

SUPPORTING INFORMATION FOR

**High Performance Single-Molecule Magnets,
Orbach or Raman Relaxation Suppression?**

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CASSCF g-VALUES AND g-VECTORS

Table S1. CASSCF+QDPT g-values and g-vectors for the eight Kramers' doublets corresponding to the ${}^6\text{H}_{15/2}$ ground multiplet for all calculated molecules.

Molecule	KD	E (cm ⁻¹)		gx	gy	gz	
1	1	0.0	g-values		0.000001	0.000001	19.887923
			g-vectors	X	0.789588	0.536789	0.297335
				Y	0.613638	-0.690705	-0.382592
			Z	0.000000	0.484546	-0.874766	
	2	554.9	g-values		0.000056	0.000062	16.962891
			g-vectors	X	0.849545	0.444755	-0.283665
				Y	-0.324623	0.864635	0.383441
			Z	0.415805	-0.233666	0.878924	
	3	835.0	g-values		0.004565	0.004851	14.391656
			g-vectors	X	0.620005	0.734743	0.275219
				Y	0.771441	-0.506905	-0.384612
			Z	-0.143081	0.450777	-0.881095	
	4	1002.7	g-values		0.003224	0.011944	11.777382
			g-vectors	X	0.803891	0.504601	-0.314862
				Y	-0.374783	0.840810	0.390611
			Z	0.461842	-0.196004	0.865035	
	5	1164.6	g-values		0.168207	0.191341	9.072690
			g-vectors	X	0.662391	0.671127	-0.332906
				Y	-0.555406	0.738145	0.382970
			Z	0.502755	-0.068778	0.861689	
	6	1333.7	g-values		0.753501	1.142417	6.323126
			g-vectors	X	0.927252	0.167798	-0.334736
				Y	-0.033292	0.927372	0.372656
			Z	0.372956	-0.334401	0.865494	
	7	1478.5	g-values		3.330960	5.168677	6.159056
			g-vectors	X	-0.288025	0.776481	-0.560464
				Y	0.378024	0.629926	0.678448
			Z	0.879852	-0.016459	-0.474963	
	8	1588.6	g-values		0.863738	4.340274	15.723468
			g-vectors	X	-0.301173	0.629140	-0.716573
				Y	0.384375	0.767806	0.512571
			Z	0.872669	-0.121060	-0.473068	
3	1	0.0	g-values		0.000002	0.000002	19.888309
			g-vectors	X	-0.290393	0.739193	0.607673
				Y	0.191682	-0.577232	0.793764

			Z	0.937512	0.346984	0.025934
2	567.5	g-values		0.000191	0.000196	16.957858
		g-vectors	X	-0.159935	0.787234	0.595552
			Y	0.059126	-0.594596	0.801848
			Z	0.985355	0.163456	0.048551
3	868.1	g-values		0.003331	0.003556	14.371674
		g-vectors	X	0.802841	-0.051453	-0.593969
			Y	-0.595748	-0.030714	-0.802584
			Z	0.023053	0.998203	-0.055311
4	1056.6	g-values		0.010477	0.017071	11.762507
		g-vectors	X	0.717004	0.321980	-0.618251
			Y	-0.569117	-0.241741	-0.785918
			Z	-0.402506	0.915364	0.009915
5	1234.7	g-values		0.393699	0.426134	9.075076
		g-vectors	X	0.564477	0.518559	0.642232
			Y	-0.435034	-0.474326	0.765350
			Z	0.701507	-0.711415	-0.042155
6	1416.3	g-values		0.048478	0.889233	6.347958
		g-vectors	X	0.080274	0.752726	0.653421
			Y	-0.012568	-0.654720	0.755767
			Z	0.996694	-0.068880	-0.043097
7	1569.0	g-values		3.382820	5.264047	5.444159
		g-vectors	X	-0.582848	0.454983	0.673260
			Y	-0.808908	-0.246185	-0.533911
			Z	-0.077174	-0.855794	0.511527
8	1680.8	g-values		0.909184	4.731612	15.435581
		g-vectors	X	0.614496	0.744239	-0.261731
			Y	0.788799	-0.573798	0.220345
			Z	0.013809	-0.341854	-0.939652
5a	1	0.0	g-values	0.000003	0.000005	19.864176
			g-vectors	X	-0.974758	-0.186804
				Y	-0.222660	0.853621
				Z	0.016408	0.486247
						-0.873667
2	452.9	g-values		0.000071	0.000078	17.007812
		g-vectors	X	0.976305	0.166608	-0.138099
			Y	0.212108	-0.863237	0.458074
			Z	-0.042893	-0.476512	-0.878121
3	742.1	g-values		0.001174	0.001298	14.383616
		g-vectors	X	-0.183213	0.972574	0.143290
			Y	-0.884396	-0.099415	-0.456027
			Z	-0.429275	-0.210275	0.878355

4	942.0	g-values		0.035959	0.040509	11.742249	
		g-vectors	X	-0.473969	0.875664	0.092554	
			Y	-0.794490	-0.379962	-0.473724	
			Z	-0.379656	-0.298063	0.875797	
5	1111.2	g-values		0.615072	0.694564	9.048552	
		g-vectors	X	0.972068	0.224394	0.068790	
			Y	-0.161632	0.852554	-0.497018	
			Z	-0.170175	0.472016	0.865009	
6	1254.9	g-values		0.152029	1.563730	6.217820	
		g-vectors	X	0.830753	0.551623	-0.074575	
			Y	0.502521	-0.685599	0.526712	
			Z	0.239418	-0.475043	-0.846766	
7	1349.3	g-values		2.603855	8.389052	8.978059	
		g-vectors	X	0.118021	0.824092	-0.554025	
			Y	-0.471943	0.537435	0.698881	
			Z	0.873694	0.178986	0.452353	
8	1482.2	g-values		0.241799	0.735500	18.215197	
		g-vectors	X	0.116691	0.345681	0.931068	
			Y	-0.479284	-0.801487	0.357640	
			Z	0.869868	-0.487979	0.072153	
5b	1	0.0	g-values		0.000008	0.000009	19.862022
			g-vectors	X	-0.868340	-0.493351	-0.050903
				Y	0.453144	-0.747451	-0.485774
				Z	0.201610	-0.444884	0.872601
2	439.1	g-values		0.000270	0.000291	17.022831	
		g-vectors	X	0.254674	0.966992	-0.008261	
			Y	-0.838035	0.216432	-0.500855	
			Z	-0.482534	0.134478	0.865492	
3	730.2	g-values		0.009214	0.010431	14.334595	
		g-vectors	X	-0.098347	0.995149	0.002439	
			Y	-0.858579	-0.083611	-0.505818	
			Z	-0.503160	-0.051840	0.862637	
4	939.3	g-values		0.134420	0.143446	11.684571	
		g-vectors	X	0.990895	0.039975	0.128564	
			Y	-0.026028	-0.880014	0.474235	
			Z	0.132095	-0.473263	-0.870961	
5	1116.4	g-values		0.797073	1.099230	9.004690	
		g-vectors	X	0.981254	-0.046323	0.187067	
			Y	-0.128964	-0.879143	0.458776	
			Z	0.143206	-0.474301	-0.868637	
6	1255.5	g-values		3.467982	5.515909	5.750712	
		g-vectors	X	0.961007	0.226315	-0.158892	

				Y	-0.164995	0.930407	0.327291
				Z	0.221905	-0.288313	0.931469
	7	1352.9	g-values		1.854668	4.846297	11.861981
			g-vectors	X	-0.076234	0.715263	-0.694686
				Y	-0.503295	0.573839	0.646068
				Z	0.860746	0.398884	0.316242
	8	1503.6	g-values		0.088300	0.190309	18.427845
			g-vectors	X	-0.122687	0.636091	-0.761798
				Y	-0.525264	0.609656	0.593648
				Z	0.842049	0.472978	0.259318
6	1	0.0	g-values		0.000002	0.000003	19.876809
			g-vectors	X	0.501577	0.478567	0.720690
				Y	0.814925	-0.540985	-0.207925
				Z	0.290376	0.691598	-0.661342
	2	564.5	g-values		0.000384	0.000411	16.943151
			g-vectors	X	0.472161	0.512936	0.716910
				Y	0.848790	-0.484073	-0.212672
				Z	0.237950	0.708922	-0.663935
	3	946.3	g-values		0.045788	0.046104	14.251066
			g-vectors	X	0.393466	0.588916	-0.705948
				Y	-0.662937	0.713767	0.225945
				Z	0.636945	0.379098	0.671257
	4	1151.3	g-values		0.051343	0.544391	11.014433
			g-vectors	X	0.716404	-0.135650	-0.684371
				Y	0.415687	0.870790	0.262544
				Z	0.560330	-0.472572	0.680225
	5	1180.8	g-values		0.482729	1.140047	16.340079
			g-vectors	X	0.749743	0.365842	-0.551402
				Y	-0.228859	-0.638498	-0.734809
				Z	-0.620894	0.677111	-0.394983
	6	1208.7	g-values		2.922972	5.232123	9.987416
			g-vectors	X	0.812811	0.120522	0.569924
				Y	0.064497	0.953729	-0.293669
				Z	-0.578947	0.275455	0.767428
	7	1227.3	g-values		0.627393	6.466121	9.977723
			g-vectors	X	0.903670	-0.149790	0.401179
				Y	0.372475	0.737173	-0.563771
				Z	-0.211291	0.658892	0.721954
	8	1243.6	g-values		1.266472	8.848429	10.956542
			g-vectors	X	-0.310862	0.935155	-0.169853
				Y	0.515056	0.315938	0.796806

				Z	0.798800	0.160213	-0.579870
7	1	0.0	g-values		0.000002	0.000002	19.874402
			g-vectors	X	0.329538	0.002092	0.944140
				Y	0.943352	0.040184	-0.329352
				Z	-0.038628	0.999190	0.011269
	2	464.3	g-values		0.000086	0.000090	17.014156
g-vectors			X	0.324460	-0.154861	0.933137	
			Y	0.853798	-0.376660	-0.359382	
			Z	0.407130	0.913316	0.010009	
	3	731.3	g-values		0.002174	0.002546	14.387818
g-vectors			X	0.006499	0.374153	-0.927344	
			Y	0.043416	0.926384	0.374070	
			Z	0.999036	-0.042692	-0.010224	
	4	906.2	g-values		0.019770	0.022624	11.750820
g-vectors			X	0.257886	-0.079279	0.962917	
			Y	0.934428	-0.232916	-0.269433	
			Z	0.245640	0.969260	0.014015	
	5	1063.2	g-values		0.065178	0.102958	9.099082
g-vectors			X	0.247226	0.037922	0.968216	
			Y	0.943833	0.216650	-0.249485	
			Z	-0.219225	0.975513	0.017769	
	6	1210.9	g-values		1.070477	1.183905	6.437814
g-vectors			X	-0.184651	0.202990	-0.961613	
			Y	-0.587835	0.761315	0.273585	
			Z	0.787626	0.615787	-0.021253	
	7	1327.5	g-values		1.985630	3.703077	4.779321
g-vectors			X	-0.212913	0.977059	-0.004911	
			Y	-0.976607	-0.212654	0.031902	
			Z	0.030126	0.011589	0.999479	
	8	1397.6	g-values		-0.867606	4.934478	11.588115
g-vectors			X	0.947805	-0.034333	-0.316996	
			Y	-0.318581	-0.061172	-0.945920	
			Z	0.013085	0.997537	-0.068917	
8	1	0.0	g-values		0.000003	0.000003	19.492969
			g-vectors	X	-0.372232	-0.915534	0.152452
				Y	0.533260	-0.345398	-0.772226
				Z	0.759656	-0.206151	0.616786
	2	385.8	g-values		0.000176	0.000180	16.759559
g-vectors			X	0.771871	0.609789	0.179926	
			Y	-0.242849	0.544322	-0.802956	
			Z	-0.587571	0.576083	0.568233	

3	624.6	g-values		0.001068	0.001315	14.160659	
		g-vectors	X	0.868683	0.458353	-0.187886	
			Y	0.400963	-0.427870	0.810035	
			Z	0.290891	-0.778999	-0.555466	
4	797.6	g-values		0.024135	0.025988	11.560561	
		g-vectors	X	-0.405565	0.901252	-0.152520	
			Y	0.525582	0.366445	0.767777	
			Z	0.747851	0.231221	-0.622299	
5	935.9	g-values		0.430897	0.455511	8.993341	
		g-vectors	X	0.205107	0.972465	-0.110651	
			Y	0.701314	-0.067167	0.709682	
			Z	0.682708	-0.223162	-0.695779	
6	1048.6	g-values		0.603221	1.430876	6.268526	
		g-vectors	X	0.164336	0.981841	-0.094775	
			Y	0.727685	-0.055806	0.683638	
			Z	0.665935	-0.181312	-0.723641	
7	1127.0	g-values		2.880222	6.791163	8.518121	
		g-vectors	X	-0.172818	-0.085553	0.981231	
			Y	0.810353	0.553931	0.191019	
			Z	-0.559876	0.828156	-0.026402	
8	1201.1	g-values		0.508490	1.899394	17.230422	
		g-vectors	X	-0.153205	0.691365	0.706075	
			Y	0.763812	0.536193	-0.359289	
			Z	-0.626993	0.484264	-0.610220	
13	1	0.0	g-values		0.000018	0.000023	19.471873
			g-vectors	X	0.184475	0.970720	-0.153857
				Y	-0.980488	0.192582	0.039434
				Z	0.067909	0.143580	0.987306
2	393.0	g-values		0.007903	0.008621	16.691997	
		g-vectors	X	0.950469	-0.271579	-0.151173	
			Y	0.279072	0.959790	0.030363	
			Z	0.136848	-0.071048	0.988041	
3	576.2	g-values		1.943614	3.902767	14.908371	
		g-vectors	X	-0.106774	-0.783588	0.612037	
			Y	0.100972	-0.620919	-0.777344	
			Z	0.989143	-0.021201	0.145418	
4	612.7	g-values		0.240349	2.583270	6.727381	
		g-vectors	X	0.852889	0.431220	0.294328	
			Y	0.445688	-0.894971	0.019729	
			Z	0.271923	0.114352	-0.955501	
5	620.0	g-values		0.629598	4.532908	8.189100	
		g-vectors	X	-0.663864	0.625457	0.409985	

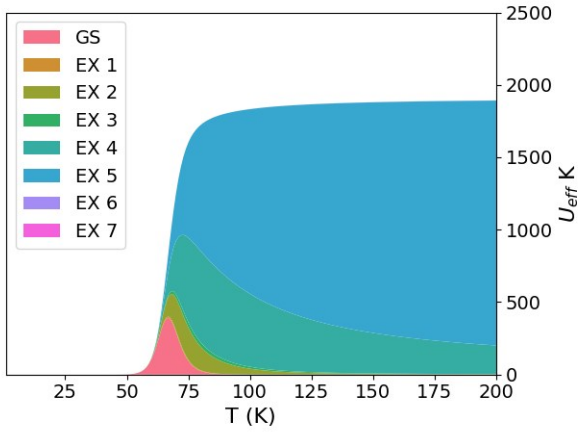
				Y	0.058765	0.590149	-0.805153
				Z	-0.745541	-0.510420	-0.428533
6	660.3	g-values			0.889914	2.604185	6.813811
		g-vectors	X		0.310226	-0.867452	-0.388956
			Y		0.944516	0.327692	0.022513
			Z		0.107929	-0.374359	0.920981
7	699.3	g-values			0.108929	2.334253	12.015781
		g-vectors	X		-0.007517	0.920263	0.391229
			Y		0.824535	-0.215651	0.523104
			Z		0.565762	0.326514	-0.757167
8	706.9	g-values			0.524841	2.777654	13.636737
		g-vectors	X		-0.093097	0.989601	-0.109651
			Y		0.730864	-0.006865	-0.682488
			Z		-0.676144	-0.143678	-0.722625
14	1	0.0	g-values		0.000010	0.000038	19.432563
			g-vectors	X	0.012926	0.999423	-0.031419
				Y	-0.999916	0.012933	0.000030
				Z	0.000436	0.031416	0.999506
2	312.8	g-values			0.016803	0.017645	16.672374
		g-vectors	X		-0.997373	0.001288	0.072426
			Y		0.001290	0.999999	-0.000009
			Z		-0.072426	0.000085	-0.997374
3	565.7	g-values			0.331687	0.644426	13.317208
		g-vectors	X		-0.997881	0.000400	0.065071
			Y		0.000398	1.000000	-0.000031
			Z		-0.065071	-0.000005	-0.997881
4	643.9	g-values			0.525699	1.838965	16.091409
		g-vectors	X		0.169394	-0.985548	-0.000193
			Y		-0.000057	0.000186	-1.000000
			Z		0.985548	0.169394	-0.000024
5	692.5	g-values			0.719981	2.421257	13.137876
		g-vectors	X		-0.993261	-0.115903	-0.000204
			Y		-0.000190	-0.000135	1.000000
			Z		-0.115903	0.993261	0.000112
6	719.0	g-values			2.808931	4.633468	8.820187
		g-vectors	X		-0.789975	-0.000267	0.613139
			Y		-0.000458	1.000000	-0.000154
			Z		-0.613138	-0.000402	-0.789975
7	761.6	g-values			1.906388	2.215257	15.170984
		g-vectors	X		-0.319779	-0.000119	0.947492
			Y		-0.000754	1.000000	-0.000129

			Z	-0.947492	-0.000756	-0.319779
	8	926.0	g-values	0.053073	0.073520	19.202293
			g-vectors	X	-0.415237	0.000144
				Y	0.000281	1.000000
				Z	0.909713	-0.000243
15	1	0.0	g-values	0.005917	0.008835	19.435605
			g-vectors	X	0.695498	-0.019043
				Y	0.043158	0.998951
				Z	0.717231	-0.041645
	2	265.1	g-values	0.293512	0.460094	16.416916
			g-vectors	X	-0.698233	0.007894
				Y	-0.016622	0.999491
				Z	-0.715677	-0.030915
	3	413.1	g-values	3.250595	4.940944	13.012518
			g-vectors	X	0.677979	0.731377
				Y	0.065086	0.040146
				Z	0.732194	-0.680791
	4	476.5	g-values	1.109208	5.432737	8.712560
			g-vectors	X	-0.101471	0.681266
				Y	-0.993091	-0.112542
				Z	0.058944	-0.723333
	5	561.1	g-values	0.553895	4.974616	12.094861
			g-vectors	X	0.651659	0.200020
				Y	-0.025503	-0.958282
				Z	-0.758084	0.204177
	6	595.6	g-values	2.565678	4.501510	10.601969
			g-vectors	X	-0.547358	0.735144
				Y	0.067929	0.515349
				Z	0.834137	0.440430
	7	647.6	g-values	0.404884	1.904744	16.273842
			g-vectors	X	-0.489168	0.729242
				Y	0.332766	0.663118
				Z	0.806214	0.168763
	8	667.9	g-values	0.077851	2.113944	16.488411
			g-vectors	X	0.916646	0.091265
				Y	-0.370706	0.558156
				Z	-0.149453	-0.824701
17	1	0.0	g-values	0.000641	0.000812	19.446300
			g-vectors	X	0.109886	-0.134341
				Y	-0.981096	0.144138
				Z	0.159299	0.980396

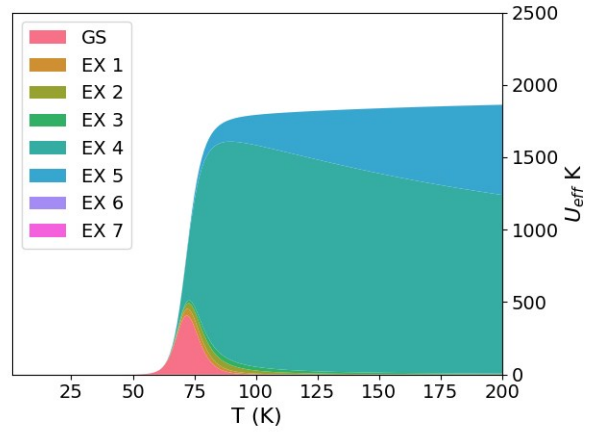
2	216.6	g-values		0.016797	0.020627	16.933402
		g-vectors	X	0.034284	0.110225	-0.993315
			Y	-0.998945	-0.026616	-0.037432
			Z	-0.030564	0.993550	0.109196
3	352.9	g-values		0.284446	0.379226	14.209798
		g-vectors	X	0.108166	-0.207300	-0.972279
			Y	0.979241	0.190863	0.068247
			Z	0.171425	-0.959478	0.223641
4	434.9	g-values		2.405283	4.001060	11.040041
		g-vectors	X	0.422605	-0.329313	-0.844368
			Y	0.903004	0.232551	0.361254
			Z	0.077393	-0.915135	0.395648
5	464.6	g-values		1.716149	7.517017	9.546554
		g-vectors	X	0.939491	-0.326418	0.103959
			Y	0.324265	0.749467	-0.577192
			Z	0.110492	0.575977	0.809964
6	491.5	g-values		0.830430	3.148175	12.401856
		g-vectors	X	0.948159	-0.304455	0.091111
			Y	0.164723	0.225654	-0.960181
			Z	0.271772	0.925412	0.264106
7	529.8	g-values		0.572503	1.229015	15.761780
		g-vectors	X	0.962213	0.272108	-0.010145
			Y	-0.050616	0.142130	-0.988553
			Z	-0.267551	0.951713	0.150532
8	650.9	g-values		0.032455	0.064246	18.979931
		g-vectors	X	0.895614	-0.339448	0.287490
			Y	-0.171763	0.332270	0.927413
			Z	-0.410333	-0.879984	0.239282

Table S2. Comparison between experimental and calculated effective demagnetization barriers and ground state tunneling relaxation time for all calculated systems.

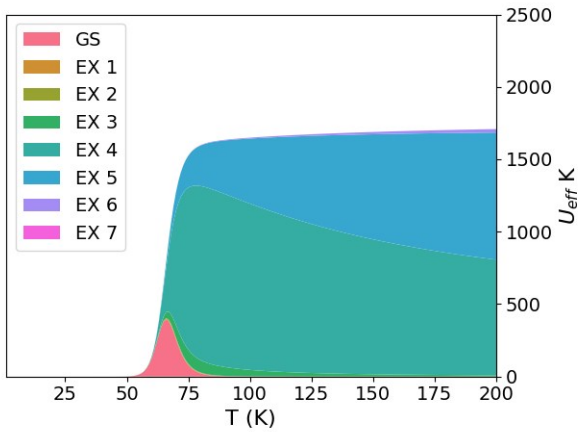
	$U_{\text{eff}}/\text{exp}$ (K)	$U_{\text{eff}}/\text{calc}$ (K)	$\log_{10}(\tau)/\text{exp}$	$\log_{10}(\tau)/\text{calc}$
1	2217	1893	4.40	4.88
3	1986	1863	2.65	4.37
5	1848	1731	2.64	3.35
6	1815	1708		3.98
7	1760	1738		4.41
8	1760	1622		3.90
13	950	906	0.15	1.94
14	944	1041	-0.19	2.12
15	803	711		-3.48
17	638	649	-1.77	-1.15



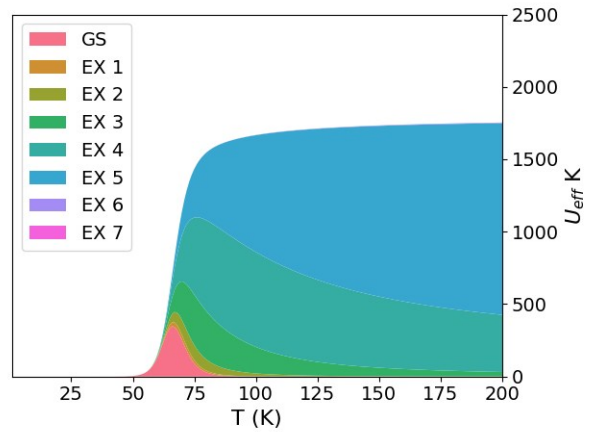
1



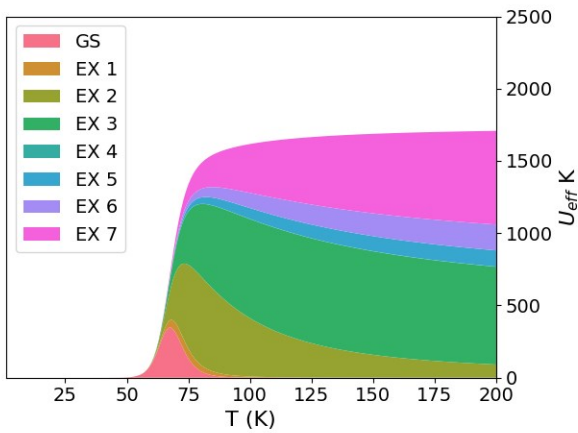
3



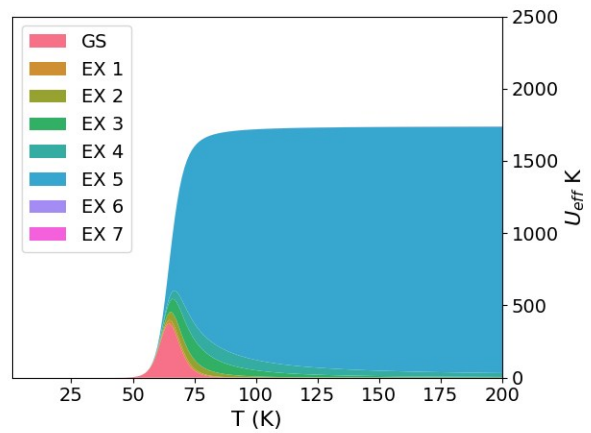
5a



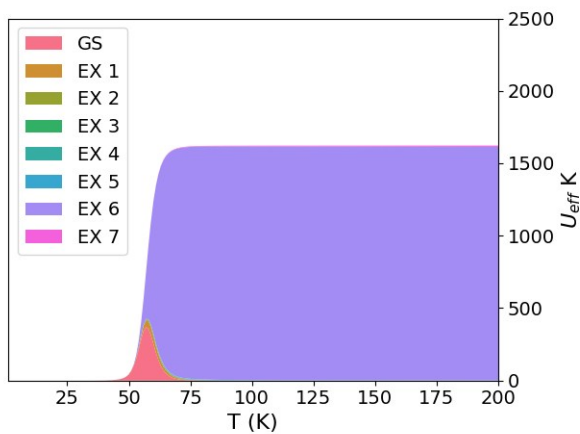
5b



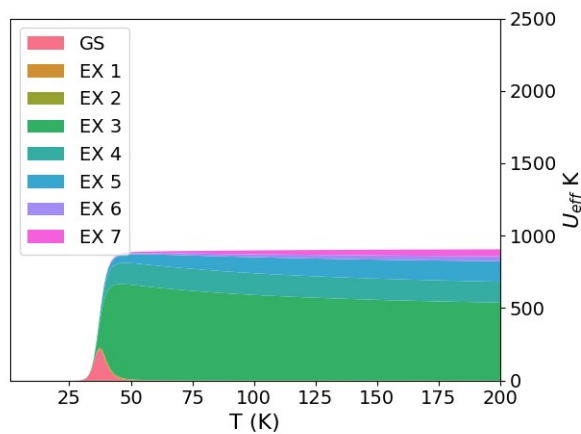
6



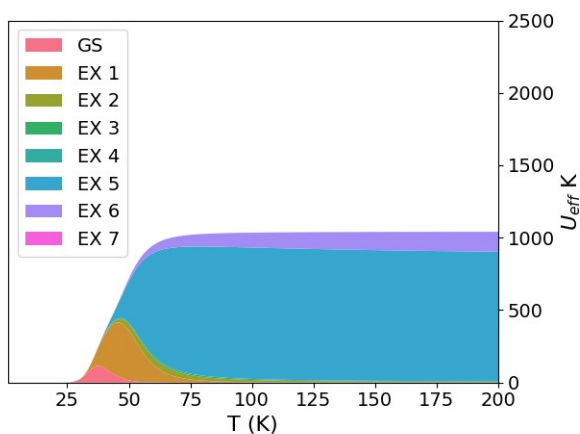
7



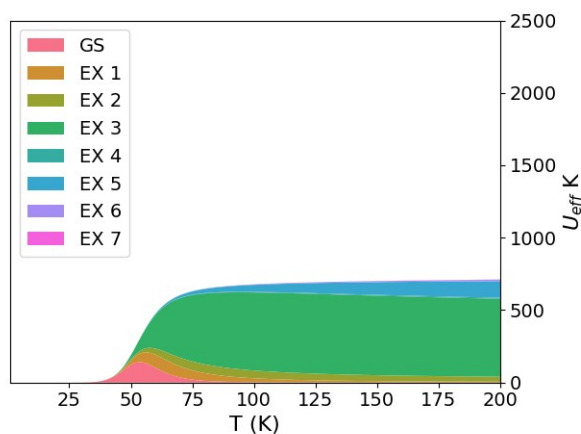
8



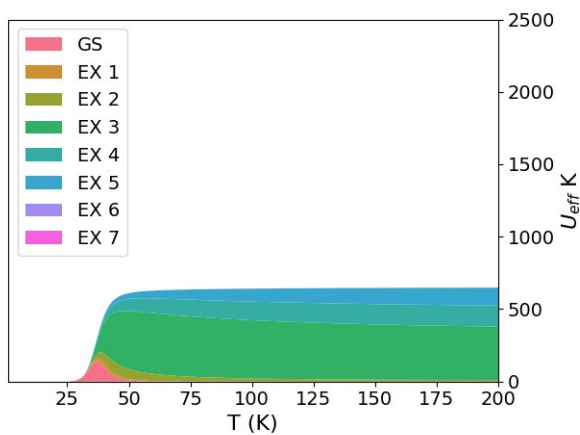
13



14



15



17

Figure S1. Effective demagnetization barrier including relative contributions from the ground state (GS) and seven lowest excited states (EX n).

Example for the calculation of tunneling rates (UandTau)

The calculation of tunneling rates requires state energies, g-values and g-vectors obtained from a CASSCF calculation. In addition, the position of the magnetic ions and their neighbors must be provided by a regular .cif file. Both files serve as input to our program “UandTau”, which can be obtained upon request to the authors.

The relevant parts of the ORCA output are indicated:

1) Relativistic state energies are listed as the Eigenvalues of the QDPT matrix.

```
*****
Doing QDPT with ONLY SOC!
*****

Lowest eigenvalue of the SOC matrix: -13311.11927091 Eh
Energy stabilization: -9255.29614 cm-1
Eigenvalues:      cm-1      eV      Boltzmann populations at T = 300.000
K
  0:           0.00          0.0000      4.54e-01
  1:           0.00          0.0000      4.54e-01
  2:          565.68          0.0701      3.01e-02
  3:          565.68          0.0701      3.01e-02
  4:          825.21          0.1023      8.67e-03
  5:          825.21          0.1023      8.67e-03
  6:          979.91          0.1215      4.13e-03
  7:          979.91          0.1215      4.13e-03
  8:         1135.22          0.1407      1.96e-03
  9:         1135.22          0.1407      1.96e-03
 10:         1299.53          0.1611      8.91e-04
 11:         1299.53          0.1611      8.91e-04
 12:         1437.17          0.1782      4.60e-04
 13:         1437.17          0.1782      4.60e-04
 14:         1562.75          0.1938      2.52e-04
 15:         1562.75          0.1938      2.52e-04
```

2) For each Kramers' doublet, we must search for the corresponding g-factors and g vectors.

```
-----
KRAMERS PAIR 1
-----

Matrix elements Re<1|S|1>  -0.770999   0.953205   2.178132
Matrix elements Re<1|S|2>   0.001310  -0.001620  -0.003701
Matrix elements Im<1|S|2>   0.000835  -0.001032  -0.002358
Matrix elements Re<1|L|1>  -1.540983   1.900426   4.345677
Matrix elements Re<1|L|2>   0.002619  -0.003229  -0.007384
Matrix elements Im<1|L|2>   0.001668  -0.002057  -0.004704

-----
ELECTRONIC G-MATRIX
-----

g-matrix:
```

0.010484	-0.006679	-6.169539		
-0.012944	0.008247	7.618094		
-0.029590	0.018851	17.413984		
g-factors:				
0.000001	0.000001	19.983669	iso =	6.661224
g-shifts:				
-2.002318	-2.002318	17.981350	iso =	4.658904
Orientation:				
X	-0.4602615	-0.8323733	-0.3087297	
Y	0.7418828	-0.5516191	0.3812167	
Z	-0.4876158	-0.0535819	0.8714125	

3) the xyz coordinate of the magnetic center.

```

| 19> actorbs forbs
| 20> rel
| 21> gtensor true
| 22> ndoubgtensor 8
| 23> dosoc true
| 24> end
| 25> end
| 26> * xyz 1 6
| 27> Dy 0.466208642603 3.09356609245 12.8240748266
| 28> C 0.0644682210099 4.83254336403 14.5794295819
| 29> C -1.26857168577 4.53969857176 14.1263920349
| 30> C -1.59477418585 3.19897238631 14.5373982324

```

This is an input file for UandTau, the corresponding cif file “molecule.cif” must be present in the same directory:

```

>RUNMODE single
>NEWJOB
-> ncenters 1
-> dilution_ratio 1
-> dilution_repetitions 1
-> print regular
-> InputMode gfactors
-> ciffile molecule.cif
-> jobtitle job1
---> center 0
--> ncoord 1
Dy 0.466208642603 3.09356609245 12.8240748266
--> end ncoord
--> energies 8
0.00
565.68
825.21
979.91

```

```

1135.22
1299.53
1437.17
1562.75
--> end energies
--> NKD 8
0.000001      0.000001      19.983669
  X      -0.4602615      -0.8323733      -0.3087297
  Y       0.7418828      -0.5516191       0.3812167
  Z     -0.4876158      -0.0535819       0.8714125
  0.000090      0.000095      17.167746
  X     -0.9345989       0.2087017      -0.2880425
  Y     -0.3142182      -0.8639265       0.3935707
  Z     -0.1667087       0.4583390       0.8730026
  0.002568      0.002861      14.557224
  X       0.9023782       0.3289903       0.2783502
  Y       0.4200429      -0.8158282      -0.3974774
  Z       0.0963198       0.4755940      -0.8743757
  0.017737      0.023243      11.908042
  X     -0.6820395       0.6566458       0.3219291
  Y       0.5480870       0.7504075      -0.3694445
  Z     -0.4841722      -0.0755306      -0.8717066
  0.084852      0.129838       9.210357
  X     -0.1168235       0.9286263       0.3521441
  Y       0.9030312       0.2469064      -0.3515279
  Z     -0.4133847       0.2769304      -0.8674230
  1.092539      1.287135       6.411262
  X     -0.1697691       0.9184407      -0.3572746
  Y     -0.9371860      -0.0383618       0.3467142
  Z       0.3047308       0.3936942       0.8672624
  3.141881      6.217129       7.951621
  X     -0.2911190       0.3156801      -0.9031034
  Y       0.3837230       0.9032593       0.1920399
  Z       0.8763598      -0.2906351      -0.3840896
  0.659835      2.755765      17.026882
  X     -0.3133455       0.8288292      -0.4635265
  Y       0.3784035       0.5566582       0.7395555
  Z       0.8709910       0.0563363      -0.4880582
--> end NKD
---> end center 0
>ENDJOB

```