F6	41482792	41481493	41481455	41481566	41481773	41481578	41482561	41482599	41485853	41486940	41482752	41483434	41487038	41483311	41483953	41482605	41484233	41483073	41482728	41484754	41483517
F7	41447274	41445975	41445937	41446048	41446255	41446060	41447043	41447081	41450335	41451422	41447234	41447916	41451520	41447793	41448435	41447087	41448715	41447555	41447210	41449236	41447999
C9	525852247	525850948	525850910	525851021	525851228	525851033	525852016	525852054	525853308	525856395	525852207	525852889	525856493	525852766	525853408	525852060	525853688	525852528	525852183	525854209	525852972
C10	525852708	525851409	525851370	525851482	525851688	525851493	525852477	525852515	525855769	525856856	525852668	525853350	525856954	525853226	525853868	525852520	525854149	525852989	525852643	525854669	525853432
C11	525852519	525851220	525851181	525851293	525851499	525851304	525852287	525852325	525855579	525856666	525852479	525853161	525856765	525853037	525853679	525852331	525853959	525852800	525852454	525854480	525853243
C12	525852643	525851344	525851306	525851417	525851624	525851429	525852412	525852450	525855704	525856791	525852603	525853285	525856889	525853162	525853804	525852456	525854084	525852924	525852579	525854605	525853368
C13	525853698	525852399	525852360	525852472	525852678	525852483	525853467	525853505	525856759	525857846	525853658	525854340	525857944	525854216	525854858	525853510	525855139	525853979	525853633	525855659	525854422
C14	525848910	525847611	525847573	525847684	525847891	525847696	525848679	525848717	525851971	525853058	525848870	525849553	525853156	525849429	525850071	525848723	525850351	525849191	525848846	525850872	525849635
C15	525843072	525841773	525841735	525841847	525842053	525841858	525842841	525842879	525846133	525847220	525843032	525843715	525847319	525843591	525844233	525842885	525844513	525843353	525843008	525845034	525843797
C16	525847470	525846171	525846133	525846244	525846451	525846256	525847239	525847277	525850531	525851618	525847430	525848112	525851716	525847989	525848631	525847283	525848911	525847751	525847406	525849432	525848195
C17	525847060	525845761	525845723	525845834	525846041	525845845	525846829	525846867	525850121	525851208	525847020	525847702	525851306	525847579	525848221	525846873	525848501	525847341	525846995	525849022	525847784
C18	525843423	525842124	525842085	525842197	525842404	525842208	525843192	525843230	525846484	525847571	525843383	525844065	525847669	525843941	525844584	525843235	525844864	525843704	525843358	525845384	525844147
H19	231	1068	1106	995	788	984	0.0000	38	3292	4379	191	873	4477	750	1392	44	1672	512	166	2193	955
H20	1763	3062	3101	2989	2783	2978	1994	1957	1298	2384	1803	1121	2483	1245	603	1951	322	1482	1828	198	1039
H21	1226	73	112	0	207	11	995	1033	4287	5374	1186	1868	5472	1744	2386	1038	2667	1507	1161	3187	1950
H22	537	762	800	688	482	677	306	344	3598	4685	497	1180	4784	1056	1698	350	1978	818	473	2499	1262
H23	1293	6	44	67	274	79	1062	1100	4354	5441	1253	1935	5539	1812	2454	1106	2734	1574	1229	3255	2018
H24	1199	1299	1338	1226	1019	1215	231	193	3061	4148	40	642	4246	518	1161	188	1441	281	65	1961	724
H25	-11.48	-95	39	73	280	84	1068	1106	4360	5447	1259	1941	5545	1817	2460	1111	2740	1580	1234	3260	2023
H26	-10.57	-12.18	-134	112	318	123	1106	1144	4399	5485	1298	1980	5584	1856	2498	1150	2778	1619	1273	3299	2062
H27	-0.08	0.19	0.17	-23	207	11	995	1033	4287	5374	1186	1868	5472	1744	2386	1038	2667	1507	1161	3187	1950
H28	-0.15	0.13	0.33	-12.01	183	195	788	826	4080	5167	979	1661	5265	1538	2180	832	2460	1300	955	2981	1744
H29	2.30	-0.30	-0.15	-11.70	-11.51	-11	984	1021	4276	5362	1175	1857	5461	1733	2375	1027	2656	1496	1150	3176	1939
H30	-0.39	-0.19	-0.51	-0.10	-0.06	0.05	969	38	3292	4379	191	873	4477	750	1392	44	1672	512	166	2193	955
H31	-0.54	-0.40	-0.62	-0.17	-0.28	-0.17	-9.09	1006	3254	4341	153	835	4439	712	1354	6	1634	474	129	2155	918
H32	-0.44	-0.36	-0.62	-0.20	-0.28	-0.11	-6.00	-9.00	4249	1087	3101	2419	1185	2542	1900	3248	1620	2780	3126	1099	2337
H33	0.56	0.24	0.19	0.00	-0.07	-0.03	-0.26	-0.40	-0.29	5332	4188	3506	98	3629	2987	4335	2707	3867	4212	2186	3423
H34	0.37	0.17	0.14	-0.01	-0.06	-0.05	-0.26	-0.33	-0.33	-12.97	1159	682	4286	559	1201	148	1481	321	25	2002	764
H35	0.21	0.08	0.02	-0.03	-0.08	-0.05	-0.17	-0.24	-0.17	-10.58	-10.45	1839	3604	124	518	830	799	361	707	1319	82
H36	-0.22	-0.15	-0.25	-0.16	-0.22	-0.18	-0.18	-0.34	-0.23	12.60	1.39	0.99	5430	3728	3086	4434	2805	3965	4311	2285	3522
H37	-0.15	-0.11	-0.18	-0.10	-0.13	-0.09	-0.06	-0.05	0.04	0.35	-0.12	0.13	0.62	1716	642	706	922	237	583	1443	206
H38	-0.32	-0.21	-0.32	-0.16	-0.21	-0.15	-0.08	-0.02	0.08	-0.10	-0.36	-0.02	1.03	-7.72	2355	1348	280	880	1225	801	436
H39	-0.15	-0.11	-0.18	-0.08	-0.11	-0.07	0.04	0.06	0.18	0.02	0.41	0.08	-0.01	5.85	0.46	1012	1628	469	123	2149	912
H40	-0.28	-0.18	-0.31	-0.14	-0.18	-0.11	0.10	0.15	0.40	0.04	-0.16	0.01	-0.05	11.64	9.26	-10.15	2635	1160	1506	521	717
H41	-0.07	-0.07	-0.16	-0.07	-0.10	-0.04	0.08	0.04	0.25	0.20	-0.03	0.10	0.48	-0.43	0.77	0.58	6.54	1479	346	1680	443
H42	-0.05	-0.06	-0.12	-0.06	-0.09	-0.05	0.01	-0.01	0.12	0.16	-0.01	0.12	0.04	-0.10	-0.29	5.82	12.82	-9.52	1135	2026	789
H43	0.10	-0.03	-0.19	-0.09	-0.16	-0.06	-0.01	-0.12	0.27	0.71	0.20	0.33	-1.06	0.22	-0.15	-0.32	0.33	6.66	11.49	3153	1237
H44	0.08	0.00	-0.08	-0.05	-0.10	-0.04	-0.05	-0.12	0.05	0.84	0.51	0.15	-0.30	-0.46	0.15	0.76	-0.18	0.38	8.00	-7.67	1921

Table S4: For Complex 2: on the diagonal are the Larmor frequencies for the nuclei, on the lower triangle of the matrix are the coupling constants between the two nuclei, on the upper triangle are the differences in Larmor frequencies between the two coupled nuclei.

	Hg1	Se2	se3	P4	Si5	F6	F7	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	H19	H20	H21	H22	H23
Hg1	125907781	8435780	8401607	158651001	13721930	535104716	535154067	50750607	50746891	50746773	50746619	50749701	50750333	50755952	50752074	50752374	50756044	576599309	576600880	576598465	576598245	576598265
Se2	-835.01	134343561	34173	150215220	5286150	526668936	526718287	42314827	42311111	42310993	42310839	42313921	42314553	42320172	42316294	42316594	42320264	568163529	568165100	568162685	568162465	568162484
Se3	-1485.00	5.75	134309388	150249393	5320323	526703109	526752460	42348999	42345284	42345165	42345011	42348093	42348725	42354344	42350467	42350767	42354437	568197702	568199273	568196857	568196637	568196657
P4	-190.65	-0.17	-607.71	284558781	144929070	376453716	376503067	107900394	107904109	107904228	107904382	107901300	107900668	107895049	107898926	107898626	107894956	417948309	417949879	417947464	417947244	417947264
Si5	-0.12	-17.68			139629711	521382786	521432137	37028676	37024961	37024843	37024688	37027770	37028402	37034022	37030144	37030444	37034114	562877379	562878950	562876534	562876314	562876334
F6	-2483.84	-6.41	-21.63		0.15	661012497	49351	484354110	484357825	484357943	484358098	484355016	484354384	484348764	484352642	484352342	484348672	41494593	41496164	41493748	41493528	41493548
F7	-2330.77	-6.49	-32.00		-0.46	-0.27	661061848	484403460	484407176	484407294	484407448	484404366	484403734	484398115	484401993	484401693	484398023	41445242	41446813	41444398	41444178	41444197
C9	-21.70	-83.82			-34.41	-0.05	4.50	176658388	3716	3834	3988	906	274	5345	1467	1768	5437	525848702	525850273	525847858	525847638	525847658
C10		-0.62			-37.33	-0.07	0.30	4.06	176654672	118	272	2810	3442	9061	5183	5483	9153	525852418	525853989	525851574	525851354	525851373
C11		3.98			-42.01	-0.03	2.58	5.07	3.31	176654554	154	2928	3560	9179	5301	5601	9271	525852536	525854107	525851692	525851472	525851492
C12		8.12			-41.88	-0.16	5.73	5.07	3.51	3.22	176654400	3082	3714	9333	5455	5756	9425	525852690	525854261	525851846	525851626	525851646
C13	-28.54	-69.38			-3.14	16.53	-0.27	2.22	0.01	0.15	-0.15	176657482	632	6251	2373	2673	6343	525849608	525851179	525848764	525848544	525848564
C14	-6.59		-10.00	28.34		0.01	27.25	-0.65	-0.01	0.01	0.01	-0.03	176658114	5619	1741	2042	5711	525848976	525850547	525848132	525847912	525847932
C15			-0.01	5.29		-0.86	-0.07	0.07	-0.01	-0.01	-0.01	-0.01	0.30	176663733	3878	3578	92	525843357	525844928	525842513	525842293	525842313
C16			0.37	5.33		13.78	-0.05	-0.01	-0.01	0.00	-0.01	0.05	0.20	26.40	176659855	300	3970	525847235	525848806	525846391	525846171	525846190
C17			-0.23			-1.02	0.45	-0.01	-0.01	0.00	-0.01	-0.01	-0.04	0.03	23.53	176660155	3670	525846935	525848506	525846090	525845870	525845890
C18			0.54	3.03		1.25	4.80	0.00	-0.01	0.01	0.01	0.00	0.50	3.76	0.08	26.82	176663825	525843265	525844836	525842421	525842201	525842220
H19		5.41			3.47	1.41	1.78	122.91	1.76	-0.28	2.47	3.15	0.01	-0.04	-0.02	-0.01	-0.01	702507090	1571	844	1064	1045
H20		0.83			4.14	1.80	2.45	136.23	3.61	1.68	-0.20	1.09	0.03	-0.03	0.00	0.03	0.06	-8.42	702508661	2415	2635	2616
H21					4.74			0.19	111.88	5.18	0.07	-0.08	-0.02	-0.04	-0.04	-0.03	-0.03	0.18	-0.04	702506246	220	200
H22					4.62			0.25	112.07	0.23	5.11	-0.03	-0.02	-0.03	-0.02	-0.02	-0.02	0.31	-0.03	-11.54	702506026	20
H23					3.82			6.76	111.99	-0.12	0.11	0.04	-0.01	-0.03	-0.03	-0.02	-0.02	0.48	1.61	-12.01	-11.73	702506045
H24					4.57			0.26	0.07	112.53	5.28	-0.06	0.02	-0.01	-0.01	0.01	0.02	0.23	0.33	-0.33	0.10	0.03
H25					3.65			8.06	-0.10	112.21	0.12	0.20	0.03	-0.02	-0.01	0.00	0.01	-0.28	0.60	-0.34	0.02	0.11
H26					7.12			0.22	5.38	118.19	0.21	-0.08	0.07	-0.01	0.00	0.02	0.04	0.25	0.51	2.10	-0.19	-0.29
H27					4.26			5.01	0.03	0.17	111.54	-0.22	0.03	-0.04	-0.04	-0.02	-0.01	0.88	-0.19	0.08	-0.27	0.18
H28					6.86			0.18	5.83	0.22	119.15	-0.17	0.11	-0.06	-0.06	-0.03	0.00	-0.26	0.32	-0.18	2.28	-0.12
H29					4.04			0.12	0.07	5.30	111.67	0.05	0.02	-0.07	-0.06	-0.04	-0.05	-0.28	0.10	0.27	-0.23	0.13
H30		7.13			0.30	0.85	1.61	1.70	-0.01	0.00	-0.01	131.56	-0.08	-0.03	0.00	-0.01	-0.03	0.38	0.17	0.01	0.07	-0.07
H31		37.71			-1.23	-0.22	-0.76	4.76	-0.02	0.39	-0.17	127.68	-0.10	-0.03	0.00	-0.02	-0.05	-0.33	-0.79	-0.18	-0.12	-0.09
H32		1.01			0.43	-5.82	0.75	0.95	-0.03	-0.05	-0.11	150.06	-0.10	0.00	0.04	0.02	0.00	0.15	0.75	-0.17	-0.06	-0.15
H33			-1.19	-20.40		-0.32	-23.90	0.00	-0.02	0.06	0.10	-0.12	133.34	-0.22	-0.02	0.10	0.23	-0.08	0.25	-0.08	-0.05	-0.01
H34			0.62	-2.34		-0.49	-0.83	-0.03	-0.02	0.02	0.05	-0.10	123.40	0.85	0.20	-0.03	0.54	-0.14	-0.05	-0.07	-0.06	-0.02
H35			-4.26	-7.32		-0.18	-0.53	-0.01	-0.02	0.03	0.02	-0.07	121.41	-0.18	0.07	0.06	0.23	-0.10	0.03	-0.08	-0.06	-0.04
H36			34.54	448.08		-0.16	1.96	-0.14	-0.06	-0.04	-0.05	-0.16	4.42	-0.26	0.08	0.40	2.90	-0.14	-0.25	-0.21	-0.18	-0.17
H37			0.33	7.23		1.11	-0.10	-0.04	-0.03	-0.01	-0.04	-0.02	-0.17	129.48	-1.89	0.13	0.13	-0.12	-0.09	-0.12	-0.09	-0.10
H38			-0.48	18.65		0.96	-0.41	-0.08	-0.05	-0.04	-0.07	-0.02	-0.27	129.07	-1.80	6.89	3.50	-0.22	-0.23	-0.20	-0.15	-0.16
H39			0.08	0.44		2.31	0.04	-0.01	-0.03	-0.01	-0.04	0.02	0.65	2.22	121.31	-1.23	7.97	-0.05	0.02	-0.10	-0.07	-0.08
H40			-0.11	-0.30		-1.72	-0.04	-0.02	-0.04	-0.02	-0.07	0.06	-0.06	-4.00	130.16	-3.58	0.76	-0.06	0.07	-0.17	-0.11	-0.13
H41			-0.37	2.30		0.57	0.47	0.03	-0.02	0.01	-0.02	0.02	0.01	8.36	-1.35	125.78	2.39	0.04	0.20	-0.09	-0.04	-0.07
H42			-0.08	-0.42		2.01	1.81	0.01	-0.02	0.01	-0.02	0.00	-0.01	0.63	-2.82	116.72	-3.50	-0.02	0.08	-0.08	-0.05	-0.06
H43			2.03	13.00		3.02	2.47	0.05	-0.04	0.05	-0.01	-0.03	0.08	0.00	0.08	-2.63	141.07	0.03	0.42	-0.15	-0.07	-0.09
H44			1.76	-0.22		1.94	-0.17	0.01	-0.02	0.03	0.00	-0.03	0.38	3.87	5.79	-1.45	129.09	-0.02	0.16	-0.10	-0.05	-0.06

cont. Table S4: For Complex 2: on the diagonal are the Larmor frequencies for the nuclei, on the lower triangle of the matrix are the coupling constants between the two nuclei, on the upper triangle are the differences in Larmor frequencies between the two coupled nuclei.

	H24	H25	H26	H27	H28	H29	H30	H31	H32	H33	H34	H35	H36	H37	H38	H39	H40	H41	H42	H43	H44
Hg1	576598220	576598182	576599093	576598171	576599371	576598267	576599394	576599488	576602241	576603257	576599357	576599687	576604109	576600116	576600817	576599306	576601072	576599745	576599438	576601511	576600277
Se2	568162440	568162401	568163313	568162391	568163591	568162487	568163614	568163707	568166461	568167476	568163577	568163907	568168329	568164336	568165037	568163525	568165292	568163965	568163658	568165731	568164497
Se3	568196613	568196574	568197486	568196564	568197764	568196660	568197787	568197880	568200633	568201649	568197749	568198080	568202501	568198509	568199209	568197698	568199464	568198138	568197831	568199903	568198670
P4	417947220	417947181	417948093	417947171	417948370	417947267	417948394	417948487	417951240	417952256	417948356	417948687	417953108	417949116	417949816	417948305	417950071	417948745	417948438	417950510	417949277
Si5	562876290	562876251	562877163	562876241	562877441	562876337	562877464	562877557	562880310	562881326	562877426	562877757	562882178	562878186	562878886	562877375	562879141	562877815	562877508	562879580	562878347
F6	41493504	41493465	41494377	41493455	41494655	41493551	41494678	41494771	41497524	41498540	41494641	41494971	41499392	41495400	41496100	41494589	41496355	41495029	41494722	41496795	41495561
F7	41444153	41444115	41445026	41444104	41445304	41444200	41445327	41445421	41448174	41449190	41445290	41445620	41450042	41446049	41446750	41445239	41447005	41445678	41445371	41447444	41446210
C9	525847613	525847575	525848487	525847564	525848764	525847661	525848787	525848881	525851634	525852650	525848750	525849080	525853502	525849510	525850210	525848699	525850465	525849139	525848832	525850904	525849670
C10	525851329	525851290	525852202	525851280	525852480	525851376	525852503	525852596	525855350	525856365	525852466	525852796	525857218	525853225	525853926	525852414	525854181	525852854	525852547	525854620	525853386
C11	525851447	525851409	525852321	525851398	525852598	525851494	525852621	525852715	525855468	525856484	525852584	525852914	525857336	525853343	525854044	525852533	525854299	525852972	525852665	525854738	525853504
C12	525851602	525851563	525852475	525851552	525852752	525851649	525852775	525852869	525855622	525856638	525852738	525853068	525857490	525853498	525854198	525852687	525854453	525853127	525852820	525854892	525853659
C13	525848519	525848481	525849393	525848470	525849670	525848566	525849693	525849787	525852540	525853556	525849656	525849986	525854408	525850415	525851116	525849605	525851371	525850045	525849738	525851810	525850576
C14	525847888	525847849	525848761	525847838	525849038	525847935	525849061	525849155	525851908	525852924	525849024	525849354	525853776	525849784	525850484	525848973	525850739	525849413	525849106	525851178	525849945
C15	525842268	525842230	525843142	525842219	525843419	525842315	525843442	525843536	525846289	525847305	525843405	525843735	525848157	525844164	525844865	525843354	525845120	525843793	525843486	525845559	525844325
C16	525846146	525846107	525847019	525846097	525847297	525846193	525847320	525847413	525850167	525851183	525847283	525847613	525852035	525848042	525848743	525847231	525848998	525847671	525847364	525849437	525848203
C17	525845846	525845807	525846719	525845797	525846997	525845893	525847020	525847113	525849866	525850882	525846983	525847313	525851734	525847742	525848442	525846931	525848697	525847371	525847064	525849137	525847903
C18	525842176	525842137	525843049	525842127	525843327	525842223	525843350	525843443	525846197	525847212	525843313	525843643	525848065	525844072	525844773	525843261	525845028	525843701	525843394	525845467	525844233
H19	1089	1128	216	1138	62	1042	85	178	2932	3948	48	378	4800	807	1508	4	1763	436	129	2202	968
H20	2660	2698	1787	2709	1509	2613	1486	1392	1361	2377	1523	1193	3229	764	63	1574	192	1135	1442	631	603
H21	244	283	629	294	906	197	929	1023	3776	4792	892	1222	5644	1652	2352	841	2607	1281	974	3046	1813
H22	25	63	849	74	1126	22	1149	1243	3996	5012	1112	1442	5864	1872	2572	1061	2827	1501	1194	3266	2032
H23	44	83	829	93	1106	3	1130	1223	3976	4992	1092	1423	5844	1852	2552	1041	2807	1481	1174	3246	2013
H24	702506001	39	873	49	1151	47	1174	1267	4021	5036	1137	1467	5889	1896	2597	1085	2852	1525	1218	3291	2057
H25	-11.91	702505962	912	11	1189	86	1213	1306	4059	5075	1175	1506	5927	1935	2635	1124	2890	1564	1257	3329	2096
H26	-11.56	-11.47	702506874	922	277	826	301	394	3147	4163	263	594	5015	1023	1723	212	1978	652	345	2417	1184
H27	-0.24	0.16	0.07	702505952	1200	96	1223	1317	4070	5086	1186	1516	5938	1945	2646	1135	2901	1574	1267	3340	2106
H28	-0.15	0.16	0.38	-11.57	702507152	1104	23	117	2870	3886	14	316	4738	745	1446	65	1701	374	67	2140	906
H29	2.29	-0.20	-0.18	-12.18	-10.61	702506048	1127	1220	3973	4989	1090	1420	5842	1849	2549	1038	2804	1478	1171	3244	2010
H30	0.00	-0.10	-0.10	-0.10	-0.31	-0.36	702507175	93	2847	3863	37	293	4715	722	1423	89	1678	351	44	2117	883
H31	-0.16	0.13	-0.26	-0.31	-0.45	-0.42	-9.56	702507268	2753	3769	131	200	4621	629	1329	182	1584	258	49	2023	790
H32	0.01	-0.14	-0.05	-0.31	-0.43	-0.48	-6.17	-9.78	702510022	1016	2884	2554	1868	2124	1424	2935	1169	2495	2802	730	1964
H33	0.14	0.18	0.34	0.21	0.52	0.15	-0.31	-0.45	-0.40	702511037	3900	3570	852	3140	2440	3951	2185	3511	3818	1746	2979
H34	0.03	0.08	0.15	0.15	0.35	0.12	-0.27	-0.34	-0.38	-12.89	702507138	330	4752	759	1460	51	1715	388	81	2154	920
H35	0.05	0.07	0.15	0.06	0.18	0.00	-0.20	-0.27	-0.24	-10.97	-10.57	702507468	4422	429	1130	381	1385	58	249	1824	590
H36	-0.16	-0.13	-0.16	-0.16	-0.24	-0.25	-0.17	-0.35	-0.29	11.64	1.35	0.51	702511890	3992	3292	4803	3037	4363	4670	2598	3832
H37	-0.05	-0.06	-0.04	-0.11	-0.17	-0.18	-0.09	-0.07	-0.02	0.34	-0.17	0.14	0.76	702507897	700	811	955	371	678	1395	161
H38	-0.11	-0.13	-0.12	-0.21	-0.34	-0.31	-0.11	-0.05	0.02	-0.14	-0.39	-0.05	1.01	-7.46	702508598	1511	255	1071	1378	694	540
H39	-0.02	-0.04	-0.02	-0.11	-0.16	-0.17	0.00	0.02	0.12	-0.01	0.42	0.08	-0.03	5.70	0.40	702507086	1766	440	133	2205	972
H40	-0.03	-0.08	-0.03	-0.19	-0.31	-0.31	0.04	0.08	0.33	-0.01	-0.18	-0.02	-0.09	11.65	9.08	-10.30	702508853	1326	1633	439	795
H41	0.04	0.01	0.08	-0.08	-0.08	-0.16	0.02	-0.02	0.16	0.17	-0.05	0.09	0.47	-0.44	0.75	0.55	6.53	702507526	307	1765	532
H42	0.02	0.00	0.05	-0.06	-0.07	-0.13	-0.03	-0.05	0.05	0.13	-0.03	0.10	0.00	-0.12	-0.32	5.86	12.92	-9.70	702507219	2072	839
H43	0.13	0.09	0.27	-0.05	0.06	-0.21	-0.11	-0.24	0.09	0.63	0.19	0.37	-0.72	0.36	-0.19	-0.36	0.27	6.70	11.51	702509292	1234
H44	0.07	0.05	0.15	-0.02	0.05	-0.10	-0.10	-0.17	-0.04	0.79	0.43	0.13	-0.13	-0.41	0.18	0.69	-0.22	0.37	8.28	-7.71	702508058

Table S5: For Complex 3: on the diagonal are the Larmor frequencies for the nuclei, on the lower triangle of the matrix are the coupling constants between the two nuclei, on the upper triangle are the differences in Larmor frequencies between the two coupled nuclei.

	Cd1	Te2	Te3	P4	Si5	F6	F7	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	H19	H20	H21	H22	H23
Cd1	155920342	66742136	66628154	128624917	16290421	505084765	505121481	20734037	20734228	20734350	20734259	20732821	20737857	20743908	20739462	20739730	20743350	546586691	546588122	546585960	546585692	546585695
Te2	-481.12	222662478	113983	61882781	83032558	438342629	438379344	46008099	46007908	46007787	46007877	46009316	46004280	45998228	46002675	46002406	45998787	479844555	479845986	479843823	479843556	479843559
Te3	-878.27	36.37	222548496	61996763	82918575	438456612	438493327	45894116	45893926	45893804	45893894	45895333	45890297	45884245	45888692	45888424	45884804	479958537	479959968	479957806	479957538	479957542
P4	60.53	1.63	1504.62	284545259	144915338	376459848	376496564	107890880	107890689	107890567	107890657	107892096	107887060	107881008	107885455	107885187	107881567	417961774	417963205	417961043	417960775	417960778
Si5	0.00	42.09			139629921	521375187	521411902	37024459	37024649	37024771	37024681	37023242	37028278	37034330	37029883	37030151	37033771	562877112	562878543	562876381	562876113	562876117
F6	783.72	14.79	30.10		0.13	661005107	36716	484350728	484350537	484350415	484350506	484351945	484346909	484340857	484345303	484345035	484341416	41501926	41503357	41501194	41500927	41500930
F7	784.66	10.85	87.43		0.68	-9.11	661041823	484387443	484387253	484387131	484387221	484388660	484383624	484377572	484382019	484381751	484378131	41465210	41466641	41464479	41464211	41464215
C9	6.48	195.52			-33.74	-0.22	0.75	176654380	191	312	222	1217	3819	9871	5424	5693	9312	525852654	525854085	525851922	525851655	525851658
C10		1.01			-38.53	-0.03	0.53	3.82	176654570	122	31	1408	3629	9680	5234	5502	9122	525852463	525853894	525851732	525851464	525851467
C11		-7.50			-40.35	-0.04	0.07	4.72	3.48	176654692	90	1529	3507	9559	5112	5380	9000	525852341	525853772	525851610	525851342	525851346
C12		-19.07			-41.38	-0.14	7.83	4.72	3.14	3.57	176654602	1439	3597	9649	5202	5470	9090	525852431	525853862	525851700	525851432	525851436
C13	8.88	163.74			-2.46	12.16	-0.20	2.96	-0.06	0.12	-0.09	176653163	5036	11088	6641	6909	10529	525853870	525855301	525853139	525852871	525852875
C14	2.59		33.48	22.47		0.02	21.23	-0.23	0.00	0.01	0.01	-0.02	176658199	6052	1605	1873	5493	525848834	525850265	525848103	525847835	525847839
C15			0.23	6.80		-0.71	-0.01	0.03	-0.01	0.00	-0.01	-0.01	0.24	176664251	4447	4179	559	525842782	525844213	525842051	525841783	525841787
C16			-1.02	4.64		14.41	-0.03	-0.01	-0.01	0.00	-0.01	0.06	0.17	26.27	176659804	268	3888	525847229	525848660	525846498	525846230	525846234
C17			0.74			-0.84	0.32	0.00	-0.01	0.00	0.00	0.00	-0.03	0.09	23.64	176660072	3620	525846961	525848392	525846230	525845962	525845965
C18			-3.11	2.94		-0.24	9.10	0.00	-0.01	0.01	0.03	-0.01	0.56	3.77	0.15	26.85	176663692	525843341	525844772	525842610	525842342	525842346
H19		-12.15			3.84	0.76	0.63	123.92	1.11	-0.22	3.62	2.50	0.00	-0.03	-0.01	0.00	0.00	702507033	1431	731	999	995
H20		3.43			4.03	1.07	1.88	133.03	4.19	1.40	-0.35	0.80	0.03	-0.01	0.01	0.03	0.06	-8.05	702508464	2162	2430	2427
H21					4.54			0.28	112.46	5.35	0.05	-0.13	-0.02	-0.04	-0.04	-0.03	-0.03	0.22	-0.17	702506302	268	264
H22					4.75			0.22	112.23	0.26	4.89	-0.04	-0.01	-0.03	-0.02	-0.02	-0.02	0.38	-0.07	-11.53	702506034	4
H23					4.02			6.78	111.84	-0.08	0.11	-0.05	0.00	-0.03	-0.02	-0.02	-0.02	0.24	1.93	-12.08	-11.80	702506038
H24					4.64			0.21	0.07	112.84	5.24	-0.06	0.01	-0.01	0.00	0.01	0.01	0.32	0.28	-0.29	0.12	0.03
H25					3.84			7.92	-0.01	112.37	0.02	0.16	0.02	-0.01	-0.01	0.00	0.01	-0.24	0.45	-0.28	0.02	0.12
H26					5.87			0.15	5.42	115.41	0.20	-0.07	0.05	0.00	0.00	0.02	0.03	0.26	0.48	2.22	-0.19	-0.30
H27					4.46			5.99	-0.24	0.43	111.82	-0.19	0.04	-0.03	-0.02	-0.01	0.00	1.54	-0.24	0.12	-0.38	0.15
H28					6.69			0.59	5.73	-0.04	119.44	-0.19	0.11	-0.03	-0.03	0.00	0.03	-0.11	0.43	-0.23	2.23	-0.12
H29					3.90			-0.07	0.35	5.48	110.88	0.06	0.04	-0.05	-0.04	-0.03	-0.02	-0.39	0.22	0.29	-0.12	0.12
H30		-12.46			0.33	0.84	0.74	1.49	-0.02	0.01	-0.04	132.76	-0.06	-0.02	0.01	-0.01	-0.02	0.51	0.06	-0.09	0.04	-0.11
H31		-92.39			-0.83	-0.29	-0.64	3.71	-0.08	0.39	-0.18	128.90	-0.07	-0.02	0.01	-0.01	-0.04	-0.50	-0.84	-0.31	-0.18	-0.19
H32		3.95			0.38	-3.68	0.33	0.61	-0.02	-0.05	-0.13	150.00	-0.07	0.01	0.05	0.02	0.00	0.05	0.72	-0.31	-0.13	-0.20
H33			3.59	-18.07		-0.30	-15.83	0.03	-0.01	0.04	0.10	-0.09	133.78	-0.23	-0.02	0.10	0.23	-0.04	0.25	-0.06	-0.05	0.00
H34			-1.76	-0.06		-0.39	-0.38	-0.01	-0.01	0.01	0.06	-0.08	123.77	0.85	0.16	-0.02	0.55	-0.11	0.01	-0.05	-0.06	-0.01
H35			20.80	-10.80		-0.22	-0.21	0.00	-0.02	0.02	0.03	-0.06	121.87	-0.18	0.07	0.06	0.20	-0.07	0.06	-0.07	-0.06	-0.03
H36			-45.38	428.45		-0.10	0.24	-0.09	-0.05	-0.04	-0.04	-0.12	3.74	-0.45	0.15	0.54	3.09	-0.21	-0.24	-0.20	-0.17	-0.15
H37			2.52	10.48		1.64	0.02	-0.02	-0.03	-0.01	-0.02	0.00	-0.14	130.37	-1.73	0.27	0.02	-0.09	-0.03	-0.12	-0.09	-0.09
H38			3.20	21.19		1.08	-0.25	-0.05	-0.05	-0.03	-0.05	0.00	-0.23	128.31	-1.75	7.38	3.99	-0.16	-0.12	-0.19	-0.14	-0.14
H39			-0.23	0.28		1.20	0.08	0.00	-0.03	-0.01	-0.02	0.03	0.65	2.06	121.09	-1.23	8.16	-0.03	0.05	-0.11	-0.07	-0.08
H40			0.12	-0.39		-2.85	0.04	0.00	-0.04	-0.01	-0.04	0.07	-0.05	-3.74	130.18	-3.34	0.76	-0.04	0.10	-0.17	-0.11	-0.12
H41			1.12	1.48		0.54	0.75	0.04	-0.02	0.01	-0.01	0.02	0.01	8.21	-1.40	125.49	2.40	0.06	0.22	-0.10	-0.05	-0.06
H42			-0.03	0.02		1.84	2.53	0.02	-0.02	0.01	0.00	0.01	0.00	0.56	-2.86	116.85	-3.41	0.00	0.10	-0.08	-0.05	-0.06
H43			-0.85	15.49		1.52	0.19	0.06	-0.03	0.04	0.03	-0.03	0.18	0.15	0.02	-2.50	138.72	0.05	0.36	-0.13	-0.07	-0.07
H44			-2.25	1.11		0.74	0.18	0.02	-0.02	0.02	0.01	-0.02	0.28	3.47	5.15	-1.49	129.06	0.00	0.16	-0.09	-0.05	-0.05

cont. Table S5: For Complex 3: on the diagonal are the Larmor frequencies for the nuclei, on the lower triangle of the matrix are the coupling constants between the two nuclei, on the upper triangle are the differences in Larmor frequencies between the two coupled nuclei.

	H24	H25	H26	H27	H28	H29	H30	H31	H32	H33	H34	H35	H36	H37	H38	H39	H40	H41	H42	H43	H44
Cd1	546585726	546585693	546586075	546585617	546587104	546585563	546586749	546586715	546589418	546590169	546586886	546587586	546591035	546587425	546588199	546586701	546588548	546587222	546586879	546588913	546587651
Te2	479843590	479843556	479843938	479843481	479844968	479843427	479844613	479844579	479847282	479848033	479844750	479845450	479848899	479845289	479846063	479844565	479846412	479845086	479844743	479846777	479845515
Te3	479957573	479957539	479957921	479957464	479958950	479957410	479958596	479958562	479961265	479962016	479958733	479959432	479962882	479959271	479960046	479958548	479960395	479959068	479958726	479960759	479959498
P4	417960809	417960776	417961158	417960701	417962187	417960646	417961832	417961799	417964501	417965252	417961969	417962669	417966118	417962508	417963282	417961785	417963631	417962305	417961962	417963996	417962734
Si5	562876148	562876114	562876496	562876039	562877525	562875985	562877171	562877137	562879840	562880591	562877308	562878007	562881457	562877846	562878621	562877123	562878970	562877643	562877301	562879334	562878073
F6	41500961	41500927	41501310	41500852	41502339	41500798	41501984	41501950	41504653	41505404	41502121	41502821	41506270	41502660	41503434	41501936	41503783	41502457	41502114	41504148	41502886
F7	41464246	41464212	41464594	41464137	41465623	41464083	41465268	41465235	41467937	41468688	41465405	41466105	41469555	41465944	41466718	41465221	41467068	41465741	41465398	41467432	41466170
C9	525851689	525851655	525852037	525851580	525853067	525851526	525852712	525852678	525855381	525856132	525852849	525853549	525856998	525853388	525854162	525852664	525854511	525853185	525852842	525854876	525853614
C10	525851498	525851465	525851847	525851389	525852876	525851335	525852521	525852487	525855190	525855941	525852658	525853358	525856807	525853197	525853971	525852473	525854320	525852994	525852651	525854685	525853423
C11	525851377	525851343	525851725	525851268	525852754	525851214	525852399	525852366	525855068	525855819	525852536	525853236	525856686	525853075	525853849	525852352	525854199	525852872	525852529	525854563	525853301
C12	525851467	525851433	525851815	525851358	525852844	525851304	525852490	525852456	525855159	525855910	525852627	525853326	525856776	525853166	525853940	525852442	525854289	525852963	525852620	525854654	525853392
C13	525852906	525852872	525853254	525852797	525854283	525852743	525853929	525853895	525856598	525857349	525854066	525854765	525858215	525854604	525855379	525853881	525855728	525854401	525854059	525856092	525854831
C14	525847870	525847836	525848218	525847761	525849247	525847707	525848893	525848859	525851561	525852312	525849030	525849729	525853179	525849568	525850343	525848845	525850692	525849365	525849022	525851056	525849795
C15	525841818	525841784	525842166	525841709	525843196	525841655	525842841	525842807	525845510	525846261	525842978	525843677	525847127	525843517	525844291	525842793	525844640	525843314	525842971	525845005	525843743
C16	525846265	525846231	525846613	525846156	525847642	525846102	525847287	525847254	525849956	525850707	525847424	525848124	525851574	525847963	525848737	525847240	525849087	525847760	525847417	525849451	525848190
C17	525845996	525845963	525846345	525845887	525847374	525845833	525847019	525846986	525849688	525850439	525847156	525847856	525851305	525847695	525848469	525846971	525848818	525847492	525847149	525849183	525847921
C18	525842377	525842343	525842725	525842268	525843754	525842214	525843400	525843366	525846069	525846820	525843537	525844236	525847686	525844075	525844850	525843352	525845199	525843872	525843530	525845563	525844302
H19	965	998	616	1073	413	1128	58	25	2727	3478	195	895	4344	734	1508	11	1857	531	188	2222	960
H20	2396	2429	2047	2505	1018	2559	1373	1406	1296	2047	1236	536	2913	697	77	1421	426	900	1243	791	471
H21	233	267	115	342	1144	396	790	756	3459	4210	927	1626	5076	1465	2240	742	2589	1262	920	2953	1692
H22	34	1	383	74	1412	129	1057	1024	3726	4477	1194	1894	5343	1733	2507	1010	2856	1530	1187	3221	1959
H23	31	3	379	78	1409	132	1054	1020	3723	4474	1191	1891	5340	1730	2504	1006	2853	1527	1184	3218	1956
H24	702506068	34	348	109	1378	163	1023	989	3692	4443	1160	1860	5309	1699	2473	975	2822	1496	1153	3187	1925
H25	-11.91	702506035	382	75	1411	129	1057	1023	3726	4477	1194	1893	5343	1732	2507	1009	2856	1529	1187	3220	1959
H26	-11.62	-11.69	702506417	457	1029	511	674	641	3343	4094	811	1511	4961	1350	2124	627	2474	1147	804	2838	1576
H27	-0.11	0.17	0.05	702505960	1487	54	1132	1098	3801	4552	1269	1968	5418	1808	2582	1084	2931	1605	1262	3296	2034
H28	-0.25	0.16	0.32	-11.67	702507446	1541	355	388	2314	3065	218	482	3931	321	1095	403	1444	118	225	1809	547
H29	2.38	-0.23	-0.14	-12.21	-10.98	702505905	1186	1152	3855	4606	1323	2023	5472	1862	2636	1138	2985	1659	1316	3350	2088
H30	0.01	-0.09	-0.08	-0.17	-0.36	-0.50	702507091	34	2669	3420	137	837	4286	676	1450	48	1799	473	130	2164	902
H31	-0.18	0.11	-0.25	-0.37	-0.48	-0.59	-9.41	702507058	2703	3454	171	870	4320	710	1484	14	1833	507	164	2198	936
H32	-0.02	-0.14	-0.03	-0.32	-0.34	-0.56	-5.70	-9.33	702509760	751	2532	1832	1617	1993	1219	2717	870	2196	2539	505	1767
H33	0.09	0.13	0.24	0.23	0.47	0.23	-0.25	-0.32	-0.26	702510511	3283	2583	866	2744	1970	3468	1621	2947	3290	1256	2518
H34	0.02	0.06	0.11	0.16	0.31	0.17	-0.24	-0.27	-0.28	-12.95	702507228	700	4149	539	1313	185	1662	336	7	2027	765
H35	0.03	0.05	0.11	0.09	0.20	0.06	-0.17	-0.21	-0.17	-10.72	-10.59	702507928	3449	161	613	884	962	364	707	1327	65
H36	-0.13	-0.11	-0.13	-0.13	-0.20	-0.21	-0.24	-0.30	-0.28	12.33	1.19	1.13	702511377	3610	2836	4334	2487	3813	4156	2122	3384
H37	-0.04	-0.04	-0.02	-0.08	-0.10	-0.13	-0.06	-0.05	0.02	0.26	-0.11	0.08	0.70	702507767	774	724	1123	203	546	1488	226
H38	-0.08	-0.09	-0.07	-0.16	-0.22	-0.24	-0.08	-0.02	0.06	-0.14	-0.38	-0.07	0.93	-8.02	702508541	1498	349	977	1320	714	548
H39	-0.02	-0.03	0.00	-0.08	-0.09	-0.13	0.02	0.04	0.14	0.00	0.39	0.08	-0.04	5.56	0.43	702507044	1847	521	178	2212	950
H40	-0.02	-0.05	0.00	-0.13	-0.17	-0.23	0.06	0.10	0.34	0.03	-0.16	-0.01	-0.09	11.84	8.85	-11.05	702508891	1326	1669	365	897
H41	0.04	0.02	0.08	-0.04	0.01	-0.10	0.03	-0.01	0.16	0.18	-0.04	0.08	0.42	-0.40	0.85	0.52	6.76	702507564	343	1691	429
H42	0.02	0.00	0.05	-0.03	-0.01	-0.08	-0.02	-0.03	0.07	0.13	-0.02	0.09	0.03	-0.12	-0.30	6.05	13.07	-9.95	702507221	2034	772
H43	0.10	0.08	0.21	0.05	0.24	-0.04	-0.10	-0.19	0.04	0.52	0.24	0.33	-1.05	0.19	-0.23	-0.43	0.22	7.15	11.26	702509255	1262
H44	0.05	0.04	0.12	0.02	0.11	-0.03	-0.08	-0.13	-0.02	0.65	0.44	0.14	-0.29	-0.39	0.13	0.60	-0.25	0.46	8.77	-8.34	702507993

Table S6: For Complex 4: on the diagonal are the Larmor frequencies for the nuclei, on the lower triangle of the matrix are the coupling constants between the two nuclei, on the upper triangle are the differences in Larmor frequencies between the two coupled nuclei.

	Cd1	Se2	Se3	P4	Si5	F6	F7	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	H19	H20	H21	H22	H23	
Cd1	155916644	21582334	21614648	128641915	16287029	505080108	505118628	20741477	20738311	20737775	20737907	20740666	20741350	20747056	20743265	20743404	20747038	546590629	546591985	546589394	546589524	546589441	
Se2	105.44	155916644	32314	150224249	5295305	526662441	526700962	42323811	42320645	42320109	42320241	42322999	42323684	42329390	42325599	42325737	42329372	568172963	568174319	568171728	568171858	568171775	
Se3	233.79	4.87	134301996	150256563	5327619	526694755	526733276	42356125	42352959	42352423	42352555	42355313	42355998	42361704	42357913	42358051	42361686	568205277	568206633	568204042	568204172	568204089	
P4	50.86	0.09	-660.24	284558559	144928944	376438192	376476713	107900438	107903604	107904140	107904008	107901250	107900565	107894859	107898650	107898512	107894877	417948714	417950070	417947479	417947609	417947526	
Si5	0.62	-15.12			139629615	521367136	521405657	37028505	37025340	37024804	37024935	37027694	37028379	37034085	37030294	37030432	37034067	562877658	562879014	562876423	562876552	562876469	
F6	677.95	-4.18	-4.62		0.12	660996751	38521	484338631	484341796	484342332	484342201	484339442	484338757	484333051	484336842	484336704	484333070	41510522	41511878	41509287	41509416	41509333	
F7	691.68	4.54	-26.06		0.51	-7.23	661035272	484377152	484380317	484380853	484380722	484377963	484377278	484371572	484375363	484375225	484371590	41472001	41473357	41470766	41470895	41470812	
C9	6.76	-81.18			-32.89	3.39	-0.31	176658121	3166	3701	3570	811	127	5579	1788	1927	5561	525849153	525850508	525847918	525848047	525847964	
C10		4.51			-39.00	0.00	0.61	5.20	176654955		536	404	2354	3039	8745	4954	5092	8727	525852318	525853674	525851083	525851213	525851130
C11		-0.26			-42.09	-0.11	9.53	3.87	3.13	176654419	131	2890	3575	9281	5490	5628	9263	525852854	525854210	525851619	525851748	525851665	
C12		7.85			-39.32	0.21	-0.01	3.87	3.34	3.56	176654551	2759	3443	9149	5358	5497	9131	525852723	525854078	525851488	525851617	525851534	
C13	9.60	-69.04			-3.37	4.42	0.05	2.53	0.13	0.02	-0.18	176657309	685	6391	2600	2738	6372	525849964	525851320	525848729	525848858	525848775	
C14	3.44		-9.21	29.75		-0.05	19.42	-0.50	0.00	0.05	0.00	-0.02	176657994	5706	1915	2053	5688	525849279	525850635	525848044	525848173	525848091	
C15			0.01	6.76		-0.83	0.02	-0.01	-0.01	0.00	-0.01	-0.01	0.22	176663700	3791	3653	18	525843573	525844929	525842338	525842467	525842384	
C16			0.45	4.92		12.12	-0.05	-0.01	0.00	0.00	-0.01	0.01	0.10	26.22	176659909	138	3773	525847364	525848720	525846129	525846259	525846176	
C17			-0.24			-0.36	0.16	0.02	0.00	0.00	-0.01	-0.01	-0.03	0.09	23.76	176660047	3634	525847226	525848582	525845991	525846120	525846037	
C18			0.16	3.76		-0.20	9.98	0.00	0.00	0.01	-0.01	-0.02	0.67	3.92	0.13	26.73	176663682	525843591	525844947	525842356	525842486	525842403	
H19		5.31			3.81	0.27	-0.12	124.00	2.00	3.10	-0.37	1.95	-0.06	-0.03	-0.01	-0.02	-0.04	702507273	1356	1235	1106	1189	
H20		2.76			3.93	0.36	-0.02	132.86	-0.29	1.26	3.27	2.72	-0.06	-0.01	0.03	0.01	-0.01	-8.83	702508629	2591	2462	2545	
H21					4.78			0.12	112.68	4.72	0.32	-0.06	-0.02	-0.02	-0.01	-0.01	-0.02	0.27	0.29	702506038	129	46	
H22					4.80			0.29	112.86	0.05	5.54	-0.05	-0.02	-0.01	0.00	0.00	-0.01	0.16	0.26	-11.66	702506168	83	
H23					3.95			7.99	112.27	0.12	-0.01	0.16	-0.01	-0.02	-0.01	-0.01	-0.01	0.62	-0.24	-11.67	-12.11	702506085	
H24					5.32			0.37	0.09	112.07	5.73	-0.05	0.00	0.00	0.02	0.03	0.03	-0.11	0.43	-0.28	0.15	0.04	
H25					4.47			6.85	0.21	110.23	-0.10	0.05	0.02	-0.01	0.00	0.01	0.02	1.29	0.26	-0.23	0.02	0.16	
H26					4.73			-0.13	6.48	120.02	0.22	-0.14	0.05	-0.01	0.01	0.02	0.07	-0.30	0.29	2.56	-0.26	-0.22	
H27					4.53			5.30	0.25	-0.10	112.22	-0.23	0.00	-0.03	-0.02	-0.01	-0.01	-0.34	1.23	-0.01	-0.24	0.10	
H28					4.53			-0.04	5.71	0.26	113.36	0.02	0.01	-0.04	-0.04	-0.02	-0.01	0.06	-0.34	-0.20	2.31	-0.32	
H29					4.62			0.33	0.06	5.22	113.30	-0.13	-0.02	-0.04	-0.03	-0.03	-0.03	0.13	-0.20	0.13	-0.32	0.04	
H30		7.24			0.40	0.21	1.35	1.04	-0.03	-0.02	-0.09	133.17	-0.07	-0.02	-0.01	-0.03	-0.05	0.63	0.26	0.02	0.01	-0.09	
H31		34.71			-1.52	0.35	-0.80	4.82	0.40	-0.03	-0.16	128.17	-0.08	-0.02	-0.02	-0.03	-0.06	-0.62	-0.30	-0.16	-0.13	0.16	
H32		1.80			0.30	0.31	-0.52	1.67	0.01	-0.04	0.01	144.53	-0.09	0.00	0.03	-0.01	-0.04	0.26	0.72	-0.04	0.03	-0.08	
H33			-1.20	-19.64		-0.49	-12.61	-0.06	-0.02	0.04	0.01	-0.11	133.42	-0.21	-0.02	0.08	0.21	-0.23	-0.23	-0.09	-0.07	-0.04	
H34			0.75	-2.40		-0.44	-0.14	-0.06	-0.03	0.00	0.00	-0.07	123.26	0.89	0.16	-0.02	0.65	-0.21	-0.25	-0.09	-0.09	-0.06	
H35			-4.23	-7.19		-0.24	-0.16	-0.05	-0.02	0.01	-0.01	-0.06	120.86	-0.17	0.08	0.08	0.26	-0.17	-0.16	-0.08	-0.06	-0.05	
H36			28.59	451.89		0.29	0.93	-0.09	-0.05	-0.05	-0.05	-0.07	5.62	-0.48	0.26	0.56	2.41	-0.15	-0.32	-0.17	-0.17	-0.15	
H37			0.18	6.72		1.24	-0.19	-0.03	-0.02	-0.01	-0.03	-0.01	-0.10	129.55	-1.64	0.38	-0.17	-0.10	-0.03	-0.07	-0.04	-0.05	
H38			-0.64	16.31		0.82	-0.32	-0.04	-0.03	-0.02	-0.05	0.01	-0.24	129.42	-1.82	7.75	4.43	-0.14	-0.04	-0.10	-0.06	-0.09	
H39			0.09	0.42		0.66	0.07	0.01	-0.01	0.01	-0.03	0.01	0.59	1.83	121.22	-1.24	8.10	-0.03	0.09	-0.04	0.00	-0.03	
H40			-0.10	-0.32		-1.23	0.07	0.03	-0.01	0.02	-0.04	0.02	-0.06	-3.80	129.51	-2.83	0.71	-0.02	0.23	-0.05	0.01	-0.04	
H41			-0.32	1.62		0.64	0.72	0.01	-0.01	0.04	-0.02	-0.02	-0.01	8.06	-1.37	124.91	2.43	-0.03	0.11	-0.03	0.02	-0.01	
H42			-0.03	0.06		2.40	2.38	0.00	-0.01	0.02	-0.02	-0.02	-0.01	0.52	-2.96	117.18	-3.42	-0.05	0.03	-0.04	-0.01	-0.02	
H43			1.52	10.80		0.49	-1.31	-0.03	-0.02	0.07	-0.02	-0.09	0.11	0.32	0.01	-2.47	137.77	-0.15	-0.02	-0.07	-0.01	-0.02	
H44			1.87	-0.30		0.24	0.56	-0.02	-0.01	0.03	-0.01	-0.05	0.41	2.88	4.69	-1.61	129.05	-0.11	-0.04	-0.06	-0.02	-0.03	

cont. Table S6: For Complex 4: on the diagonal are the Larmor frequencies for the nuclei, on the lower triangle of the matrix are the coupling constants between the two nuclei, on the upper triangle are the differences in Larmor frequencies between the two coupled nuclei.

	H24	H25	H26	H27	H28	H29	H30	H31	H32	H33	H34	H35	H36	H37	H38	H39	H40	H41	H42	H43	H44
Cd1	546589425	546589256	546591168	546589463	546589585	546589430	546590711	546590704	546592099	546593453	546590488	546590849	546595138	546591216	546592117	546590450	546592156	546590870	546590608	546592801	546591417
Se2	568171759	568171590	568173502	568171797	568171919	568171764	568173045	568173038	568174433	568175787	568172821	568173183	568177472	568173550	568174451	568172783	568174490	568173204	568172942	568175135	568173751
Se3	568204073	568203904	568205816	568204111	568204233	568204078	568205359	568205352	568206747	568208101	568205135	568205497	568209786	568205864	568206765	568205097	568206804	568205518	568205256	568207449	568206065
P4	417947510	417947341	417949253	417947548	417947670	417947515	417948796	417948789	417950184	417951538	417948572	417948934	417953223	417949301	417950202	417948534	417950241	417948955	417948693	417950886	417949502
Si5	562876454	562876285	562878197	562876492	562876613	562876459	562877740	562877733	562879128	562880482	562877516	562877878	562882167	562878245	562879145	562877478	562879185	562877898	562877637	562879830	562878446
F6	41509318	41509148	41511061	41509356	41509477	41509323	41510603	41510596	41511992	41513345	41510380	41510742	41515031	41511108	41512009	41510342	41512048	41510762	41510501	41512693	41511309
F7	41470797	41470628	41472540	41470835	41470956	41470802	41472082	41472075	41473471	41474824	41471859	41472221	41476510	41472588	41473488	41471821	41473528	41472241	41471980	41474173	41472789
C9	525847948	525847779	525849691	525847986	525848108	525847953	525849234	525849227	525850622	525851976	525849011	525849372	525853661	525849739	525850640	525848973	525850679	525849393	525849131	525851324	525849940
C10	525851114	525850945	525852857	525851152	525851274	525851119	525852400	525852393	525853788	525855142	525852176	525852538	525856827	525852905	525853806	525852138	525853845	525852559	525852297	525854490	525853106
C11	525851650	525851481	525853393	525851688	525851809	525851655	525852936	525852928	525854324	525855677	525852712	525853074	525857363	525853441	525854341	525852674	525854381	525853094	525852833	525855026	525853642
C12	525851518	525851349	525853261	525851556	525851678	525851523	525852804	525852797	525854192	525855546	525852581	525852942	525857231	525853309	525854210	525852543	525854249	525852963	525852701	525854894	525853510
C13	525848760	525848590	525850503	525848798	525848919	525848765	525850045	525850038	525851434	525852787	525849822	525850184	525854473	525850551	525851451	525849784	525851491	525850204	525849943	525852135	525850751
C14	525848075	525847906	525849818	525848113	525848235	525848080	525849361	525849354	525850749	525852103	525849137	525849499	525853788	525849866	525850767	525849099	525850806	525849520	525849258	525851451	525850067
C15	525842369	525842200	525844112	525842407	525842528	525842374	525843655	525843648	525845043	525846397	525843431	525843793	525848082	525844160	525845060	525843393	525845100	525843813	525843552	525845745	525844361
C16	525846160	525845991	525847903	525846198	525846320	525846165	525847446	525847439	525848834	525850188	525847222	525847584	525851873	525847951	525848852	525847184	525848891	525847605	525847343	525849536	525848152
C17	525846022	525845853	525847765	525846060	525846181	525846027	525847307	525847300	525848696	525850049	525847084	525847446	525851735	525847813	525848713	525847046	525848753	525847466	525847205	525849397	525848013
C18	525842387	525842218	525844130	525842425	525842547	525842392	525843673	525843666	525845061	525846415	525843450	525843811	525848100	525844178	525845079	525843412	525845118	525843832	525843570	525845763	525844379
H19	1204	1373	539	1166	1045	1199	81	74	1470	2823	142	220	4509	587	1487	180	1527	240	21	2172	788
H20	2560	2729	817	2522	2401	2555	1274	1281	114	1468	1498	1136	3153	769	131	1536	171	1116	1377	816	568
H21	31	138	1774	69	190	36	1317	1310	2705	4059	1093	1455	5744	1822	2722	1055	2762	1475	1214	3407	2023
H22	98	268	1645	60	61	93	1187	1180	2575	3929	964	1326	5615	1692	2593	926	2632	1346	1085	3277	1893
H23	15	185	1728	22	144	11	1270	1263	2658	4012	1047	1409	5698	1775	2676	1009	2715	1429	1168	3360	1976
H24	702506069	169	1743	38	159	5	1286	1279	2674	4028	1062	1424	5713	1791	2691	1024	2731	1444	1183	3376	1992
H25	-11.56	702505900	1912	207	329	174	1455	1448	2843	4197	1232	1593	5882	1960	2861	1194	2900	1614	1352	3545	2161
H26	-12.28	-12.61	702507812	1705	1583	1738	457	464	931	2285	681	319	3970	48	948	719	988	299	560	1633	249
H27	-0.29	0.16	0.14	702506107	122	33	1248	1241	2636	3990	1024	1386	5675	1753	2653	986	2693	1406	1145	3338	1954
H28	-0.20	0.11	0.32	-12.38	702506229	155	1126	1119	2514	3868	903	1265	5553	1631	2532	865	2571	1285	1024	3216	1832
H29	2.28	-0.33	-0.23	-11.78	-11.31	702506074	1281	1274	2669	4023	1057	1419	5708	1786	2686	1019	2726	1439	1178	3371	1987
H30	-0.12	-0.15	-0.25	-0.19	-0.35	-0.14	702507355	7	1388	2742	223	138	4427	505	1406	261	1445	159	103	2090	706
H31	-0.22	-0.15	-0.39	-0.26	-0.40	-0.27	-9.57	702507348	1395	2749	216	145	4434	512	1413	254	1452	166	96	2097	713
H32	0.01	-0.15	-0.20	-0.11	-0.40	-0.24	-6.69	-9.39	702508743	1354	1612	1250	3039	883	18	1650	57	1229	1491	702	682
H33	0.08	0.11	0.31	0.04	0.10	-0.03	-0.30	-0.33	-0.40	702510097	2965	2604	1685	2237	1336	3003	1297	2583	2845	652	2036
H34	-0.04	0.01	0.05	0.00	0.03	-0.05	-0.23	-0.23	-0.31	-12.87	702507131	362	4651	729	1629	38	1669	382	121	2313	929
H35	0.01	0.03	0.08	-0.01	0.00	-0.06	-0.20	-0.23	-0.25	-11.02	-10.90	702507493	4289	367	1267	400	1307	20	241	1952	568
H36	-0.21	-0.17	-0.28	-0.17	-0.23	-0.21	-0.29	-0.30	-0.31	11.24	1.20	0.51	702511782	3922	3022	4689	2982	4269	4530	2337	3721
H37	0.00	-0.03	-0.04	-0.08	-0.12	-0.11	-0.07	-0.06	0.00	0.22	-0.16	0.07	0.94	702507860	901	766	940	346	608	1585	201
H38	-0.03	-0.07	-0.14	-0.14	-0.22	-0.18	-0.04	0.01	0.13	-0.17	-0.39	-0.10	0.86	-7.85	702508761	1667	39	1247	1508	684	700
H39	0.06	0.01	0.02	-0.07	-0.11	-0.10	-0.02	-0.02	0.09	-0.03	0.39	0.09	-0.04	5.37	0.38	702507093	1706	420	159	2351	967
H40	0.15	0.03	0.06	-0.11	-0.18	-0.16	-0.02	-0.04	0.21	-0.01	-0.18	-0.03	-0.14	11.69	8.56	-11.31	702508800	1286	1548	645	739
H41	0.15	0.08	0.16	-0.04	-0.05	-0.08	-0.08	-0.12	0.00	0.15	-0.05	0.07	0.34	-0.40	0.88	0.46	6.84	702507514	261	1931	547
H42	0.07	0.04	0.07	-0.04	-0.06	-0.07	-0.07	-0.09	-0.02	0.11	-0.04	0.07	-0.01	-0.13	-0.33	6.23	13.31	-10.14	702507252	2193	809
H43	0.23	0.15	0.31	-0.02	-0.02	-0.10	-0.25	-0.33	-0.24	0.41	0.24	0.41	-0.55	0.26	-0.28	-0.49	0.14	7.37	11.10	702509445	1384
H44	0.09	0.06	0.13	-0.03	-0.03	-0.07	-0.15	-0.19	-0.14	0.52	0.35	0.09	0.16	-0.26	0.14	0.47	-0.31	0.51	9.19	-8.01	702508061

Table S7: For molecule 1: ratio analysis, $\Delta\omega_0/J \geq 10$ (Data from **Table S3**).

	Te2	Te3	P4	Si5	F6	F7	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	H19	H20	H21	H22	H23
Hg	29310	18947	-954054	102521625	-204150	-222502	-3208381				-2093433	-13437359									
Te2		6073	35344100	2148306	8917308	12762856	235997	-6085068	-1968591	26627853	280189						-30419886	506133807			
Te3			43897		5266997	4369172						1358546	429106449	-47881948	48233590	-14456782					
P4												5172500	18571555	20264192		37933373					
Si5					3430227374	43452506571	-1076875	-892397	-886886	-986484	-15413678						174752289	122365025	123410683	83475725	153080245
F6						19045	-4248854868	-19374796618	-3104934142	-9314804826	31475138	6458214907	-706064548	40757714	-447656440	135561330	33480679	22656775			
F7							93858743	481995456	85568847	1150606577	-3363933496	15424348	-6458610641	-17300007002	1086098174	139635673	19056112	17452226			
C9								94	101	148	372	-16602	101943	-530772	-5187222	1764871	4251611	3876607	2782280537	2247229530	65193523
C10									54	19	9612	345217	-3211785	-2618701	2823836	1547468	-2111857336	318121277	4663044	4490587	4686106
C11										37	-14558	257725	-787177	-458924	-909740	1299368	162903435	-1954848632	99442378	2616179011	5535276055
C12											-31954	-1244300	-870079	-574768	-797597	-1317188	384114253	128288462	6741684838	97905810	-6260135118
C13												-227970	-1770890	132498	-6637658	570822	225204911	525855461	-9560954034	-7303516116	3459555292
C14													20925	6372	-57821	11408	18132713078	8481462480	18132678775	6829199649	14212097758
C15														166	265846	96	-16432588791	-43820402982	-47803804229	-105168507000	-35056118605
C16															17	53965	-43820603271	35056615582	-131461561119		-47804197912
C17																136	105169365797	12229042406	65730729276	27676132773	525845766763
C18																	52584319185	6114478911	27675905109	13146072139	47803829966
H19																		-259	3168	1035	-4763
H20																			8258	3953	4899
H21																				-59	-6
H22																					-66
H23																					
H24																					
H25																					
H26																					
H27																					
H28																					
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H37																					
H38																					
H39																					
H40																					
H41																					
H42																					
H43																					
H44																					

cont. **Table S7:** For molecule 1: ratio analysis, $\Delta\omega_0/J \geq 10$ (Data from **Table S3**).

	H24	H25	H26	H27	H28	H29	H30	H31	H32	H33	H34	H35	H36	H37	H38	H39	H40	H41	H42	H43	H44
Hg																					
Te2							-28254202	-5319433	548988726												
Te3										135650885	-339172185	23583751	-8715595	206066638	146454026	-1889482263	2473866615	377006256	10907468584	-266184495	-210865293
P4										-22140325	3799644285	-38600070	989934	45233921	18936303	1034556247	-1177358739	200557194	-1077218677	26801082	1222110046
S15	81399473	131882862	150380982	143407931	122577599	121231130	1737275068	-656799487	1489101625												
F6							78714537	-166596784	-6552812												
F7							35978336	-57405930	50921788	-387728412	-108593592	-307284700	-68123216	45636206	46663614	16566535	-69604418	75423770	25496452	13339149	13556705
C9	1506739964	91261879	4140558344	77719631	2078463352	2368698345	365682904	153220295	873513801	15935042275	-87642034549	65731611181	-4310299126	-20225106377	-8481506579	-105170411953	-87642281371	11951193826	27676430669	6044301251	13838236096
C10	4014142808	1976884996	98881416	-5654317009	101222654	2379418521	23902385303	1460701429	-13483481249	7406434585	17528422258	17528444997	-13838340891	-47804838750	-16963028012	-75121788602	-37561010620	40450229908	65731580395	11188397218	16963013939
C11	4404051	4700010	4751481	4310256497	7303493044	104273509	-10310829165	-2767643818	-3529232077	5155457513	8764207975	18780470024	-10310916954	-15466265795	-7848562375	-15024352314	-8481515475	-22863165199	-32865778370	525854480015	262926621431
C12	90617378	-5842792715	2812039068	4694138	4708472	4686608	-30932494833	-9066421553	-15024448692	-35057119402	-35056840217	-29214071412	-9561034352	-16432911305	-10112573151	-19476016879	-12229164748	-23902405650	-26292628933	-16432956399	-25040636553
C13	-2540356028	-2797087228	9738006670	-25040593898	-4572631986	-14607013420	3976538	4060927	3479983	-5206513322	-5477642268	-8764238998	-3626606509	-105170843248	-105170971670	13146337755	5778627897	12229162297	5155428	30932685837	-262927211041
C14	4533180262	13146190286	21033902911	-175282561496	-26292394552	-43820641311	-7512123990	-6044238129	-6829246381	3915860	4259817	4315973	171511140	-2782272110	-1947592855	771039183	-9560915478	19475895978	-175282948589	4653547539	1669363920
C15	-9737834675	-13837941407	-8089872843	-16432557704	-11950955751	-17528061925	-29213491183	-37560205660	32865383334	-2358059283	638159020	-2873462921	-1741216286	4047255	4099670	237400851	-132956893	62914974	830715652	-11431413780	123815351
C16	-10955155633	-15466063865	-8912646318	-19475786832	-14212066244	-22862880683	58427471028	37560519799	8912720870	-40450124470	2577683482	7512115893	10731667683	-287820465	-288610665	4331598	4055192	-372941668	-193113260	3838317021	87219803
C17	-27676161059	-27676092692	-12520136250	-26292291710	-18132622095	-35056389696	131461707246	-175282288974	12825612708	4737398269	-18780250717	9921654759	1355286872	6573094732	78979907	-428214066	-143049103	4172332	4506011	-183734808	-402024300
C18	58427046998	-47803829455	-13483130394	-26292109854	-15934618291	-32865138020	-52584319185	-18780115350	18132637376	2286293786	1037166436	2401114452	164945944	1898353579	160907155	66562435	718367300	221314690	-149642390	3707131	4062549
H19	-1384	771	-3652	2842	3153	2535	0	-83	32595	1459619	-1873	-17465	-28159	-7649	-7248	-1361	-42872	6025	11893	19403	23886
H20	3636	-18014	13424	1603	-79506	-229078	19364	-2480	1833	5704	34026	9190	-13206	-31920	-3815	41509	3014	5594	13744	360	3981
H21	-8455	-474	46	0	-712	95	99478	-5706	4286827	32371	20446	26686	-41771	-47145	-25121	-57685	-91959	62788	48387	22135	23217
H22	1265	8189	-6506	-2541	225	-3721	-3690	-1275	-97253	12801	2703	6740	-37964	-43996	-17152	-38873	-94206	9629	8596	8989	7466
H23	6532	28	-287	531	-892	2186	-11935	12793	-30664	27903	11936	22247	-49905	-36236	-21526	-27644	-39061	131197	307180	34261	31041
H24		-113	-127	-15921	-6841	528	-590	-356	-6941	7420	108	3117	-18956	-3389	-3616	-1259	-5183	-4323	-1267	19813	8833
H25			-3	385	2151	-283	-5680	-2764	-12077	23177	7277	24571	-37467	-16674	-11825	-10485	-14972	-21351	-21655	-98801	-674427
H26				677	961	-804	-2153	-1855	-7060	29491	9403	89987	-22070	-10198	-7931	-6534	-9110	-10443	-10434	-17642	-25456
H27					-17	-1	-10471	-6111	-21761		-118587	-62267	-33778	-17983	-14823	-12361	-19754	-22832	-19355	-36636	-37504
H28					-17	-17	-14076	-2940	-14469	-75987	-15302	-21301	-24043	-11739	-10430	-7427	-13668	-13546	-10849	-19108	-18163
H29							19671	-6009	-38869	-178747	-23493	-37136	-30338	-19257	-15835	-14673	-24141	-37392	-23001	-52936	-48474
H30								-4	-548	-16587	-727	-5107	-25295	-12493	-17182	1210	17061	6170	18500	-182716	-19499
H31									-362	-10880	-463	-3510	-13252	-15142	61	14	11116	10777	-9183	-17376	-7521
H32										-3748	-9397	-14228	-5153	63561	23754	18047	4050	11120	26046	4072	46732
H33												-323		10340	-30481	255018	71233	19728	26661	3101	4056
H34												-65	3084	-4616	-3298	358	-9198	-10033	-3074	9811	1502
H35												3651	966	-27288	9877	99847	3611	5939	3950	544	
H36														5974	2999	-492628	-57249	8278	100249	-2166	-11858
H37															-83	121	79	-551	-5831	6529	-447
H38																2918	30	1136	-4284	-5339	2851
H39																	-160	809	21	-6822	1194
H40																		177	117	1582	-3981
H41																			-36	252	1173
H42																				176	99
H43																					-161
H44																					

Table S8: For molecule 2: ratio analysis, $\Delta\omega_0/J \geq 10$ (Data from **Table S4**).

	Se2	Se3	P4	Si5	F6	F7	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	H19	H20	H21	H22	H23
Hg	-10103	-5658	-832154	-113404384	-215435	-229604	-2339061				-1778445	-7706960									
Se2		5946	-904910966	-299058	-82214945	-81108452	-504812	-68575545	10638922	5211978	-609930						104962780	685362002			
Se3			-247240		-24348332	-16459986						-4236567	-3850394951	113845341	-181762948	78872322					
P4												3807363	20411473	20228520		35585408					
Si5					3571114972	-1123776156	-1076259	-991961	-881397	-884003	-11777281						162119061	136059693	118875720	121861077	147195694
F6						-184834	-10305406588	-7338754927	-15624449788	-2971522072	29296257	48435438367	-564509049	35146408	-474390149	388722851	29491537	23027838			
F7							107621298	1614690586	187827567	84568339	-1827941004	17776284	-6727751599	-10306425381	1066964081	100832228	23323153	16951662			
C9								916	756	786	408	-425	82234	-112877	-353518	5437413	4278184	3860160	2753130146	2128937806	77811136
C10									36	78	561940	-688308	-823706	-575887	-783311	-1144125	299289936	145544973	4700055	4692336	4695521
C11										48	19012	323613	-1835794	-1767062	2800690	1545200	-1878044772	313755434	101496177	2247228512	-4456368572
C12											-20686	337636	-717940	-454620	-822233	942545	212551613	-2642483725	7848535015	102926527	4780469507
C13												-24301	-568279	50495	-445579	6343295	167201783	483319098	-6573109548	-15934804362	13483296503
C14													18920	8795	-49796	11377	37560641175	16962920881	-23902187819	-32865494507	-87641321965
C15														147	143104	25	-12825447737	-17528164269	-12228895646	-16962654609	-15934615532
C16															13	47262	-29213735278	175282935286	-15024182588	-22862876986	-19475784828
C17																137	-75120990687	20224942526	-18780217513	-32865366905	-26292294508
C18																	-105168652998	8912624336	-15465953546	-29213455592	-23901919106
H19																		-186	4691	3433	2176
H20																			-61931	-97599	1623
H21																				-19	-17
H22																					-2
H23																					
H24																					
H25																					
H26																					
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H44																					

cont. **Table S8:** For molecule 2: ratio analysis, $\Delta\omega_0/J \geq 10$ (Data from **Table S4**).

	H24	H25	H26	H27	H28	H29	H30	H31	H32	H33	H34	H35	H36	H37	H38	H39	H40	H41	H42	H43	H44
Hg																					
Se2							79663995	15065460	565339762												
P4									-479495063	914972221	-133254709	16448660	1706301829	-1186219644	6764258312	-4984205827	-1544016679	-7192377607	279488393	323023689	
S15	123140733	154128218	79111337	132099564	82064068	139429363	1876258212	-456881134	1299954527	-20488860	-178686771	-57135842	932758	57823619	22407775	954219875	-1379373172	181558968	-1007104670	32162409	-1865844985
F6							48588616	-187759146	-7126485	-128877454	-85379919	-233117813	-261002468	37349595	43405963	18001991	-24111770	73312772	20623619	13731567	21411538
F7							25774457	-54461788	55338016	-1734203	-50115224	-78199283	21158776	-436274203	-102085590	986791395	-1151305688	87438140	22910653	-238203700	-238196610
C9	2007051960	65249730	2347537887	104917710	2970896973	4572588353	309687154	110518890	554695817	131463162477	-21033950007	-40449929259	-3783118720	-14212148908	-6829223507	-40449899915	-32865654065	18132728920	87641471945	9921715172	37560690749
C10	7848527300	-5311629196	97778394	16962944513	90213155	7967445093	-52585250299	-30932505672	-21034213985	-27676650815	-29214025876	-29214044219	-9066503753	-16432913287	-10112575493	-20225092864	-12520337634	-23902402466	-25040597488	-15024417706	-21910557753
C11	4672947	4686273	4449212	3093243518	2445826037	99198546		1358792544	-11431640605	8216507558	23902390180	21034116566	-11951303088	-37560953100	-14607056773	-58428059187	-32865893677	43821081038	87642110909	11431624737	20225134780
C12	99536551	4240738410	2528136898	4714635	4413442	4708894	-75121825064	-3039611959	-4653589576	5365884061	9738013671	22863176887	-10955364377	-14212256693	-7406397156	-14607019081	-7848573927	-21910546946	-30932518806	-87642482027	-131463414631
C13	-8481427732	2590386605	-6491967810	-2358064889	-3022124541	10955178467	3997155	4118530	3504329	-4310275047	-5155388785	-7203424469	-3206429317	-29213911972	-25040529329	21910400199	8620514278	29213891364	5155390	-15466229706	-17528352546
C14	22862951632	16432745278	7106064335	15466112893	4737378723	27676207084	-6656317234	-5421125308	-5311635435	3943611	4261406	4331365	118863873	-3039594125	-1919162351	806516830	-8481463534	65731176590	-58427678413	6335556364	1398537087
C15	-37560162022	-29213457204	-47803921959	-13146055478	-8620383919	-7848392767	-18780122937	-21033741427	-175282096291	-2434478263	619367968	-2889251292	-2014743896	4061325	4074043	236866376	-131395582	62869894	829406130	-131461389736	135947344
C16	-75120878012	-40449700573	-131461754832	-14606836025	-9560859942	-8764103219	-262923660006			12520242063	-26292559126	2655794357	7106048824	6492000428	-278816565	-292300580	4334739	4039958	-390674347	-186669281	6573117959
C17	87640974315		32865419946	-25040276034	-21033879865	-11951043022	-52584701982	-30932183133	25040469832	5258508823	-17528232753	9066332979	1311350959	4140533402	76309453	-426132035	-147090545	4180725	4505394	-200323481	-361656054
C18	32865136005	58426904159	13146076233	-40449394377	525843326813	-11685382736	-17528111667	-11188158371	-262923098321	2337098722	970190614	2337082858	181514693	4108156814	150284302	65977825	696483480	219834323	-150112302	3727656	4073375
H19	4818	-3970	852	1301	-234	-3708	223	-536	19808	-50609	-332	-3818	-33331	-6727	-6916	-72	-29875	10907	-6463	84682	-46099
H20	8036	4505	3517	-14036	4745	27216	9005	-1758	1814	9507	-29290	47716	-12712	-8678	-279	98398	2701	5562	18020	1520	3791
H21	-752	-825	300	3496	-5120	745	84495	-5812	-22344	-60658	-13317	-14728	-26498	-13320	-11939	-8326	-15800	-15247	-11592	-19910	-18495
H22	251	3328	-4375	-277	493	-99	17682	-10714	-66600	-98271	-17377	-24446	-32044	-20124	-16701	-15833	-26924	-36600	-23872	-48030	-38347
H23	1526	761	-2820	516	-9377	22	-17379	-13295	-27050	-356583	-57496	-37437	-35420	-19290	-15952	-12854	-21267	-22784	-19245	-35675	-34702
H24		-3	-76	-203	-7723	21	-293481	-7921	446730	36233	35522	31210	-37991	-40343	-23605	-49337	-83869	34663	81212	25119	31646
H25			-80	66	7528	-431	-12126	9969	-29847	29000	13992	21204	-44903	-34549	-21081	-26141	-38536	156383	-628411	37833	40301
H26				12465	725	-4515	-3165	-1499	-61712	12281	1756	4011	-30581	-26918	-13898	-12480	-61822	8252	7665	9020	7998
H27					-104	-8	-11875	-4220	-13171	24333	7700	24064	-38063	-17369	-12659	-10704	-15267	-20715	-20776	-72605	-123893
H28						-104	-75	-259	-6643	7501	41	1776	-19417	-4411	-4203	-401	-5434	-4566	-992	34515	19282
H29							-3139	-2892	-8227	33262	9005	473270	-22998	-10104	-8119	-6002	-8960	-9536	-9369	-15669	-20302
H30								-10	-462	-12623	-137	-1480	-28063	-8301	-12590	44259	39944	19515	-1383	-18568	-8743
H31									-281	-8357	-385	-753	-13091	-8613	71	415	18860	-15166	-946	-8395	-4618
H32										-2540	-7629	-10867	-6441	-124967	94935	23671	3542	15404	51896	8488	-49089
H33												-326	73	9318	-18073	-493877	-312123	20654	28709	2754	3781
H34																					
H35												-31	3528	-4494	-3772	123	-9422	-7471	-3018	11218	2125
H36													8603	3066	-24558	4541	-81452	678	2438	4916	4647
H37														5260	3250	-177896	-34512	9284	1167602	-3593	-30170
H38															-94	142	82	-839	-5603	3874	-397
H39																3740	28	1423	-4376	-3752	3014
H40																	-171	797	23	-6092	1404
H41																		203	126	1608	-3645
H42																			-32	263	1449
H43																				180	101
H44																					-160

Table S9: For molecule 3: ratio analysis, $\Delta\omega_0/J \geq 10$ (Data from **Table S5**).

	Te2	Te3	P4	Si5	F6	F7	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	H19	H20	H21	H22	H23	
Hg	-138723	-75863	2125154	-8145210711	644468	643749	3197723				2333989	8013082										
Te2		3134	37941619	1972645	29629757	40399903	235308	45642766	-6132736	-2412452	280987						-39509638	139896789				
Te3			41204		14566665	5015479						1370514	203027633	-45121624	62263804	-14763450						
P4												4801596	15855527	23241158		36706896						
Si5					4137898307	771319382	-1097314	-961055	-917568	-894727	-15050098						146735431	139672095	123899710	118400529	140158396	
F6						-4032	-2162280035	-15624210877	-13454178207	-3535405151	39821750	24217345426	-684097255	33607085	-580053934	-2018089232	54751881	38643721				
F7							642423665	922642386	6545772041	61878797	-2484044412	22814923	-60547196544	-15625226422	1537719844	53245920	66132711	22021583				
C9								50	66	47	411	-16751	308471	-678042	-5692551	2328048	4243519	3953047	1891553677	2434498400	77570683	
C10									35	10	-23458	-1814326	-968041	-654211	-785986	-1824309	475884582	125562057	4675775	4685564	4701693	
C11										25	12960	500988	-3186224	-2555976	2690083	1799961	-2368704239	375878322	98216588	2062162126	-6919096653	
C12											-15813	276708	-1206120	-650280	-1823485	363604	145383586	-1515428998	11685593335	107558076	4780467599	
C13												-251808	-1847985	118593	-2303135	-1504150	210678634	656498504	-4076380923	-15024367753	-10731691324	
C14													25007		9278	-56765	9862	-175282944734	15934856523	-30932241345	-37560559658	-175282612907
C15														169	48029	148	-18132509739	-47804019408	-13146051278	-18780063695	-18780063820	
C16																11	25578	-47804293560	40449896940	-15024185652	-23902101371	-21910259737
C17																	135		16432762250	-18780222486	-32865372622	-29213664748
C18																		262921670655	9225346883	-17528086999	-30931902489	-29213463657
H19																			-178	3339	2622	4114
H20																				-12948	-34226	1261
H21																					-23	-22
H22																						0
H23																						
H24																						
H25																						
H26																						
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H44																						

cont. **Table S9:** For molecule 3: ratio analysis, $\Delta\omega_0/J \geq 10$ (Data from **Table S5**).

	H24	H25	H26	H27	H28	H29	H30	H31	H32	H33	H34	H35	H36	H37	H38	H39	H40	H41	H42	H43	H44
Hg																					
Te2							-38504623	-5193966	121634292												
Te3										133656924	-273014069	23073863	-10577694	190535638	150128260	-2095888855	4102225597	428152603	-14116433105	-563996192	-213790422
P4										-23134181	-7463606594	-38711000	975526	39893339	19725484	1471696424	-1085619822	282406963	21997998013	26975861	376543004
S15	121335665	146735170	95939406	126262010	84137149	144364192	1700535259	-682275317	1497020850												
F6							49702975	-145111714	-11287640	-139279879	-105335332	-186949643	-402973496	25368374	38358072	34613792	-14572958	76856401	22543245	27323336	55783449
F7							56415331	-65196910	127593653	-2620123	-109696840	-198402417	175718451	2764396282	-165206049	499580971	1011391892	55067385	16415439	230374623	230367614
C9	2480432495	66428961	3459552878	87788244	894307936	-7512164656	353633296	141815717	862058001	16963101023	-65731606101	525853548523	-5842855533	-23902426711	-10517083237	-262926332020	-262927255493	13483414990	35056856119	9066463372	22863200603
C10	7621036207	-87641910760	97056450	-2181955973	91739860	1493895839	-26292626058	-6919111677	-27676588951	-37561138648	-37560904154	-37560954134	-10731771577	-18132868862	-11431608069	-21034089936	-13146358008	-23902408817	-27676455323	-18132920171	-25040639201
C11	4660357	4679475	4556458	1231501798	-14212236600	95958251	47804763584	1334650674	-11431631920	13146395483	37560895459	30932543302	-14212342853	-52585307526	-21034153978	-105170470331	-52585419860	37560919445	87642088232	15024416092	26292665074
C12	100410820	25040544434	2577704977	4702575	4402542	4742355	-13483397172	-2873510688	-3983751202	5056306823	9390225477	15934949286	-11951290360	-22863181111	-10731713056	-21910518414	-12520340212	-65731620314	-175284206561	16963053339	40450260905
C13	-9225489575	3370851744	-7512189346	-2738816650	-2842455586	8620536767	3960817	4079676	3505711	-5778652182	-6335591153	-9066461472	-4494514656	-131463651124	-131463844671	18780495746	7848592953	22863234846	5155432	-18780574730	-23902492305
C14	37560562117	21910326496	11431483002	12825555140	4653533162	14606880740	-8481433750	-7203409025	-7733111197	3930871	4248461	4314912	140527306	-3783090420	-2337112633	804050221	-9921711164	47804487756	525849022480	2857886176	1912181071
C15	-52584181787	-40449368012	-131460541582	-19475618851	-15934642289	-11188120317	-27675938987	-32865175439	75120787094	-2316503351	617186594	-3004821014	-1163378599	4033563	4098105	255635777	-140449957	64056927	944062784	3529161104	151409082
C16	-131461566148	-58427358986	262923306523	-21910256488	-18780272938	-12228979107	87641214579	87641208959	11431520791	-30932394552	3286546403	7848479465	3601723107	-304134160	-300141973	4342471	4039524	-374535442	-183605942	26292472563	102047000
C17	105169199276	525845962658	32865396552	-4780471590	-262923687019	-19475771607	-105169403852	-47804271413	22863029920	5056254223	-22862919837	9390140285	970205360	1976871034	71262836	-428912701	-157392642	4190354	4500228	-210423843	-352681369
C18	404494113595	58426927002	15934628036	175280755949	15934659224	-29213456320	-22862756505	-15024096169	525846068524	2256853303	959568497	2669260083	170122189	35056271697	131889854	64473192	692813174	218828078	-154432755	3790588	4074417
H19	3052	-4212	2388	698	-3656	-2876	115	-49	52446	-96617	-1759	-13359	-21089	-8343	-9197	-390	-53071	8430	94139	49380	960356
H20	8465	5363	4292	-10264	2367	11901	21790	-1684	1800	8222	176535	8934	-12139	-21778	-639	28990	4100	4054	12066	2185	2942
H21	-802	-971	52	2759	-5086	1371	-9290	-2470	-11157	-76537	-18533	-23570	-25128	-12315	-11977	-6933	-15051	-15029	-10948	-22041	-19008
H22	287	37	-2026	-199	634	-1037	28576	-5816	-28229	-95260	-21327	-34437	-31066	-20153	-18169	-15068	-27205	-34002	-24230	-47369	-37680
H23	997	23	-1265	523	-11546	1065	-9941	-5514	-18897	-1491233	-132309	-67518	-35838	-20112	-17884	-13065	-23385	-24622	-21523	-45318	-39915
H24		-3	-30	-1027	-5489	69	170480	-5588	-246119	49364	72492	61986	-39917	-48535	-30911	-65007	-134384	34783	76857	33544	40956
H25			-33	447	9047	-552	-11611	9471	-26802	35812	19567	35061	-47703	-41248	-26953	-32543	-54919	89965	395523	41287	45550
H26				9731	3196	-3706	-8326	-2615	-98333	17423	7728	13864	-38454	-79427	-29506	626655	2473602	13657	17115	13325	13590
H27					-127	-4	-6542	-2936	-12027	19964	7736	22118	-41999	-22595	-16136	-14078	-22204	-43367	-40701	73235	92446
H28						-140	-985	-814	-6887	6522	694	2459	-19657	-3344	-4978	-4574	-8701	19671	-44962	7506	5067
H29							-2358	-1949	-6871	20025	7874	32622	-26563	-13893	-10892	-8622	-13035	-17278	-17089	-93046	-83517
H30								-4	-468	-13902	-578	-4951	-17638	-11079	-19079	2275	29986	14775	-8665	-21424	-11276
H31									-290	-10726	-628	-4125	-14257	-14782	70	49	19294	-101305	-5115	-11566	-7368
H32										-2877	-9108	-10652	-5735	132872	20659	19267	2581	13556	37895	12952	-110429
H33											-254	-241	70	10434	-14172	1155893	54024	16745	24924	2430	3856
H34												-66	3498	-4854	-3446	477	-10135	-9076	-370	8516	1747
H35													3047	2089	-9435	11196	-137495	4332	7599	3973	484
H36														5172	3056	-105705	-27329	9101	134070	-2023	-11589
H37															-97	130	95	-506	-4626	7710	-586
H38																3508	39	1150	-4357	-3063	4315
H39																	-167	1001	29	-5108	1583
H40																			196	128	1673
H41																				-34	237
H42																					181
H43																					-151
H44																					

Table S10: For molecule 4: ratio analysis, $\Delta\omega_0/J \geq 10$ (Data from Table S6).

	Se2	Se3	P4	Si5	F6	F7	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	H19	H20	H21	H22	H23	
Hg	204682	92454	2529433	26184933	745010	730280	3069628				2161161	6036481										
Se2		6631	1615314506	-350265	-126025949	116090139	-521383	9383735	-160912963	5393862	-612995						107061045	206009543				
Se3			-227580		-114027875	-20210002						-4599913	6051672030	94972899	-176491881	264760536						
P4												3626910	15956057	21935078		28680191						
Si5					4533627271	1018370424	-1125863	-949465	-879700	-941727	-10993971						147581976	143116963	117879879	117265948	142572561	
F6						-5331	142957093	-484341796417	-4363444434	2295460667	109653485	-10305079944	-587070365	39974979	-1337946696	-2446126614	152053194	114991351				
F7							-1567563597	790179963	50837621	-80730120260	8969962276	24938335	21059633569	-9885211496	3008541770	48543956	-360626096	-2764890458				
C9								609	957	923	321	-251	-464956	-178826	120413	-1853698	4240753	3957840	4572590587	1838629534	65788560	
C10									171	121	18686	-1013014	-1457533	-1651331	-1697447	-2181706	263321141	-1832242767	4666724	4659530	4683766	
C11										37	125656	77712	-9280919	2744856	1407015	712503	169849113	417676100	111409241	11685594405	4345881532	
C12											-15498	-1721653	-914946	-669782	-916101	-1826217	-1417392783	161008597	1648437265	94953344	-52585153388	
C13												-28528	-912975	324952	-342246	-398278	269528428	193612415	-9560885980	-10310761924	3245980094	
C14													25703	18413	-73332	8451	-9225425952	-8481461857	-22862958444	-26292408673	-37560577898	
C15														145	39278	5	-15465987444	-43820410748	-23901924457	-43820205609	-30931904966	
C16																6	28582	-43820613692	18132714489	-37560437804	-262923129260	-52584617562
C17																	136	-29213734775	58427620203	-40449691608	-262923060086	-87641006212
C18																		-15024102613	-43820412279	-30931903319	-87640414281	-65730300349
H19																			4541	6826	1923	
H20																			-154	8873	-10471	
H21																					-4	
H22																				-11	-7	
H23																						
H24																						
H25																						
H26																						
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H40																						
H41																						
H42																						
H43																						
H44																						

cont. **Table S10:** For molecule 4: ratio analysis, $\Delta\omega_0/J \geq 10$ (Data from **Table S6**).

	H24	H25	H26	H27	H28	H29	H30	H31	H32	H33	H34	H35	H36	H37	H38	H39	H40	H41	H42	H43	H44
Hg																					
Se2							78466102	16368674	315827923												
Se3										-475090385	759632534	-134454685	19872339	3228442409	-887823070	6313389972	-5516570912	-1759150209	-19593284698	372839533	304178836
P4										-21282795	-174290481	-58169650	924904	62231879	25628538	1007104902	-1314308934	257834025	6965811554	38691991	-1397824421
S15	105823736	125951283	119026897	124392595	124145702	121940307	1425006936	-370558086	1863838171												
F6							200534316	118263807	135218214	-85068331	-94772557	-173685112	141689525	33557889	50501228	62894458	-33667517	65166032	17296042	85593182	170128317
F7							30742834	-51582183	-80374943	-3290347	-290013001	-264154273	44598398	-217133967	-129200898	609879723	638054271	57600335	17417883	73535767	73533313
C9	1421210671	76754894	-4108200714	99179175	-14606891886	1613030532	507087015	109052100	315447284	-8912745356	-8346809693	-11431508097	-6044294959	-21033989567	-13838174732	75121281817	20225026121	47804490257	-525849131488	-20225050926	-23902270004
C10	5908439485	2528129543	81150132	2103404608	92173755	8912730832	-15934921206	1314630982	105170757596	-21910630906	-19476006533	-19476019933	-10731771982	-29214050272	-18780493055	-52585213844	-40450295760	-105170511711	-58428033024	-35056965987	-40450238910
C11	4692339	4770623	4381272	-5421151421	1999436537	100737865	-22863171109	-16962997693	-13483444197	12825748231	525852712101	40450236454	-9921837035	-105170688125	-26292717063	52585267416	22863233939	14607030397	29214046274	7512214650	20225140059
C12	91755631	-5258513491	2401156445	4685857	4638899	4641231	-5975600046	-3370851263	75122027463	65731943252	-175284193548	-65731617806	-9738096877	-17528443639	-10731718568	-20225097796	-12825713394	-29214053490	-30932511852	-35056992938	-40450270007
C13	-10731607343	10955178968	-3895188909	-2266589645	22862996489	-4206790118	3948713	4102690	3638254	-4869007291	-7106078676	-8216409122	-7303534344	-65731318816	87641908528	105169956814	27676394237	-21910425174	5155392	-5778594895	-10310799048
C14	-525848075116	29213772545	10516996362	525848113052	65731029324	-35056538669	-7512133725	-6829212386	-5778579659	3941358	4266178	4350826	93634934	-5535261746	-2209457002	895824701	-9225452734	-52584951951	-87641543029	4737400457	1276335114
C15	175280789653	-75120314236	-40449547072	-18780085961	-11950966555	-13483137792	-21910152274	-23901983980	525845042782	-2528107676	591499923	-3148765227	-1102406880	4059005	4063247	287503222	-138453159	65249263	1019076651	1664068812	182584847
C16	26292308008	175281996952	87641317190	-23902099914	-15024180561	-16432692659	-43820620483	-32865464923	21033953360	-21910424490	3349345366	6656298534	2030316112	-320638994	-288769276	4337957	4060452	-384672717	-177651129	65731191977	112025597
C17	20224846993	47804168410	27676198147	-37560432840	-25040294347	-21033841069	-21033892298	-15934766679	-75121242234	6260119636	-32865442753	6573093073	937347121	1387461247	67895250	-425098663	-185812280	4209844	4487478	-212980720	-327019909
C18	18132496115	22862705132	7512059004	-52584242527	-37560181915	-20224707394	-10955076520	-8764061099	-12825489297	2492163104	812741035	2054077388	217832684	-3130024870	118620591	64942993	737510685	216842817	-153575809	3816727	4074639
H19	-10751	1062	-1784	-3481	16849	8949	129	-120	5763	-12276	-669	-1293	-30059	-5986	-11017	-7194	-76330	-8285	-398	-14193	-7159
H20	5954	10378	2837	2057	-7040	-13103	4939	-4229	158	-6409	-6089	-6969	-9853	-23311	-3754	17255	759	10142	44418	-54376	-13532
H21	-111	-612	693	-6885	-966	267	69291	-8134	-65969	-45601	-11882	-19144	-33787	-27601	-28065	-27056	-51141	-38824	-31947	-46665	-36117
H22	660	12746	-6230	-253	26	-289	169610	-9442	88809	-56946	-10710	-21732	-34028	-44537	-43217	-925932	219364	67302	-216941	-297936	-82318
H23	351	1192	-7961	229	-449	245	-14943	7944	-34082	-102875	-16615	-31302	-37732	-34140	-31115	-34787	-71455	-285788	-61453	-186677	-79048
H24		-15	-142	-131	-810	2	-10452	-5919	243075	50345	-24141	129457	-27076	447686	-96121	16521	18833	9441	15987	14936	23159
H25			-152	1312	2910	-530	-9635	-9783	-19210	37472	153941	48283	-34602	-78402	-39732	170514	93550	19679	38639	23019	34301
H26				11923	5027	-7623	-1822	-1191	-4585	7346	13893	3938	-14078	-1165	-6974	42276	16463	1878	7999	5216	1898
H27					-10	-3	-6465	-4699	-23747	107829	-256072	-99006	-33580	-21118	-18556	-14295	-24705	-40185	-27930	-185428	-75143
H28						-14	-3190	-2770	-6349	38681	27356	-632275	-23835	-13155	-11509	-8159	-24244	-160809	-55521		
H29							-9148	-4717	-11120	-125709	-22985	-23652	-27709	-15804	-14925	-10509	-17473	-18221	-16139	-33374	-27216
H30								-1	-208	-9110	-993	-699	-15373	-7653	-36045	-15373	-72255	-1936	-1425	-8294	-4676
H31									-149	-8381	-957	-643	-14781	-8129	87	613	-41489	-1348	-1027	-6279	-3793
H32										-3376	-5182	-5019	-9772	294359	138	17930	274	-307356	-82820	-2900	-4873
H33											-230	-236	150	10076	-8049	-115512	-117897	16884	26835	1590	3930
H34												-33	3869	-4700	-4177	99	-9534	-7211	-3452	9803	2671
H35													8476	5093	-13341	4491	-50258	287	3394	4725	6307
H36														4164	3522	-130241	-21610	12555	-377492	-4257	22830
H37															-115	143	80	-862	-4639	6026	-785
H38																4364	5	1420	-4627	-2444	5107
H39																	-151	909	26	-4789	2071
H40																		188	116	4707	-2407
H41																			-26	262	1071
H42																				197	88
H43																					-173
H44																					