Supporting information for "Understanding the magnetic blocking mechanism in N_2^{3-}-radical-bridged dilanthanide single-molecule magnets"

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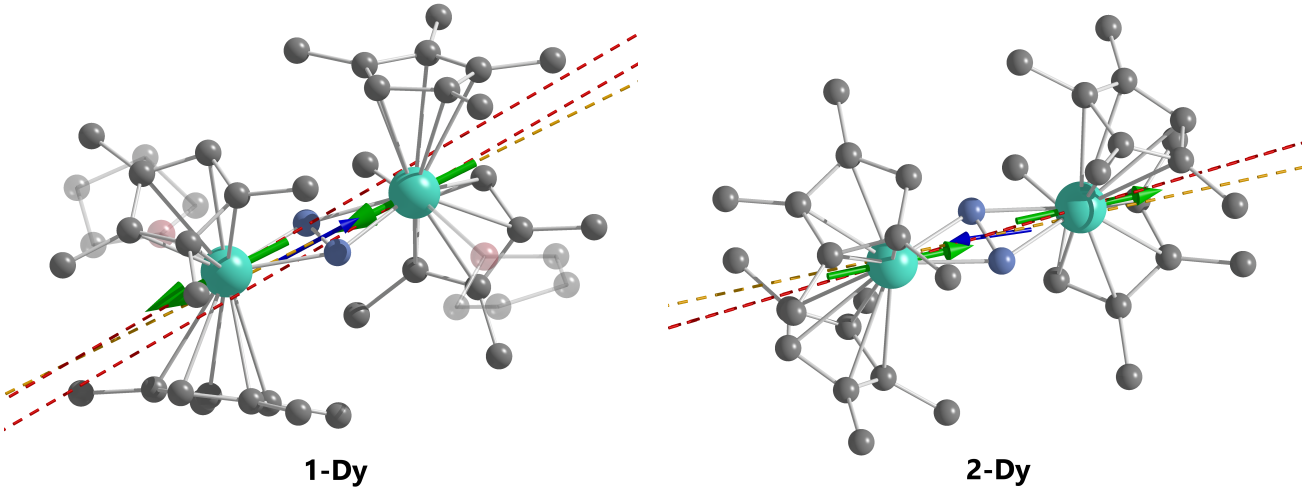

Figure S1: Molecular structure of **1-Tb** (left) and **2-Tb** (right). Cyan, blue, red and gray spheres illustrate Tb, N, O and C atoms, respectively. Hydrogen atoms are omitted and THF groups are faded for clarity. Red dash line indicates magnetic anisotropy axis of the ground doublet on each Ln ion while the yellow one is for the ground exchange doublet. Green and blue arrows demonstrate magnetic moments of the Ln ions and the radical, respectively.

Table S1: Contribution of local CF doublet on each lanthanide center to exchange doublet for **1-Tb** (only the contribution larger or equal to 5% is reported).

Local CF doublet	Exchange doublet					
	1	2	3	4	5	6
$\|\pm6\rangle$	94%	49%	85%	85%	50%	46%
$\|\pm5\rangle$	6%	50%	14%	15%	49%	8%
$\|\pm4\rangle$						42%
$\|\pm3\rangle$						
$\|\pm2\rangle$						
$\|\pm1\rangle$						
$\|0\rangle$						

Table S2: Contribution of local CF doublet on each lanthanide center to exchange doublet for **1-Dy** (only the contribution larger or equal to 5% is reported).

Local CF doublets	Exchange doublet					
	1	2	3	4	5	6
$\|\pm 15/2\rangle$	97%	98%	98%	95%	50%	54%
$\|\pm 13/2\rangle$					48%	44%
$\|\pm 11/2\rangle$						
$\|\pm 9/2\rangle$						
$\|\pm 7/2\rangle$						
$\|\pm 5/2\rangle$						
$\|\pm 3/2\rangle$						
$\|\pm 1/2\rangle$						

Table S3: Contribution of local CF doublet on each lanthanide center to exchange doublet for **2-Tb** (only the contribution larger or equal to 5% is reported).

Local CF doublet	Exchange doublet					
	1	2	3	4	5	6
$\|\pm 6\rangle$	98%	95%	95%	49%	50%	52%
$\|\pm 5\rangle$		5 %	5%	51%	49%	47%
$\|\pm 4\rangle$						
$\|\pm 3\rangle$						
$\|\pm 2\rangle$						
$\|\pm 1\rangle$						
$\|0\rangle$						

Table S4: Contribution of local CF doublet on each lanthanide center to exchange doublet for **2-Dy** (only the contribution larger or equal to 5% is reported).

Local CF doublet	Exchange doublet					
	1	2	3	4	5	6
$\|\pm 15/2\rangle$	96%	96%	96%	50%	49%	49%
$\|\pm 13/2\rangle$				37%	37%	34%
$\|\pm 11/2\rangle$				11%	11%	10%
$\|\pm 9/2\rangle$						5%
$\|\pm 7/2\rangle$						
$\|\pm 5/2\rangle$						
$\|\pm 3/2\rangle$						
$\|\pm 1/2\rangle$						