The Mechanism of Spin-Phonon Relaxation in Endohedral Metallofullerene Single Molecule Magnets

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Table S1: Summary of all the Endohedral metallofullerene based SMMs along with blocking temperature and the U_{eff}.

Sr. No.	Molecule	$T_{B,100s}$ (K)	$T_{B,hys}$ (K)(Field sweep mTs−1)is given in bracket)	$T_{B,ZFC}$ (K)(temperature sweep (K min-1) used is given in bracket)	U_{eff} (K)	Ref
1	$DySc_2N@D_3(6140)$-C_{68}	2.3	5 (2.9)	3.8 (5)	23.6	[1]
2	$DySc_2N@D_{5h}(6)$-C_{80}	3.6	7 (2.9)	5.9 (5)	17.7	[1]
3	$DySc_2N@I_h(7)$-C_{80}	4.6	7 (2.9)	6.9 (5)	23.6	[2]
4	$DyY_2N@I_h(7)$-C_{80}	~6	8 (2.9)	8.4 (5)	929	[3]
5	$DyLu_2N@I_h(7)$-C_{80}	~6.5	9 (2.9)	9.5 (5)	24.2	[3, 4]
6	HoSc2N@Ih(7)-C_{80}	—	—	—	16.5	[5]
7	$Dy_2ScN@I_h(7)$-C_{80}	5	7 (2.9)	8 (5)	10.7/1735	[6]
8	$Dy_2YN@I_h(7)$-C_{80}	~3.5	5 (2.9)	4.7 (5)	43.8/680	[3]
9	$Dy_2LaN@I_h(7)$-C_{80}	~2	4 (2.9)	3.3 (5)	—	[3]
10	$Dy_2LuN@I_h(7)$-C_{80}	5.2	8 (2.9)	8 (5)	4.3	[3, 4]
11	$Dy_2GdN@I_h(7)$-C_{80}	~1.5	~1.8 (5.3)	—	15.1	[7]
12	$DyErScN@I_h(7)$-C_{80}	~4.5	9 (33)	~8 (3)	12.5	[8]
13	$Tb_2ScN@I_h(7)$-C_{80}	0.4	~0.4 (3.3)	—	1/10.5/56.4	[9]
14	$Dy_2ScN@D_{5h}(6)$-C_{80}	2.6	7 (2.9)	5.3 (5)	8.4	[1]
15	$Dy_2ScN@D_s(51365)$-C_{84}	~1.8	5 (2.9)	3.3 (5)	—	[1]
16	$Dy_3N@I_h(7)$-C_{80}	—	~2 (0.8)	—	—	[10]
17	TbCN@C2v(19138)-C76b	—	—	—	12	[11]
18	TbCN@C2(5)-C82b	—	—	—	10–20	[12]
19	TbCN@Cs(6)-C82b	—	—	—	10–20	[12]
20	TbCN@C2v(9)-C82b	—	—	—	10–20	[12]
21	$Dy_2O@C_s(10528)$-C_{72}	3.4	7 (2.9)	8 (5)	—	[13]
22	$Dy_2O@C_2(13333)$-C_{74}	5.0	14 (2.9)	14 (5)	—	[13]
23	$Dy_2O@C_{2v}(5)$-C_{80}	3.2	6 (2.9)	11 (5)	25.9	[14]
24	$Dy_2O@C_s(6)$-C_{82}	2.8	6 (2.9)	10 (5)	10.8	[15]
25	$Dy_2O@C_{3v}(8)$-C_{82}	5.9	7 (2.9)	9 (5)	7.8	[15]
26	$Dy_2O@C_{2v}(9)$-C_{82}	3.7	7 (2.9)	8 (5)	18.6	[15]
27	$Dy_2O@C_1(26)$-C_{88}	6	8 (2.9)	10.5 (5)	20.4	[16]
28	$Dy_2O@C_s(32)$-C_{88}	4.6	8 (2.9)	8.5 (5)	—	[16]
29	$Dy_2O@D_2(35)$-C_{88}	3.9	8 (2.9)	8.5 (5)	—	[16]
30	$Dy_2S@C_s(10528)$-C_{72}	—	3.0 (8.33)	—	—	[17]
31	$Dy_2S@C_s(6)$-C_{82}	—	3.0 (8.33)	—	17.8	[17, 18]

32	$Dy_2S@C_{3v}(8)$-C_{82}	2	5 (8.33)	4.0 (5)	6	[17, 18]
33	$DyScS@C_s(6)$-C_{82}	~4	9 (10)	7.3 (5)	15.2	[19]
34	$DyScS@C_{3v}(8)$-C_{82}	~2	9 (10)	7.3 (5)	6.5	[19]
35	$DyYTiC@I_h(7)$-C_{80}	~5	7 (2.9)	8 (5)	14.9	[20]
36	$Dy_2TiC@I_h(7)$-C_{80}	1.7	3 (5)	—	9.5	[21]
37	$Dy_2TiC_2@I_h(7)$-C_{80}	—	1.8 (5)	—	—	[21]
38	$Dy_2TiC@D_{5h}(6)$-C_{80}	—	1.8 (5)	—	—	[21]
39	$Dy_2C_2@C_s(6)$-C_{82}	—	3.0 (8.33)	—	17.4	[17]
40	$Dy_2C_2@C_s(32)$-C_{88}	—	2.1 (2.9)	—	—	[16]
41	$Dy_2C_2@D_2(35)$-C_{88}	—	2.1 (2.9)			[16]
42	$Dy@C_s(6)$-$C_{81}N$	45	39 (3.5)/60 (10)	69 (1)	—	[22]
43	$Dy_2@C_{80}(CH_2Ph)$	18	22 (2.9)	21.9 (5)	613	[23]
44	$Dy_2@C_{79}N$	12	24 (20)	21 (3)	669	[24]
45	$Tb_2@C_{79}N$	24	26 (2.9)	28 (5)	757	[25]
46	Tb2@C80(CH2Ph)	25.2	27 (9.5)	28.9 (5)	799	[26]
47	$Tb_2@C_{80}(CF_3)$	25	26 (2.9)	28.5 (5)	801	[27]
48	$Ho_2@C_{80}(CH_2Ph)$	—	—	—	334	[26]
49	Er2@C80(CH2Ph)a	—	—	—	—	[26]
50	$TbGd@C_{80}(CH_2Ph)$	—	—	14.4 (5)	—	[26]
51	$TbY@C_{80}(CH_2Ph)$	—	5 (2.9)	5 (5)	—	[26]
52	Nd2@C80(CF3)a	—	—	—	—	[28]
53	Gd2@C79Na	—	—	—	6.5	[29, 30]
54	$DyEr@C_{3v}(8)$-C_{82}	—	3 (33)	5 (3)		[31]

Table S2: |V(r)/G(r)| ratio of $DySSc@C_{82}$ and Fragment $DyScS(C_8H_6)_2$. (Here V(r) is the Virial Field function, G(r) is the electronic kinetic energy density, |V(r)/G(r)| is the ratio of Virial field function to Electronic kinetic energy.

Bond	V(r)	G(r)	$(\nabla^2\rho(r)$	H(r)	|V(r)/G(r)|
$DySSc@C_{82}$					
Dy-S	−0.071	0.056	0.159	−0.015	1.285
Dy-C	−0.074	0.062	0.202	−0.008	1.189
Dy-S	−0.081	0.043	0.137	−0.011	1.143
Dy-C	−0.076	0.062	0.194	−0.014	1.219

Note: |V(r)/G(r)| < 1 – ionic interaction, |V(r)/G(r)| > 2 – covalent interaction, 1<|V(r)/G(r)<2 – intermediate interaction.

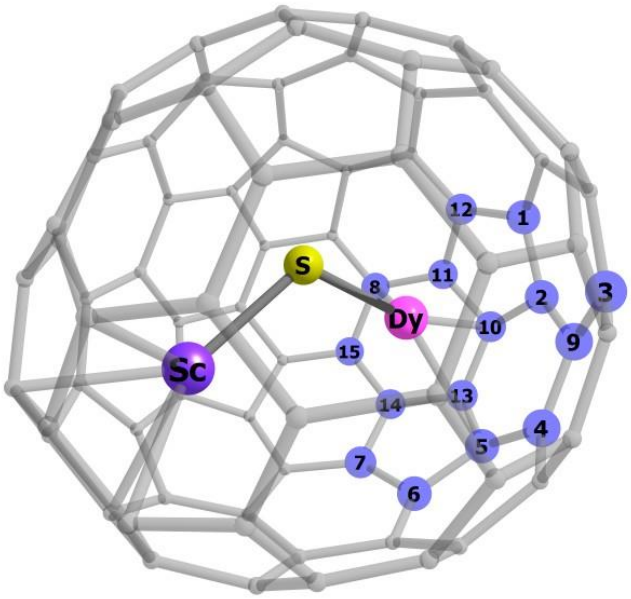

Figure S1:$DyScS@C_{82}$ structure showing the marked C atoms as the one having considerable delocalization indices.

Table S3: Delocalisation index $\delta(Dy, C_{cage})$ between Dy^{III} and the cage carbon atoms.	
Carbon number	$\delta(Dy, C_{cage})$
1	0.236
2	0.315
3	0.101
4	0.208
5	0.276
6	0.163
7	0.163
8	0.237
9	0.237
10	0.345
11	0.315
12	0.236
13	0.328
14	0.276
15	0.208

Table S4: Energies, g-tensor, angle of the ground excited g_{zz} with the ground g_{zz} in $DyScS@C_{82}$ molecule and the $DyScS(C_8H_6)$.					
KD	Energies (cm^{-1})	g_{xx}	g_{yy}	g_{zz}	Angle (°)
$DyScS@C_{82}$					
1	0.0	0.002	0.003	19.925	
2	239.3	0.009	0.012	17.078	2.5
3	471.0	0.190	0.235	14.133	5.9
4	659.7	0.249	0.567	11.697	20.1
5	800.4	0.641	1.288	8.531	4.4
6	889.7	6.186	5.695	3.801	45.7
7	941.6	0.996	3.247	14.668	96.1
8	1011.6	0.182	1.136	18.890	89.8
$DyScS(C_8H_6)_2$					
1	0.0	0.001	0.001	20.032	
2	271.9	0.012	0.018	17.726	27.8
3	389.9	0.058	0.079	14.218	21.5
4	520.3	0.875	1.029	12.453	16.6
5	596.8	1.725	3.809	10.140	36.5
6	671.5	3.383	5.859	9.881	86.8
7	764.8	0.909	1.938	16.382	87.9
8	988.9	0.043	0.075	20.059	93.4

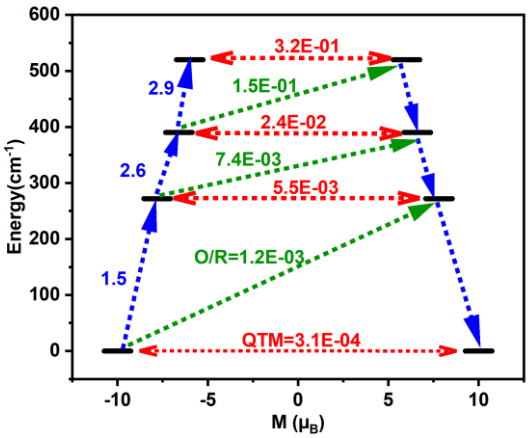

Figure S2: Relaxation mechanism of spin reversal in fragment $DyScS(C_8H_6)_2$

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