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Single-ion magnet behaviour in highly axial lanthanide mononitrides encapsulated in boron nitride nanotubes: a quantum chemical investigation

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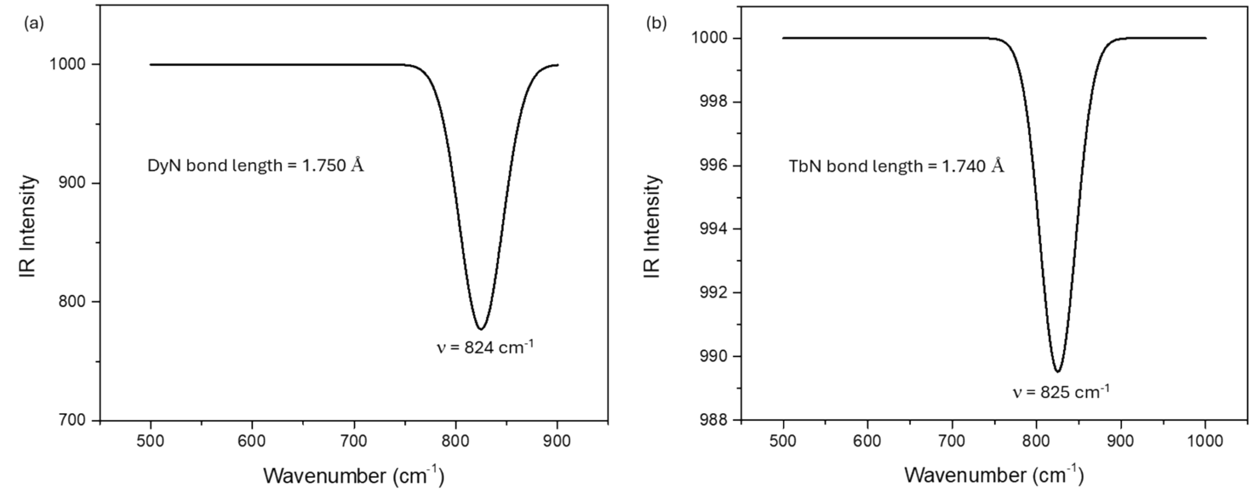

Fig. S1 B3LYP computed IR-frequencies along with the optimized bond lengths (inset).

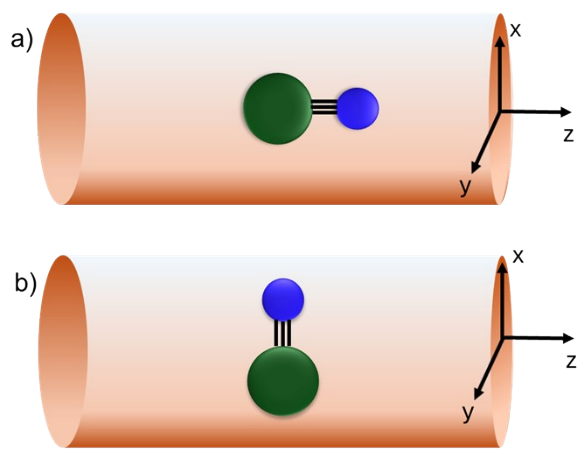

Fig. S2 Schematic representation of parallel($_{||}$) and perpendicular($_{\perp}$) arrangement of **[LnN]** inside BNNT. The tube is periodic along the z-direction.

Table S1 The diameters (Å) of non-optimized, optimized pristine, and fully optimized DyN@BNNT.

	(8,0)		(9,0)	
Pristine-non optimised[1]	6.73		7.33	
Pristine optimised	6.77		7.34	
DyN@BNNT	**8Dy$_{\|\|}$**	**8Dy$_{\perp}$**	**9Dy$_{\|\|}$**	**9Dy$_{\perp}$**
	6.79 Å	6.71 Å	7.33 Å	7.36 Å

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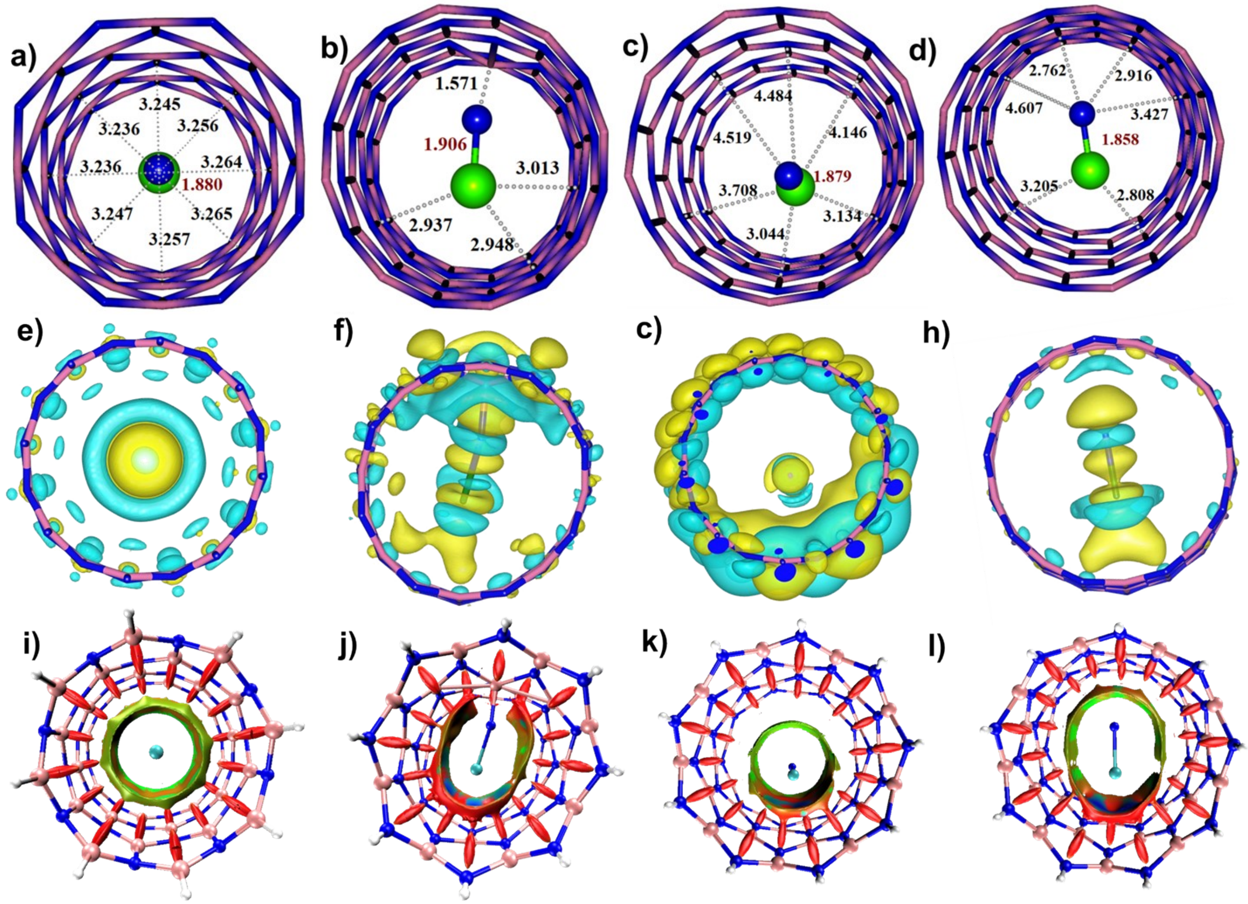

Fig. S3 pDFT optimized structures of a) **$8Tb_{\parallel}$** ; b) **$8Tb_{\perp}$**; c) **$9Tb_{\parallel}$** and d) **$9Tb_{\perp}$** with relevant bond parameters (bond distance in red color represents the Tb-N bond distance of the **[TbN]** molecule; (e)-(h) CDD plots corresponding to optimized structures plotted with an isosurface= 0.00186 e Å^{-3}; (i)-(l) NCI-plots for above structures. Color code: Tb (light-green), N(blue), B(pink).

Table S2 pDFT computed binding energies of **[LnN]**@BNNT assemblies.

LnN@BNNT(n,0)	**$Ln_{\parallel}$**	**$Ln_{\perp}$**
DyN@BNNT(8,0)	-217.75	-175.97
DyN@BNNT(9,0)	-183.95	-130.32
TbN@BNNT(8,0)	-214.19	-166.97
TbN@BNNT(9,0)	-180.16	-128.52

B.E. = $E_{LnN@BNNT} - E_{LnN} - E_{BNNT}$

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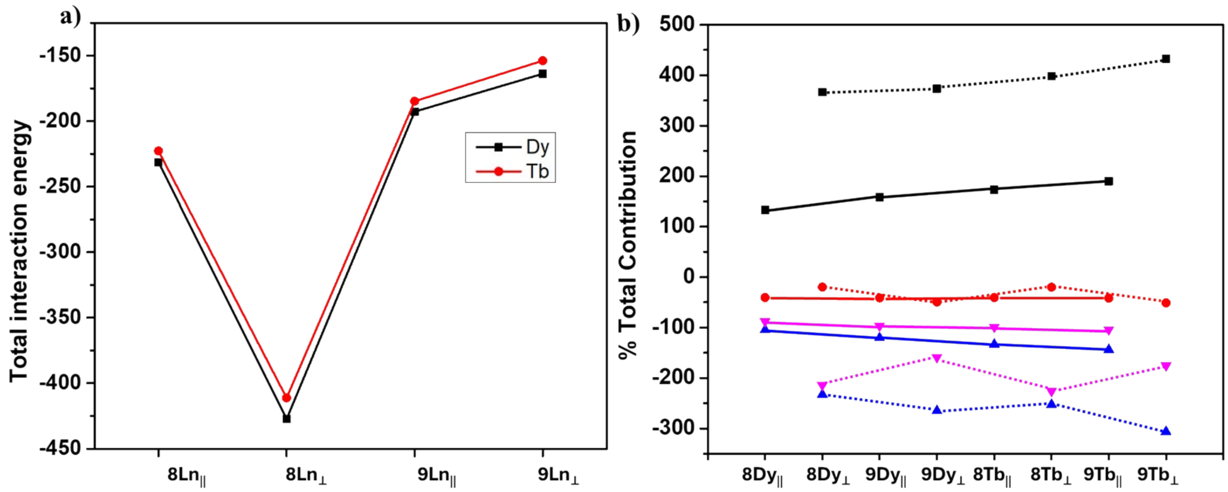

Fig. S4 PBE-D3BJ/TZ2P computed trends in the total interaction energy a), with the corresponding %contribution b) for [LnN]@BNNTs.

Table S3 PBE-D3BJ/TZ2P computed PEDA energies for **[LnN]**@BNNT. All energies are in kJ/mol.

Energy	8Dy		8Tb		9Dy		9Tb	
Assemblies	**$8Dy_{\|\|}$**	**$8Dy_{\perp}$**	**$8Tb_{\|\|}$**	**$8Tb_{\perp}$**	**$9Dy_{\|\|}$**	**$9Dy_{\perp}$**	**$9Tb_{\|\|}$**	**$9Tb_{\perp}$**
Pauli	307.8	1565.7	385.6	1638.9	305.3	631.5	351.1	665.5
Dispersion	-93.7	-84.5	-90.6	-81.8	-79.4	-80.5	-77.3	-78.4
Electrostatic	-242.2	-993.3	-297.1	-1038.3	-232.2	-446.2	-266.1	-471.1
Orbital	-203.2	-915.2	-220.5	-929.9	-186.4	-266.2	-192.5	-269.8
Total Interaction	**-231.4**	**-427.3**	**-222.7**	**-411.2**	**-192.7**	**-161.4**	**-184.8**	**-153.8**

Table S4 Contribution (%) of decomposition energies to Total Binding Energy for complexes.

Assemblies	E_Pauli	E_disp	E_elstat	E_orb
$8Dy_{\|\|}$	133.0	-40.5	-104.7	-87.8
$8Dy_{\perp}$	366.4	-19.8	-232.5	-214.2
$9Dy_{\|\|}$	158.4	-41.2	-120.5	-96.7
$9Dy_{\perp}$	373.4	-49.5	-264.9	-159.0
$8Tb_{\|\|}$	173.1	-40.7	-133.4	-99.0
$8Tb_{\perp}$	398.6	-19.9	-252.5	-226.1
$9Tb_{\|\|}$	190.0	-41.8	-144.0	-104.2
$9Tb_{\perp}$	432.7	-51.0	-306.3	-175.4

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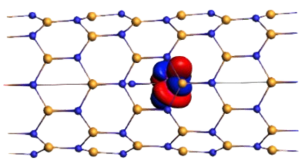
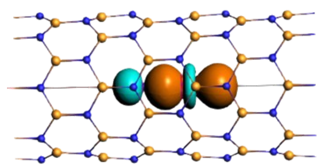
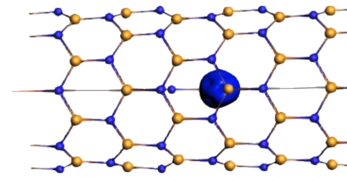
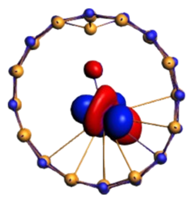
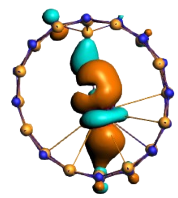
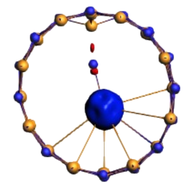
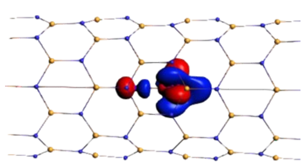
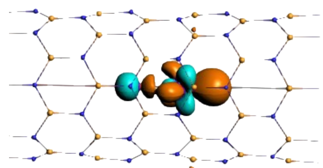
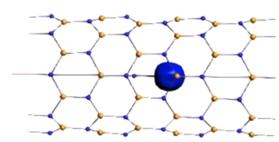
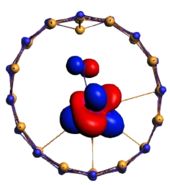
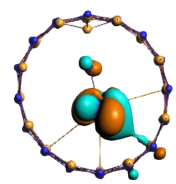
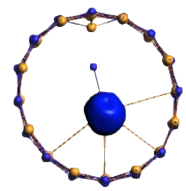
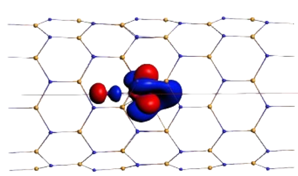
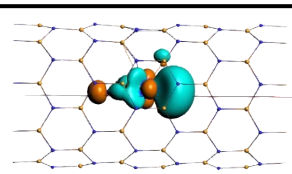
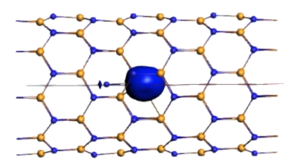
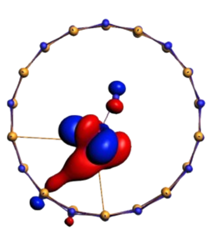
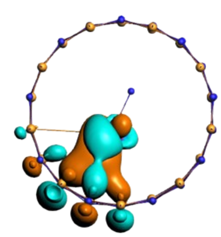
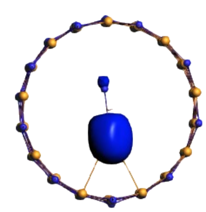
Table S5 PBE-D3BJ/TZ2P computed HOMO, LUMO, and spin densities of **[LnN]**@BNNT.

Complex	HOMO	LUMO	Spin-density
$8Dy_{\|\|}$			
$8Dy_{\perp}$			
$8Tb_{\|\|}$			
$8Tb_{\perp}$			
$9Dy_{\|\|}$			
$9Dy_{\perp}$			

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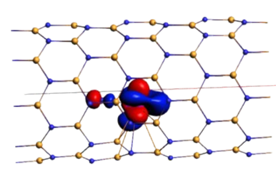
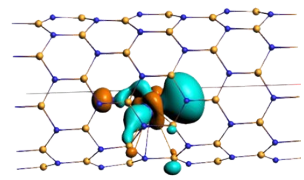
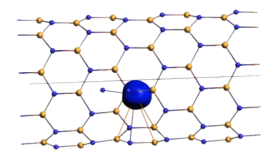
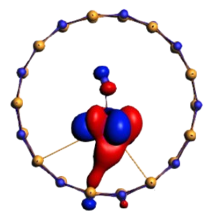
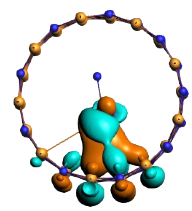
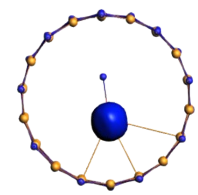
$9Tb_{\parallel}$			
$9Tb_{\perp}$			

Periodic Energy Decomposition Analysis:

The total interaction energy ΔE_{int} is broken down into four components within the ETS energy breakdown scheme[2] as shown in equation **2**;

$$\Delta E_{\text{int}} = \Delta E_{\text{elstat}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}} \qquad \ldots \textbf{(2)}$$

ΔE_{elstat} represents the classical electrostatic interaction between the charge densities of the fragments within the promolecule, directly correlating with the ionic bonding between the fragments. On the other hand, ΔE_{Pauli} accounts for Pauli repulsion, reflecting the energy increase due to enforcing the Pauli exclusion principle on the promolecular densities, which are intrinsically repulsive. ΔE_{disp} includes the DFT-D3 dispersion correction[3] contribution, which is always stabilizing in nature. ΔE_{orb} represents the orbital interaction term, reflecting the reduction in energy as promolecular densities mix and relax, linked to the covalent bonding between metal and ligands. It describes the stabilization due to the relaxation of fragment wavefunctions (Ψ^0) into the combined wavefunction (Ψ) during bonding. Using NOCV within EDA, ΔE_{orb} is broken into contributions from interacting orbitals. Pairs of complementary orbitals (Ψ_{-k}, Ψ_k) with non-zero eigenvalues represent the deformation density ($\Delta\rho_{orb}$), showing electron density redistribution.

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Non-interacting orbitals have zero eigenvalues and contribute no deformation, as shown in equation **3**.

$$\Delta\rho^{orb}(r) = \rho - \rho^{o} = \sum_{k=1}^{\frac{N}{2}} \nu_k[-\Psi_{-k}^{2}(r) + \psi_k^2(r)] + \sum_{k=1}^{N/2} \Delta\rho_k(r) \quad \dots (\mathbf{3})$$

This includes contributions from charge transfer, electron pair bonding, and polarization. This systematic breakdown into physical components offers insights into bonding, especially in systems with distinct σ and π characters, showing how electron density redistributes and stabilizes the interaction.

We performed PEDA calculations to decompose further the nature of interactions between the **[LnN]** and BNNT rings. The computed interaction energy (ΔE_{int}) is always stabilizing in nature for all eight hybrid assemblies. The computed ΔE_{int} value is significant for the **[LnN]**@BNNT (8,0) compared to **[LnN]**@BNNT (9,0), which aligns with the observed trend in the binding energy. Among all the studied eight assemblies, the Pauli interactions are the strongest, followed by the electrostatic and orbital interactions, which are stabilizing in nature. As we move from the **8Dy**$_{||}$(**8Tb**$_{||}$) to **9Dy**$_{||}$(**9Tb**$_{||}$) complexes, both the electrostatic and orbital interaction decreases due to an increase in the diameter of the tube, resulting in a weaker ΔE_{int} value for the **[LnN]**@BNNT (9,0) assemblies. For **8Dy**$_{\perp}$ and **8Tb**$_{\perp}$ assemblies, we observed giant ΔE_{int} values of -427.3 kJ/mol and -411.2 kJ/mole, nearly two times larger than any other computed ΔE_{int} values. This exceptionally high ΔE_{int} value in **8Dy**$_{\perp}$ and **8Tb**$_{\perp}$ is attributed to the formation of the B-N bond between the B atom of the BNNT ring and the N atom of **[LnN]**. Next, we decomposed the orbital component of the interaction energy (ΔE_{orb}) into its corresponding NOCV donor/acceptor pairs to understand the nature of the interaction. Table S6 summarizes the first three deformation densities with the corresponding energy value. Notably, we observed the strong *s*-type orbital interaction with ΔE_{orb1} value of -261.7(-248.5) kJ/mol for the **8Dy**$_{\perp}$(**8Tb**$_{\perp}$), which is ~29(27)% of the total ΔE_{orb} value. Visual inspection of the NOCV pair reveals an electron flow from the **[LnN]** orbital to the vacant *2p* orbital of the B atoms in the BNNT ring. For **9Dy**$_{\perp}$(**9Tb**$_{\perp}$), we observed a similar NOCV pair corresponding to the ΔE_{orb1} value; however, the strength of the ΔE_{orb1} value is decreased to -63.1(-47.0) kJ/mol as a result of the decreased orbital overlap in the BNNT (9,0) tube (see Fig. S5). Contrarily, the ΔE_{orb1} value for the **8Dy**$_{||}$(**8Tb**$_{||}$) and **9Dy**$_{||}$(**9Tb**$_{||}$) assemblies is extremely weak, indicating a weaker orbital overlap interaction between the **[LnN]** and BNNT rings in the parallel arrangement. The computed deformation density from the PEDA calculation nicely matches the computed CDD plots (see Fig. 2, S2 and S5). The dispersion interaction is always stabilizing in nature and contributes around ~19% to 50% of the total interaction energy. The strength of the dispersion interaction is more dominant in the **8Dy**$_{||}$(**8Tb**$_{||}$) and **9Dy**$_{||}$(**9Tb**$_{||}$) assemblies. The presence of the dispersion interaction can be directly verified from the NCI plots, which show weak van der Waals interaction between the tube and **[LnN]** molecule.

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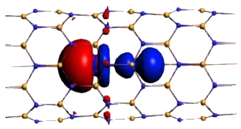
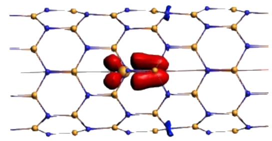
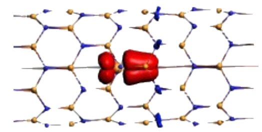
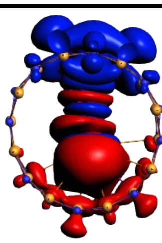
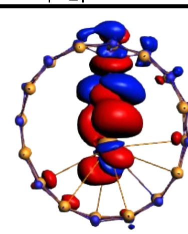
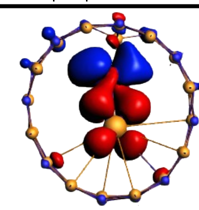
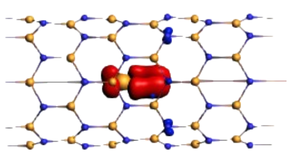
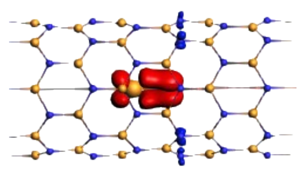
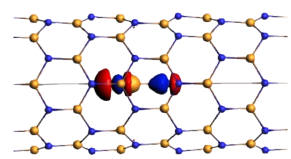
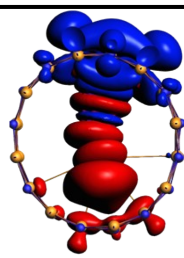
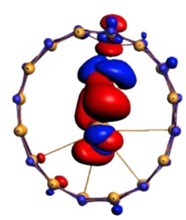
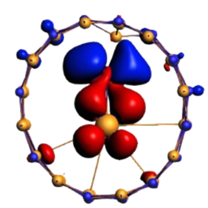
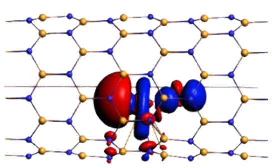
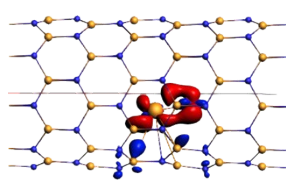
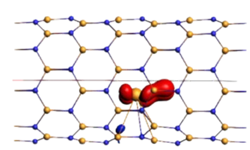
Table S6 ETS-NOCV derived the first three strongest electron deformation densities ($\Delta E_{orb(1)}$ to $\Delta E_{orb(3)}$) at the PBE-D3(BJ)/TZ2P level. Isosurface values are 0.0001 a.u. The direction of the charge flow of the deformation densities is from red to blue. The ΔE_{orb} energies are in kJ/mol. The eigenvalues ν_i give the size of the charge migration.

Complex	$\Delta \boldsymbol{E}_{\mathbf{orb(1)}}$	$\Delta \boldsymbol{E}_{\mathbf{orb(2)}}$	$\Delta \boldsymbol{E}_{\mathbf{orb(3)}}$
8Dy∥	 $\Delta r_{(1)}$ $\Delta E_{orb(1)}$ =-11.8; $\lvert n_1 \rvert$ =0.25	 $\Delta r_{(2)}$ $\Delta E_{orb(2)}$ = -14.5; $\lvert n_2 \rvert$ =0.17	 $\Delta r_{(3)}$ $\Delta E_{orb(3)}$ = -14.4; $\lvert n_3 \rvert$ =0.17
8Dy⊥	 $\Delta r_{(1)}$ $\Delta E_{orb(1)}$ =-261.7; $\lvert n_1 \rvert$ = 0.53	 $\Delta r_{(2)}$ $\Delta E_{orb(2)}$ =-39.9 $\lvert n_2 \rvert$ = 0.23	 $\Delta r_{(3)}$ $\Delta E_{orb(3)}$ =-29.7; $\lvert n_3 \rvert$ = 0.19
8Tb∥	 $\Delta r_{(1)}$ $\Delta E_{orb(1)}$ =-15.0; $\lvert n_1 \rvert$ = 0.17	 $\Delta r_{(2)}$ $\Delta E_{orb(2)}$ =-15.0; $\lvert n_2 \rvert$ = 0.17	 $\Delta r_{(3)}$ $\Delta E_{orb(3)}$ =-9.3; $\lvert n_3 \rvert$ = 0.15
8Tb⊥	 $\Delta r_{(1)}$ $\Delta E_{orb(1)}$ =-248.5; $\lvert n_1 \rvert$ = 0.46	 $\Delta r_{(2)}$ $\Delta E_{orb(2)}$ =-29.9; $\lvert n_2 \rvert$ = 0.21	 $\Delta r_{(3)}$ $\Delta E_{orb(3)}$ =-31.4; $\lvert n_3 \rvert$ = 0.19
9Dy∥			 $\Delta r_{(3)}$

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<table>
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$|n_1|$ = 0.23</th><th>$\Delta r_{(2)}$
$\Delta E_{orb(2)}$ =-13.8;
$|n_2|$ = 0.18</th><th>$\Delta E_{orb(3)}$ =-11.0;
$|n_3|$ =0.15</th></tr>
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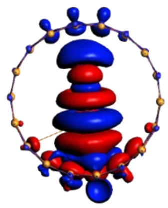

$\Delta r_{(1)}$
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$|n_1|$ = 0.47</td>
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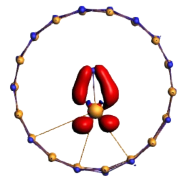
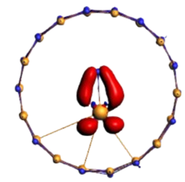
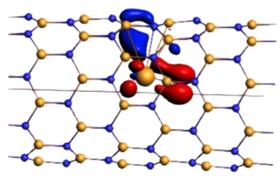
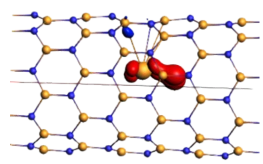
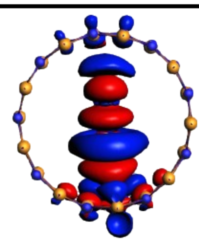


$\Delta r_{(2)}$
$\Delta E_{orb(2)}$ =-11.1;
$|n_2|$ = 0.14</td>
<td>


$\Delta r_{(3)}$
$\Delta E_{orb(3)}$ =-4.6;
$|n_3|$ = 0.11</td>
</tr>
<tr>
<td>9Tb||</td>
<td>


$\Delta r_{(1)}$
$\Delta E_{orb(1)}$ =-16.1;
$|n_1|$ = 0.18</td>
<td>


$\Delta r_{(2)}$
$\Delta E_{orb(2)}$ =-11.1;
$|n_2|$ = 0.14</td>
<td>

$\Delta r_{(3)}$
$\Delta E_{orb(3)}$ =-8.2;
$|n_3|$ = 0.12</td>
</tr>
<tr>
<td>9Tb⊥</td>
<td>


$\Delta r_{(1)}$
$\Delta E_{orb(1)}$ =-47.0;
$|n_1|$ = 0.36</td>
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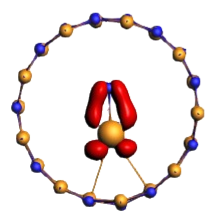
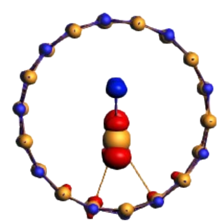


$\Delta r_{(2)}$
$\Delta E_{orb(1)}$ =-11.8;
$|n_2|$ = 0.13</td>
<td>


$\Delta r_{(3)}$
$\Delta E_{orb(3)}$ =-5.8;
$|n_3|$ = 0.11</td>
</tr>
</table>

SUPPORTING INFORMATION

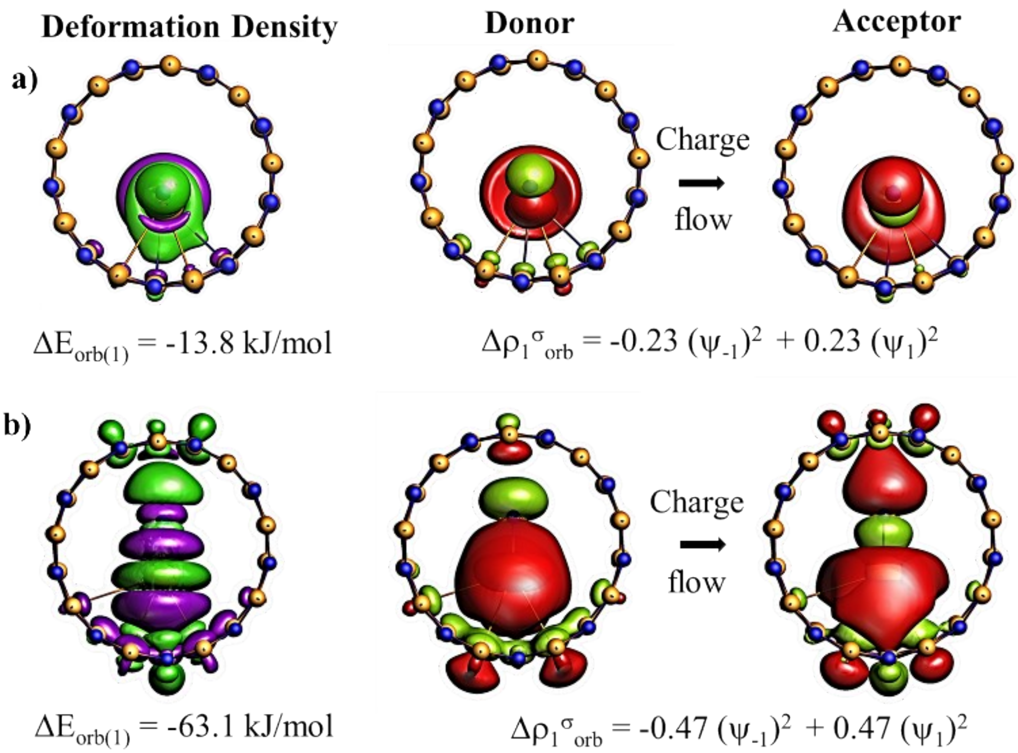


Fig. S5 ETS-NOCV computed electron deformation density (EDD) plots along with corresponding donor and acceptor for **9Dy**$_{||}$ and **9Dy**$_{\perp}$ computed at PBE-D3BJ/TZ2P level of theory. The EDD is plotted with an isosurface value of 0.00001 a.u., where the violet region shows charge depletion and the green region shows charge accumulation

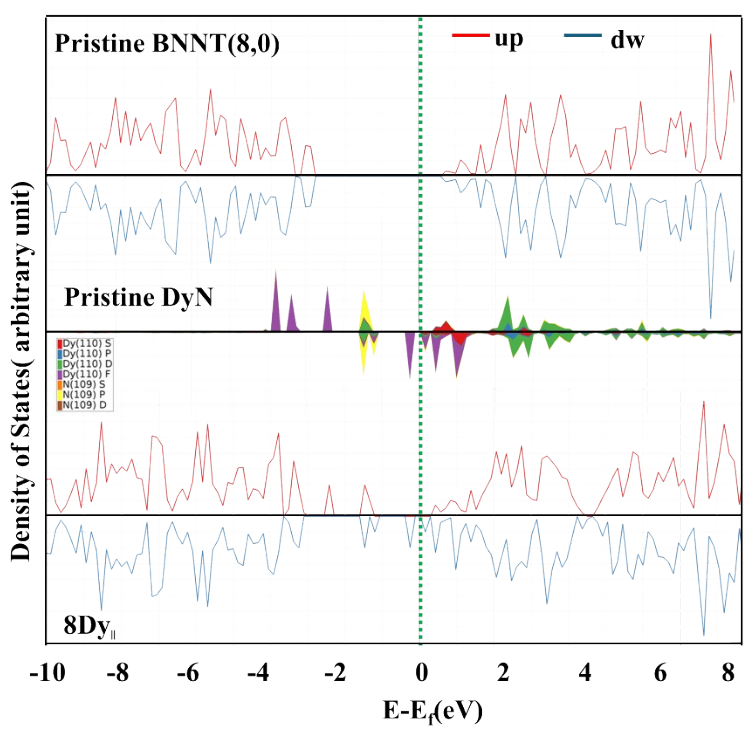


Fig. S6 Density of States plot for **8Dy**$_{||}$. The green dotted line shows the fermi-level.

SUPPORTING INFORMATION

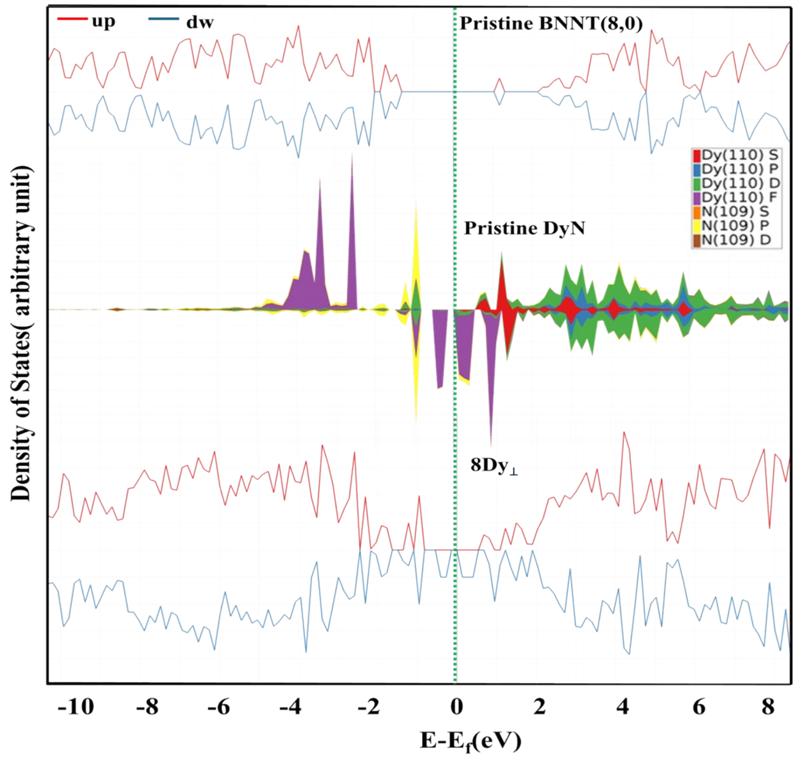


Fig. S7 Density of States plot for **8Dy$_{\perp}$.**The green dotted line shows the fermi-level.

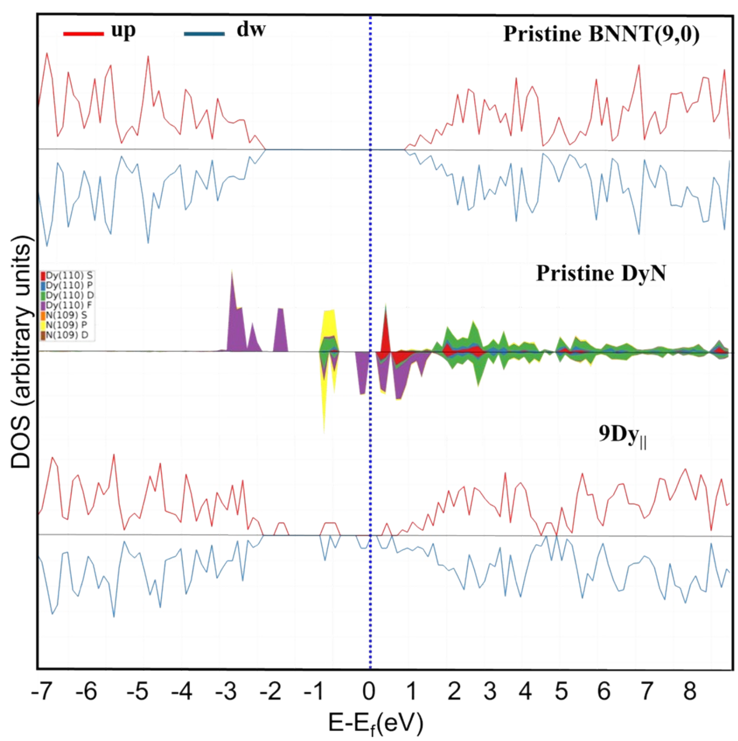


Fig. S8 Density of States plot for **9Dy$_{||}$.**The green dotted line shows the fermi-level.

Table S7 Basis set specification of several atoms in OpenMolcas.

Atoms	ANO-RCC basis functions
H	2s
B	3s2p
N of [LnN]	3s2p1d
N	3s2p
Dy, Tb	7s6p4d2f1g

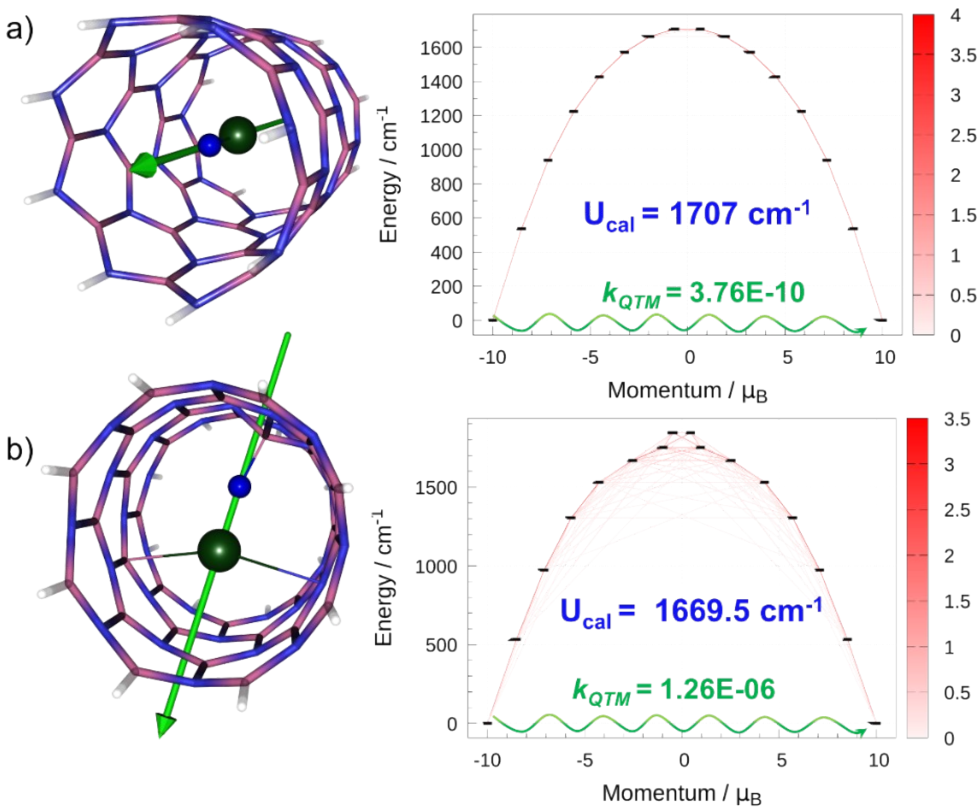


Fig. S9 CASSCF computed *g*-tensor orientation in **8Dy**$_{\parallel}$ and **8Dy**$_{\perp}$. The solid arrow denotes the main magnetic anisotropy axis (g_{zz}). Color code: Dy (green), N(blue), B(pink).

SUPPORTING INFORMATION

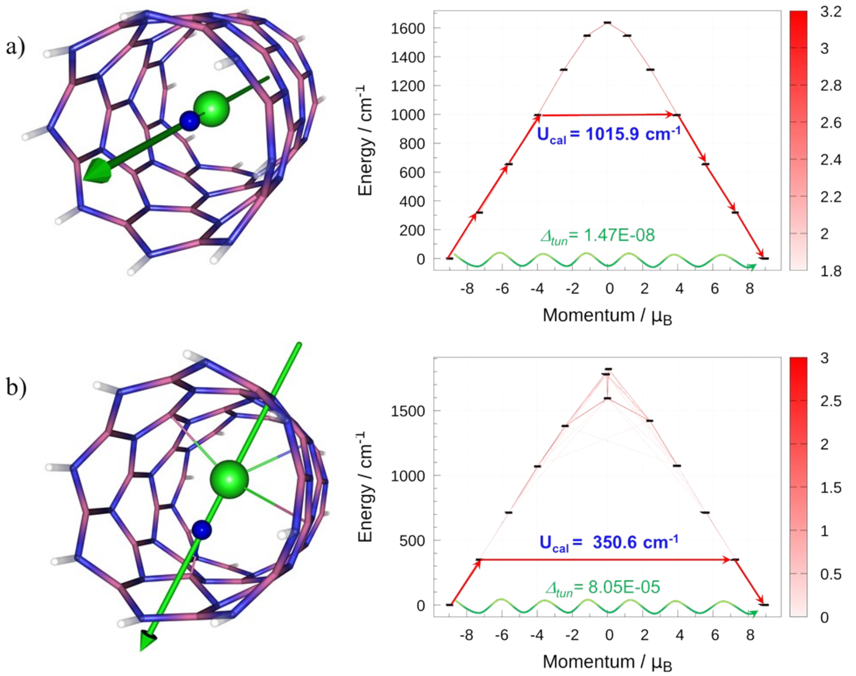


Fig. S10 CASSCF computed *g*-tensor orientation in **8Tb**$_{||}$ and **8Tb**$_{\perp}$. The solid arrow denotes the main magnetic anisotropy axis (g_{zz}). Color code: Tb (light- green), N(blue), B(pink).

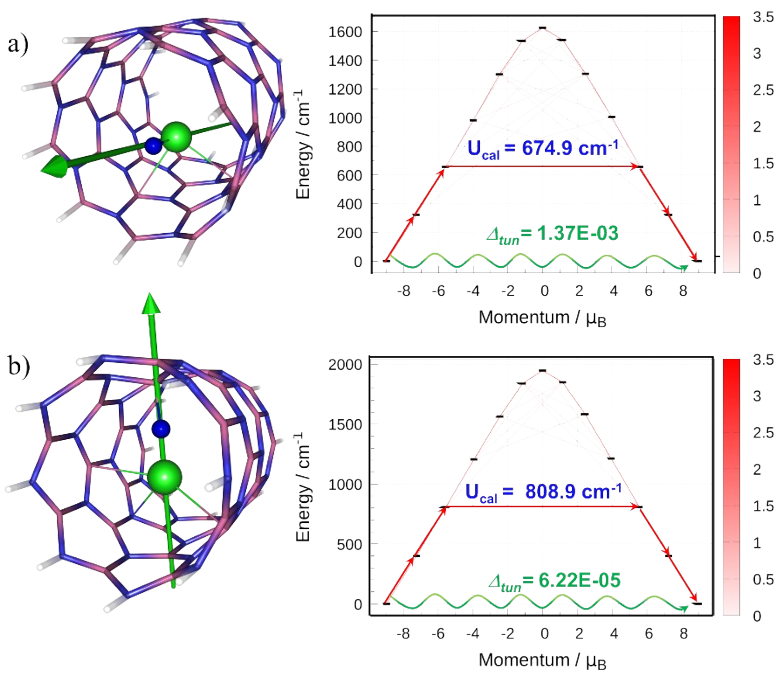


Fig. S11 CASSCF computed *g*-tensor orientation in **9Tb**$_{||}$ and **9Tb**$_{\perp}$. The solid arrow denotes the main magnetic anisotropy axis (g_{zz}). Color code: Tb (light- green), N(blue), B(pink).

SUPPORTING INFORMATION

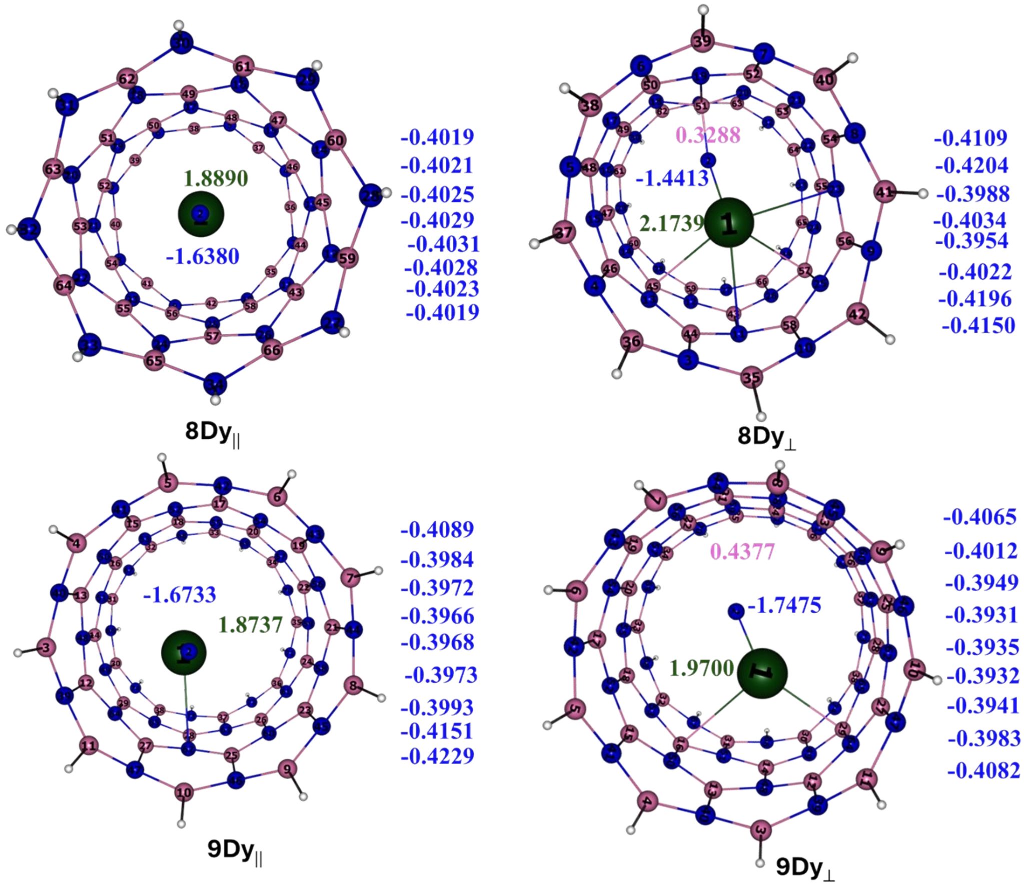


Fig. S12 CASSCF computed LoProp charges on the neareast boron and nitrogen atoms of the [DyN] molecule. Color code: Dy (green), N(blue), B(pink).

Table S8 SINGLE_ANISO computed span of the eight low-lying KDs for complexes **[DyN]**@BNNT reported in cm^{-1}.

Free	$8Dy_{\parallel}$	$9Dy_{\parallel}$	$8Dy_{\perp}$	$9Dy_{\perp}$
0.0	0.0	0.0	0.0	0.0
521.6	537.4	513.8	533.4	569.5
934.9	938.3	905.7	972.7	1038.6
1250.7	1223.9	1194.3	1304.2	1400.6
1487.4	1427.5	1397.0	1531.0	1661.9
1657.5	1570.4	1537.6	1669.5	1835.8
1767.5	1662.2	1619.6	1752.2	1939.7
1821.4	1707.0	1666.8	1844.7	1989.1

Table S9 CASSCF computed SOC states and corresponding g-tensor values **[DyN]** and **[TbN]** molecules and encapsulated **[LnN]@BNNT**. All the energies are reported in cm^{-1}.

Pristine DyN	Pristine TbN

SUPPORTING INFORMATION

SOC states ($^6H_{15/2}$)	g-values				SOC states ($^7F_6$)	g-values			
	g_{xx}	g_{yy}	g_{zz}	k_{QTM}		g_{xx}	g_{yy}	g_{zz}	Δ_{tun}
0.0	0.000	0.000	20.012	6.4E-20	0.00	0.000	0.000	18.014	0.00E+00
521.6	0.000	0.000	17.051	2.0E-17	373.97	0.000	0.000	14.514	0.00E+00
934.9	0.000	0.000	14.293	8.2E-13	756.30	0.000	0.000	11.098	0.00E+00
1250.8	0.000	0.000	11.638	2.5E-09	1133.32	0.000	0.000	7.843	0.00E+00
1487.4	0.000	0.000	9.023	4.4E-09	1475.36	0.000	0.000	4.875	6.23E-07
1657.5	0.000	0.000	6.431	6.5E-09	1726.91	0.000	0.000	2.297	1.79E-07
1767.6	0.000	0.000	3.855	3.4E-08	1820.91				
1821.4	10.598	10.598	1.284	3.5E+00					

Calculations for [DyN]@BNNT									
8Dy$_{\parallel}$						**8Dy$_{\perp}$**			
SOC states ($^6H_{15/2}$)	**g-values**				**SOC states ($^6H_{15/2}$)**	**g-values**			
	g_{xx}	g_{yy}	g_{zz}	k_{QTM}		g_{xx}	g_{yy}	g_{zz}	k_{QTM}
0.0	0.000	0.000	20.009	3.76E-10	0.0	0.000	0.000	20.005	1.26E-06
537.4	0.000	0.000	17.037	2.40E-08	533.4	0.000	0.000	17.022	9.99E-05
938.3	0.000	0.000	14.308	1.15E-07	972.7	0.008	0.009	14.177	2.96E-03
1223.9	0.001	0.001	11.679	3.36E-04	1304.2	0.167	0.181	11.398	5.80E-02
1427.5	0.013	0.015	9.071	4.64E-03	1531.0	1.244	1.337	8.564	4.32E-01
1570.4	0.012	0.016	6.471	4.67E-03	1669.5	5.790	5.251	4.262	1.70E+00
1662.2	0.106	0.110	3.880	3.60E-02	1752.2	1.664	4.514	13.479	2.76E+00
1707.0	10.713	10.496	1.293	3.53E+00	1844.7	0.110	0.252	19.413	4.93E-01
9Dy$_{\parallel}$						**9Dy$_{\perp}$**			
SOC states ($^6H_{15/2}$)	**g-values**				**SOC states ($^6H_{15/2}$)**	**g-values**			
	g_{xx}	g_{yy}	g_{zz}	k_{QTM}		g_{xx}	g_{yy}	g_{zz}	k_{QTM}
0.0	0.000	0.000	20.007	3.91E-07	0.0	0.000	0.000	20.009	1.27E-07
513.8	0.002	0.002	17.064	7.02E-04	569.5	0.000	0.000	17.015	2.35E-05
905.7	0.003	0.004	14.325	1.22E-03	1038.6	0.003	0.003	14.227	9.06E-04
1194.3	0.031	0.036	11.650	1.12E-02	1400.6	0.003	0.008	11.576	1.82E-03
1397.0	2.318	2.343	8.904	7.78E-01	1661.9	0.383	0.400	8.985	1.31E-01
1537.6	1.727	2.859	6.469	7.98E-01	1835.8	1.202	2.044	6.364	5.43E-01
1619.6	5.604	4.634	3.350	1.66E+00	1939.7	5.050	3.684	1.512	1.10E+00
1666.8	1.013	5.319	15.261	3.58E+00	1989.1	1.172	7.197	13.682	3.47E+00

Calculations for [TbN]@BNNT									
8Tb$_{\parallel}$					**8Tb$_{\perp}$**				
SOC states ($^7F_6$)	**g-values**				**SOC states ($^7F_6$)**	**g-values**			
	g_{xx}	g_{yy}	g_{zz}	Δ_{tun}		g_{xx}	g_{yy}	g_{zz}	Δ_{tun}
0.00, 0.00	0.000	0.000	17.939	1.47E-08	0.00, 0.00	0.000	0.000	17.937	8.05E-05
329.10, 329.10	0.000	0.000	14.587	1.98E-07	350.55, 350.56	0.000	0.000	14.555	1.09E-02
674.52, 674.52	0.000	0.000	11.268	5.43E-04	712.33, 712.73	0.000	0.000	11.214	4.02E-01
1015.87, 1015.94	0.000	0.000	8.071	6.73E-02	1069.82, 1074.66	0.000	0.000	7.957	4.84E+00
1321.96, 1321.98	0.000	0.000	5.104	2.15E-02	1382.25, 1421.98	0.000	0.000	4.820	3.97E+01

1544.09, 1626.48	0.000 0.000 13.370	8.24E+01	1779.79, 1821.02	0.000 0.000 15.403	4.12E+01
9Tb$_{\|\|}$			**9Tb$_{\perp}$**		
SOC states ($^7F_6$)	**g-values**		**SOC states ($^7F_6$)**	**g-values**	
	g_{xx} g_{yy} g_{zz}	***Δ_{tun}***		**g_{xx} g_{yy} g_{zz}**	***Δ_{tun}***
0.00, 0.00	0.000 0.000 17.938	1.37E-03	0.00, 0.00	0.000 0.000 17.941	6.22E-05
331.90, 331.90	0.000 0.000 14.583	6.18E-03	400.80, 400.80	0.000 0.000 14.498	2.85E-03
674.69, 674.93	0.000 0.000 11.269	2.42E-01	808.90, 808.91	0.000 0.000 11.122	1.62E-02
1001.35, 1022.20	0.000 0.000 8.083	2.09E+01	1206.21, 1212.29	0.000 0.000 7.886	6.08E+00
1311.13, 1315.53	0.000 0.000 5.115	4.40E+00	1564.06, 1581.49	0.000 0.000 4.908	1.74E+01
1529.51, 1535.73	0.000 0.000 2.452	6.22E+00	1839.15, 1848.82	0.000 0.000 2.299	9.66E+00

Table S10 SINGLE_ANISO computed wave function decomposition analysis for the **DyN@BNNT** centre.

±mJ	**[DyN]**	**8Dy$_{\|\|}$**	**8Dy$_{\perp}$**	**9Dy$_{\|\|}$**	**9Dy$_{\perp}$**
KD1	100 % |±15/2〉	100 % |±15/2〉	100 % |±15/2〉	100 % |±15/2〉	100 % |±15/2〉
KD2	100 % |±13/2〉	100 % |±13/2〉	99.7 % |±13/2〉	99.7 % |±13/2〉	100 % |±13/2〉
KD3	100 % |±11/2〉	99.9 % |±11/2〉	98.4 % |±11/2〉	98.1 % |±11/2〉	100 % |±11/2〉
KD4	100 % |±9/2〉	99.9 % |±9/2〉	95.1 % |±9/2〉	96.0 % |±9/2〉	100 % |±9/2〉
KD5	99.9 % |±7/2〉	100 % |±7/2〉	98.1 % |±7/2〉	95.3 % |±7/2〉	99.7 % |±7/2〉
KD6	99.9 % |±5/2〉	99.6 % |±5/2〉	98.6 % |±5/2〉	98.6 % |±5/2〉	98.2 % |±5/2〉
KD7	99.8 % |±3/2〉	100 % |±3/2〉	94.2 % |±3/2〉	98.1 % |±3/2〉	92.1 % |±3/2〉
KD8	99.8 % |±1/2〉	95.8 % |±1/2〉	98.4 % |±1/2〉	97.8 % |±1/2〉	93.0 % |±1/2〉

Table S11 SINGLE_ANISO computed wave function decomposition analysis for the **TbN@BNNT** centre.

±mJ		**8Tb$_{\|\|}$**	**8Tb$_{\perp}$**	**9Tb$_{\|\|}$**	**9Tb$_{\perp}$**
KD1	100 % |±6〉	100 % |±6〉	100 % |±6〉	100 % |±6〉	100 % |±6〉
KD2	100 % |±5〉	100 % |±5〉	100 % |±5〉	100 % |±5〉	100 % |±5〉
KD3	100 % |±4〉	100 % |±4〉	100 % |±4〉	100 % |±4〉	100 % |±4〉
KD4	100 % |±3〉	100 % |±3〉	100 % |±3〉	100 % |±3〉	100 % |±3〉
KD5	100 % |±2〉	100 % |±2〉	100 % |±2〉	100 % |±2〉	100 % |±2〉
KD6	100 % |±1〉	100 % |±1〉	100 % |±1〉	100 % |±1〉	100 % |±1〉
KD7	100 % |0〉	100 % |0〉	100 % |0〉	100 % |0〉	100 % |0〉

Table S12 SINGLE_ANISO computed crystal field parameters for **[DyN]@BNNT.** The CF parameters were computed using the following equation, $\hat{H}_{CF} = \Sigma \sum_{k=-q}^{q} B_k^q O_k^q$ and here B_k^q and O_k^q are the crystal field parameters and Steven's operator, respectively.

k	**q**	**[DyN]**	**8Dy$_{\|\|}$**	**8Dy$_{\perp}$**	**9Dy$_{\|\|}$**	**9Dy$_{\perp}$**

2	-2	2.13E-08	1.37E-02	-2.44E-01	1.10E-01	-4.31E-02
2	-1	-1.92E-09	1.16E-01	5.84E-01	-5.42E-01	-5.89E-02
2	0	**-2.43E+01**	**-2.24E+01**	**-2.26E+01**	**-9.75E+00**	**-1.19E+01**
2	1	2.16E-08	-1.01E-01	-1.37E+00	1.29E+00	1.27E-01
2	2	-8.42E-09	-7.19E-03	4.82E-01	-1.96E-01	1.29E-01
4	-4	-2.21E-10	8.29E-06	-6.05E-04	2.25E-04	-3.53E-04
4	-3	-2.82E-09	1.02E-05	-5.48E-05	-1.47E-03	6.30E-04
4	-2	-1.21E-11	-6.17E-05	-1.17E-03	-1.21E-03	-6.55E-04
4	-1	-4.04E-11	3.89E-04	7.94E-05	1.37E-03	4.10E-05
4	0	**-3.57E-02**	**-4.76E-02**	**-4.72E-02**	**-4.98E-03**	**-4.90E-03**
4	1	1.57E-11	-3.15E-04	-2.20E-05	-3.31E-03	-3.08E-03
4	2	1.39E-10	4.46E-05	7.41E-04	1.29E-03	-1.87E-05
4	3	8.11E-10	1.66E-05	-3.04E-04	4.60E-04	-1.91E-03
4	4	3.84E-10	2.62E-05	-1.57E-04	8.77E-04	1.30E-03
6	-6	5.60E-12	1.66E-05	-6.35E-04	1.30E-05	-8.19E-06
6	-5	4.32E-11	-8.78E-07	-3.70E-04	3.40E-05	1.37E-05
6	-4	-5.37E-12	3.40E-07	-2.62E-05	3.05E-07	-6.77E-06
6	-3	-7.67E-12	2.61E-07	-1.71E-05	-1.98E-05	1.07E-05
6	-2	-1.05E-12	7.04E-07	1.82E-04	6.67E-06	1.49E-06
6	-1	4.92E-12	-1.55E-04	**-6.64E-04**	4.48E-05	7.68E-06
6	0	**-2.23E-04**	**-3.40E-04**	-4.29E-04	1.63E-07	1.39E-05
6	1	-2.51E-11	1.33E-04	1.55E-03	**-1.06E-04**	4.71E-05
6	2	4.68E-11	1.37E-06	-2.80E-04	-3.10E-06	4.22E-05
6	3	-5.16E-11	1.35E-07	4.00E-05	-4.01E-07	**-4.40E-05**
6	4	1.15E-11	-3.02E-07	-4.35E-06	3.58E-06	-3.97E-05
6	5	1.78E-10	8.40E-07	-2.36E-04	1.09E-04	-9.93E-05
6	6	2.32E-11	-9.93E-06	-7.95E-04	-1.49E-04	3.77E-05
8	-8	-2.45E-13	1.33E-07	5.58E-08	-7.15E-10	-1.50E-10
8	-7	-3.32E-12	2.85E-08	-2.14E-07	2.65E-09	1.40E-09
8	-6	-2.58E-13	6.05E-08	-2.27E-06	-5.67E-09	3.52E-09
8	-5	3.85E-13	-1.05E-08	-3.69E-06	-5.01E-08	-2.73E-08
8	-4	7.53E-14	4.26E-09	-2.87E-07	-1.14E-09	1.71E-08
8	-3	8.95E-15	4.21E-09	2.21E-08	1.00E-07	-6.25E-08
8	-2	4.62E-13	5.90E-09	1.47E-06	-1.61E-08	4.21E-09
8	-1	-6.47E-15	-2.98E-07	-1.33E-06	-4.36E-08	-9.05E-09
8	0	**-7.18E-07**	**-8.98E-07**	-1.04E-06	4.02E-09	-3.01E-09
8	1	-6.07E-14	2.57E-07	**3.13E-06**	1.02E-07	-4.23E-08
8	2	8.24E-13	1.43E-08	-2.39E-06	1.59E-09	-2.22E-07
8	3	-1.86E-12	1.86E-09	2.90E-07	-1.35E-08	**2.59E-07**
8	4	8.62E-13	-1.83E-09	-3.51E-08	-8.26E-09	1.02E-07
8	5	5.99E-12	1.25E-08	-2.35E-06	**-1.71E-07**	2.03E-07
8	6	5.25E-13	-3.46E-08	-2.85E-06	4.93E-08	-1.58E-08
8	7	-1.73E-12	-6.07E-10	-1.01E-06	-5.42E-09	-6.41E-09
8	8	9.04E-13	1.43E-07	-7.25E-08	1.24E-09	-2.07E-10

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Table S13 SINGLE_ANISO computed crystal field parameters for **[TbN]@BNNT.** The CF parameters were computed using the following equation, $\hat{H}_{CF} = \Sigma \sum_{k=-q}^{q} B_k^q O_k^q$ and here B_k^q and O_k^q are the crystal field parameters and Steven's operator, respectively.

k	q	[TbN]	8Tb$_{\parallel}$	8Tb$_{\perp}$	9Tb$_{\parallel}$	9Tb$_{\perp}$
2	-2	5.51E-09	4.07E-03	-5.58E-03	-4.76E-02	-9.62E-02
2	-1	3.98E-09	8.22E-04	-1.90E-01	1.67E-03	1.14E-02
2	0	**-1.66E+01**	**-1.49E+01**	**-1.53E+01**	**-1.48E+01**	**-1.82E+01**
2	1	4.70E-09	-9.56E-03	-4.79E-02	-9.78E-01	-2.52E-01
2	2	9.07E-09	6.00E-03	-2.31E-01	-2.97E-01	5.91E-02
4	-4	-1.03E-10	-5.27E-06	-8.14E-05	-1.96E-03	3.28E-03
4	-3	-2.03E-10	2.80E-05	-1.57E-05	4.77E-04	-2.70E-03
4	-2	-8.74E-11	1.77E-06	-1.83E-05	1.45E-04	1.96E-03
4	-1	-3.26E-11	2.57E-05	2.29E-03	-3.03E-05	-2.97E-05
4	0	**2.19E-02**	**2.17E-02**	**2.22E-02**	**2.10E-02**	**2.82E-02**
4	1	-5.18E-11	1.13E-04	5.67E-04	1.24E-02	4.61E-03
4	2	-8.17E-11	-1.84E-05	7.54E-04	-8.79E-04	-2.63E-04
4	3	-5.10E-11	6.42E-06	-1.48E-04	-4.44E-03	1.01E-03
4	4	-2.05E-10	-6.71E-06	-1.43E-04	6.43E-04	-3.40E-03
6	-6	6.66E-14	1.14E-06	-1.32E-06	2.34E-04	8.98E-05
6	-5	8.21E-12	-6.25E-07	5.19E-06	-1.71E-04	-1.10E-04
6	-4	4.51E-13	-1.72E-08	-9.68E-08	1.02E-05	-2.35E-05
6	-3	3.24E-12	-2.26E-07	-1.58E-06	1.79E-06	3.38E-07
6	-2	1.41E-12	-1.04E-07	7.64E-07	-2.72E-06	-2.14E-05
6	-1	5.62E-14	-1.72E-06	-4.16E-06	4.72E-07	-5.35E-06
6	0	**-7.97E-05**	**-7.99E-05**	**-8.08E-05**	**-7.95E-05**	**-1.31E-04**
6	1	3.32E-13	-1.49E-07	-6.91E-07	-5.81E-05	-8.61E-05
6	2	4.33E-13	1.75E-07	-1.11E-05	3.33E-05	-1.85E-05
6	3	7.90E-13	5.12E-08	1.29E-06	1.68E-05	1.28E-05
6	4	1.12E-12	1.13E-07	5.11E-07	-6.50E-06	6.72E-05
6	5	-2.02E-11	2.13E-07	8.64E-07	1.94E-04	6.86E-05
6	6	2.77E-13	8.90E-08	2.33E-05	-2.67E-04	-6.38E-05
8	-8	-1.13E-19	3.46E-12	6.12E-11	-4.09E-08	2.51E-09
8	-7	-4.48E-15	4.24E-12	1.75E-09	1.74E-07	4.05E-08
8	-6	-1.45E-15	-4.75E-09	5.59E-09	-9.67E-07	-3.85E-07
8	-5	-1.10E-13	1.18E-08	-1.04E-07	3.27E-06	2.25E-06
8	-4	6.08E-15	6.75E-10	7.77E-09	-8.33E-08	2.34E-07
8	-3	-1.38E-13	5.03E-09	6.64E-08	-9.92E-08	4.48E-07
8	-2	-1.62E-14	2.97E-09	-1.95E-08	5.26E-08	2.64E-07
8	-1	-8.03E-15	8.91E-09	-4.18E-08	-8.50E-10	3.70E-08
8	0	**8.45E-08**	**9.32E-08**	9.15E-08	9.69E-08	2.01E-07
8	1	-4.96E-15	-2.16E-09	-1.16E-08	5.65E-09	4.00E-07
8	2	6.68E-15	-1.77E-09	**1.88E-07**	**-8.08E-07**	**7.21E-07**
8	3	-2.64E-14	-2.60E-09	-2.78E-08	-1.29E-07	-7.16E-07
8	4	-3.41E-15	-1.79E-09	3.06E-10	1.12E-07	-1.30E-06
8	5	3.53E-13	-4.18E-09	-1.61E-08	-3.68E-06	-1.43E-06
8	6	-2.62E-15	-3.65E-10	-9.84E-08	1.10E-06	2.74E-07
8	7	-2.95E-14	-1.61E-12	6.41E-10	-2.05E-07	-2.33E-08
8	8	-7.53E-20	-2.48E-12	-2.51E-09	5.74E-08	-5.14E-09

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Table S14 pDFT optimized coordinates of LnN@BNNT.

8Dy$_{\parallel}$				8Dy$_{\perp}$			
N	11.5037	4.8163	1.3907	N	11.5909	4.8027	1.3922
N	11.0168	6.0059	3.5189	N	11.0497	5.9535	3.5251
N	10.1046	6.9108	1.3908	N	10.0889	6.8252	1.3996
N	8.9190	7.4085	3.5186	N	8.8892	7.2644	3.5272
N	7.6342	7.4021	1.3904	N	7.6179	7.3287	1.3930
N	6.4434	6.9171	3.5182	N	6.3996	6.8872	3.5135
N	5.5394	6.0034	1.3902	N	5.4637	6.0227	1.3801
N	5.0397	4.8188	3.5181	N	4.9380	4.8420	3.5064
N	5.0470	3.5329	1.3901	N	4.9856	3.5555	1.3768
N	5.5322	2.3423	3.5181	N	5.4894	2.3756	3.5062
N	6.4469	1.4384	1.3903	N	6.4548	1.5138	1.3821
N	7.6318	0.9403	3.5182	N	7.6445	1.0737	3.5181
N	8.9176	0.9470	1.3902	N	8.9320	1.0405	1.3980
N	10.1070	1.4331	3.5183	N	10.1367	1.4953	3.5271
N	11.0124	2.3459	1.3903	N	11.0909	2.3370	1.3944
N	11.5085	3.5311	3.5187	N	11.6548	3.5086	3.5169
N	11.4608	4.8078	5.6552	N	11.6841	4.7998	5.6527
N	11.0302	6.0147	7.7878	N	11.0161	5.9191	7.7854
N	10.0801	6.8740	5.6552	N	10.0284	6.6945	5.6588
N	8.9228	7.4246	7.7878	N	8.8773	7.2580	7.7796
N	7.6434	7.3577	5.6552	N	7.5941	7.3090	5.6499
N	6.4346	6.9315	7.7879	N	6.3584	6.9814	7.7814
N	5.5793	5.9776	5.6551	N	5.4031	6.0687	5.6434
N	5.0242	4.8225	7.7880	N	4.9039	4.8985	7.7839
N	5.0959	3.5429	5.6552	N	5.0566	3.5751	5.6365
N	5.5198	2.3338	7.7880	N	5.4899	2.3188	7.7850
N	6.4743	1.4784	5.6551	N	6.4050	1.4508	5.6432
N	7.6293	0.9245	7.7877	N	7.6310	0.9515	7.7797
N	8.9094	0.9912	5.6549	N	8.9032	1.1844	5.6558
N	10.1167	1.4195	7.7874	N	10.0916	1.5675	7.7801
N	10.9761	2.3703	5.6548	N	11.1338	2.3438	5.6554
N	11.5245	3.5281	7.7875	N	11.6823	3.5058	7.7955
N	11.5026	4.8161	9.9146	N	11.6068	4.8012	9.9231
N	11.0116	6.0020	12.0431	N	11.0348	5.9633	12.0465
N	10.1044	6.9100	9.9148	N	10.0751	6.8023	9.9107
N	8.9184	7.4009	12.0430	N	8.9000	7.2999	12.0434
N	7.6348	7.4015	9.9146	N	7.6108	7.3319	9.9110
N	6.4490	6.9099	12.0427	N	6.4147	6.8999	12.0407
N	5.5405	6.0033	9.9145	N	5.4425	6.0536	9.9124
N	5.0492	4.8170	12.0427	N	4.9727	4.8410	12.0269
N	5.0491	3.5336	9.9146	N	5.0238	3.5634	9.8923
N	5.5404	2.3475	12.0428	N	5.5299	2.3887	12.0279

N	6.4483	1.4401	9.9146	N	6.4430	1.4690	9.9128
N	7.6340	0.9486	12.0427	N	7.6554	1.0379	12.0429
N	8.9177	0.9480	9.9144	N	8.9259	1.0398	9.9092
N	10.1037	1.4391	12.0427	N	10.1340	1.4763	12.0449
N	11.0118	2.3465	9.9143	N	11.0858	2.3444	9.9179
N	11.5026	3.5325	12.0427	N	11.6135	3.5130	12.0479
N	8.2577	4.1735	7.3393	N	7.0977	4.0286	7.0065
B	11.4359	4.8030	2.8135	B	11.5351	4.7823	2.8116
B	10.9503	5.9611	0.6855	B	10.9760	5.9242	0.6932
B	10.0663	6.8539	2.8135	B	10.0464	6.7586	2.8234
B	8.9039	7.3288	0.6854	B	8.8786	7.2372	0.6923
B	7.6471	7.3355	2.8130	B	7.6085	7.2485	2.8176
B	6.4896	6.8486	0.6848	B	6.4437	6.8270	0.6839
B	5.5954	5.9658	2.8127	B	5.5099	5.9674	2.8075
B	5.1210	4.8025	0.6849	B	5.0410	4.8216	0.6689
B	5.1132	3.5461	2.8127	B	5.0463	3.5730	2.8089
B	5.6011	2.3881	0.6850	B	5.5759	2.4361	0.6702
B	6.4844	1.4948	2.8129	B	6.4661	1.5791	2.8082
B	7.6481	1.0206	0.6850	B	7.6566	1.1141	0.6882
B	8.9040	1.0140	2.8129	B	8.9059	1.1185	2.8221
B	10.0627	1.5004	0.6850	B	10.0929	1.5349	0.6925
B	10.9547	2.3842	2.8130	B	11.0398	2.3804	2.8149
B	11.4304	3.5469	0.6852	B	11.5312	3.5289	0.6917
B	11.3936	4.7945	7.0976	B	11.5963	4.7798	7.0870
B	10.9514	5.9618	4.9453	B	11.0100	5.8953	4.9429
B	10.0420	6.8174	7.0978	B	10.0263	6.7383	7.0933
B	8.9046	7.3308	4.9450	B	8.8393	7.1861	4.9467
B	7.6563	7.2914	7.0983	B	7.5800	7.2596	7.0839
B	6.4885	6.8515	4.9443	B	6.3964	6.8306	4.9460
B	5.6349	5.9403	7.0987	B	5.4832	6.0154	7.0867
B	5.1189	4.8036	4.9442	B	5.0270	4.8216	4.9489
B	5.1612	3.5560	7.0989	B	5.5652	3.6948	7.0697
B	5.6000	2.3869	4.9442	B	5.5458	2.4350	4.9487
B	6.5114	1.5344	7.0985	B	6.4497	1.5206	7.0877
B	7.6486	1.0184	4.9444	B	7.6103	1.1440	4.9434
B	8.8958	1.0577	7.0978	B	8.8746	1.1203	7.0931
B	10.0641	1.4991	4.9447	B	10.1022	1.5695	4.9445
B	10.9191	2.4082	7.0973	B	11.0783	2.3766	7.0907
B	11.4315	3.5467	4.9451	B	11.6283	3.5199	4.9367
B	11.4286	4.8014	11.3376	B	11.5118	4.7839	11.3525
B	10.9484	5.9600	9.2124	B	10.9671	5.9003	9.2273
B	10.0623	6.8470	11.3377	B	10.0440	6.7655	11.3437
B	8.9037	7.3271	9.2124	B	8.8612	7.2147	9.2154
B	7.6496	7.3269	11.3374	B	7.6207	7.2636	11.3383
B	6.4904	6.8481	9.2124	B	6.4127	6.8575	9.2051

B	5.6037	5.9608	11.3373	B	5.5254	5.9844	11.3266
B	5.1228	4.8027	9.2124	B	5.0083	4.8474	9.1784
B	5.1233	3.5481	11.3374	B	5.0809	3.5773	11.3051
B	5.6032	2.3896	9.2124	B	5.5569	2.4012	9.1819
B	6.4903	1.5029	11.3374	B	6.4882	1.5589	11.3297
B	7.6488	1.0226	9.2122	B	7.6354	1.0729	9.2094
B	8.9029	1.0225	11.3373	B	8.9128	1.0966	11.3408
B	10.0617	1.5019	9.2120	B	10.0697	1.5721	9.2245
B	10.9487	2.3886	11.3372	B	11.0191	2.3833	11.3494
B	11.4281	3.5473	9.2122	B	11.5576	3.5275	9.2307
Dy	8.2454	4.1736	5.4630	Dy	8.9196	4.0638	6.4642
	$9Dy_{\parallel}$				**$9Dy_{\perp}$**		
B	12.3524	5.7330	0.6458	B	12.4001	5.7324	0.6456
B	11.1150	7.8703	0.6477	B	11.1420	7.8627	0.6429
B	11.9328	6.9083	2.7743	B	11.9775	6.9180	2.7646
B	8.7945	8.7157	0.6482	B	8.8066	8.6873	0.6417
B	10.0296	8.4955	2.7754	B	10.0464	8.4744	2.7725
B	6.4729	7.8711	0.6492	B	6.4790	7.8473	0.6377
B	7.5600	8.4978	2.7767	B	7.5657	8.4637	2.7702
B	5.2387	5.7325	0.6500	B	5.2410	5.7102	0.6344
B	5.6712	6.9095	2.7790	B	5.6703	6.8822	2.7677
B	5.6687	3.3003	0.6492	B	5.6579	3.2777	0.6348
B	5.2423	4.4784	2.7787	B	5.2337	4.4566	2.7673
B	7.5622	1.7138	0.6483	B	7.5526	1.6952	0.6389
B	6.4770	2.3418	2.7764	B	6.4615	2.3233	2.7688
B	10.0329	1.7166	0.6473	B	10.0262	1.7179	0.6417
B	8.8004	1.4990	2.7756	B	8.7847	1.4956	2.7704
B	11.9258	3.3017	0.6461	B	11.9316	3.3008	0.6434
B	11.1328	2.3369	2.7737	B	11.1119	2.3493	2.7736
B	12.3848	4.4736	2.7704	B	12.3922	4.4768	2.7669
B	12.3211	5.7321	4.8737	B	12.4496	5.7478	4.8832
B	11.0753	7.8595	4.8898	B	11.1586	7.8560	4.8944
B	11.9133	6.9060	7.0434	B	12.0249	6.9048	7.0364
B	8.7798	8.7231	4.8984	B	8.7906	8.6572	4.8991
B	10.0212	8.5111	7.0365	B	10.0370	8.4471	7.0369
B	6.4699	7.8727	4.9028	B	6.4667	7.8297	4.9003
B	7.5475	8.5163	7.0356	B	7.5558	8.4483	7.0267
B	5.2435	5.7320	4.9041	B	5.2271	5.7020	4.9018
B	5.6593	6.9153	7.0357	B	5.6775	6.8686	7.0230
B	5.6617	3.3007	4.9020	B	5.6468	3.2819	4.9021
B	5.2281	4.4775	7.0360	B	5.2713	4.4604	7.0199
B	7.5439	1.7183	4.8971	B	7.5364	1.7089	4.9025

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B	6.4569	2.3295	7.0357	B	6.4640	2.3370	7.0228
B	9.9974	1.7488	4.8863	B	9.9995	1.7341	4.9007
B	8.7865	1.4939	7.0379	B	8.7679	1.5053	7.0269
B	11.8983	3.3186	4.8709	B	11.9255	3.3180	4.8984
B	11.1156	2.3493	7.0458	B	11.0772	2.3777	7.0352
B	12.3716	4.4761	7.0478	B	12.4280	4.5132	7.0387
B	12.3710	5.7352	9.1723	B	12.4890	5.7510	9.1773
B	11.1128	7.8730	9.1699	B	11.1490	7.8379	9.1759
B	11.9204	6.9126	11.2970	B	11.9786	6.9126	11.3026
B	8.7896	8.7220	9.1689	B	8.8039	8.6668	9.1639
B	10.0284	8.5020	11.2981	B	10.0453	8.4641	11.2947
B	6.4673	7.8752	9.1683	B	6.4732	7.8430	9.1532
B	7.5565	8.5019	11.2990	B	7.5691	8.4670	11.2884
B	5.2329	5.7337	9.1679	B	5.2320	5.7081	9.1478
B	5.6633	6.9127	11.2987	B	5.6722	6.8874	11.2830
B	5.6613	3.2985	9.1685	B	5.6466	3.2716	9.1472
B	5.2344	4.4784	11.2990	B	5.2356	4.4553	11.2805
B	7.5556	1.7108	9.1694	B	7.5420	1.6926	9.1527
B	6.4714	2.3384	11.2989	B	6.4599	2.3128	11.2834
B	10.0312	1.7136	9.1705	B	10.0126	1.7333	9.1615
B	8.7951	1.4954	11.2979	B	8.7875	1.4930	11.2887
B	11.9472	3.2907	9.1732	B	11.9113	3.3377	9.1751
B	11.1162	2.3417	11.2970	B	11.1073	2.3600	11.2940
B	12.3527	4.4804	11.2973	B	12.3951	4.4800	11.3014
N	11.9829	6.9445	1.3469	N	12.0241	6.9466	1.3431
N	12.4806	5.7505	3.4665	N	12.4901	5.7506	3.4647
N	10.0531	8.5615	1.3487	N	10.0713	8.5360	1.3462
N	11.1703	7.9300	3.4751	N	11.1952	7.9127	3.4737
N	7.5364	8.5626	1.3493	N	7.5514	8.5345	1.3423
N	8.7944	8.7953	3.4772	N	8.8118	8.7378	3.4759
N	5.6088	6.9447	1.3513	N	5.6164	6.9231	1.3382
N	6.4266	7.9289	3.4797	N	6.4410	7.8929	3.4708
N	5.1724	4.4661	1.3510	N	5.1711	4.4469	1.3370
N	5.1709	5.7446	3.4810	N	5.1712	5.7225	3.4676
N	6.4327	2.2885	1.3494	N	6.4235	2.2654	1.3394
N	5.6037	3.2618	3.4793	N	5.5966	3.2443	3.4681
N	8.7989	1.4292	1.3484	N	8.7970	1.4243	1.3422
N	7.5355	1.6396	3.4769	N	7.5320	1.6394	3.4714
N	11.1652	2.2881	1.3466	N	11.1596	2.2993	1.3463
N	10.0676	1.6351	3.4742	N	10.0480	1.6694	3.4759
N	12.4300	4.4664	1.3438	N	12.4485	4.4634	1.3445
N	12.0466	3.2370	3.4647	N	11.9891	3.2793	3.4772
N	11.8960	6.9026	5.6121	N	12.0630	6.9529	5.6001
N	12.4513	5.7484	7.7420	N	12.6222	5.7754	7.7516
N	10.0337	8.5590	5.6103	N	10.0570	8.4680	5.6088

N	11.1503	7.9199	7.7389	N	11.1671	7.8457	7.7379
N	7.5263	8.5724	5.6100	N	7.5423	8.5215	5.6018
N	8.7881	8.7914	7.7401	N	8.8079	8.7182	7.7335
N	5.6120	6.9433	5.6109	N	5.5887	6.9266	5.5973
N	6.4255	7.9267	7.7399	N	6.4274	7.9017	7.7305
N	5.1735	4.4675	5.6109	N	5.1244	4.4385	5.5943
N	5.1723	5.7444	7.7397	N	5.1543	5.7245	7.7300
N	6.4167	2.2836	5.6102	N	6.3973	2.2513	5.5965
N	5.6033	3.2649	7.7401	N	5.5727	3.2287	7.7308
N	8.7802	1.4557	5.6106	N	8.7827	1.4258	5.6021
N	7.5304	1.6478	7.7400	N	7.5185	1.6186	7.7311
N	11.0913	2.3702	5.6130	N	11.1233	2.3484	5.6092
N	10.0515	1.6554	7.7395	N	10.0364	1.6761	7.7340
N	12.3569	4.4810	5.6120	N	12.4526	4.4843	5.6037
N	12.0236	3.2477	7.7425	N	11.9119	3.3514	7.7354
N	11.9808	6.9443	9.8668	N	12.0595	6.9536	9.8747
N	12.4138	5.7458	11.9962	N	12.4774	5.7459	12.0022
N	10.0501	8.5633	9.8681	N	10.0702	8.5070	9.8632
N	11.1579	7.9244	11.9972	N	11.1843	7.9042	11.9964
N	7.5330	8.5646	9.8696	N	7.5513	8.5265	9.8609
N	8.7936	8.7855	11.9988	N	8.8123	8.7450	11.9925
N	5.6051	6.9459	9.8696	N	5.6137	6.9223	9.8591
N	6.4286	7.9236	11.9997	N	6.4413	7.9005	11.9904
N	5.1686	4.4666	9.8697	N	5.1703	4.4447	9.8582
N	5.1711	5.7447	12.0004	N	5.1812	5.7230	11.9879
N	6.4280	2.2872	9.8697	N	6.4151	2.2588	9.8598
N	5.6085	3.2661	11.9998	N	5.6006	3.2414	11.9886
N	8.7954	1.4302	9.8677	N	8.7906	1.4286	9.8620
N	7.5372	1.6490	11.9982	N	7.5329	1.6303	11.9919
N	11.1636	2.2891	9.8671	N	11.1420	2.3310	9.8620
N	10.0536	1.6525	11.9972	N	10.0503	1.6673	11.9928
N	12.4309	4.4660	9.8681	N	12.4786	4.4731	9.8723
N	11.9790	3.2698	11.9963	N	11.9848	3.2785	11.9960
N	9.3465	4.9557	4.1270	N	7.9844	4.8453	6.5487
Dy	9.6464	4.8756	5.9794	Dy	9.7704	5.3195	6.7278
	$8Tb_{\parallel}$				**$8Tb_{\perp}$**		
N	11.5081	4.8168	1.3905	N	11.5975	4.7977	1.3926
N	11.0121	6.0021	3.5172	N	11.0502	5.9492	3.5243
N	10.1076	6.9149	1.3905	N	10.0914	6.8172	1.3993
N	8.9182	7.4025	3.5177	N	8.8886	7.2589	3.5274
N	7.6333	7.4063	1.3911	N	7.6215	7.3179	1.3920
N	6.4473	6.9107	3.5181	N	6.3952	6.8867	3.5120
N	5.5348	6.0060	1.3912	N	5.4645	6.0206	1.3787
N	5.0451	4.8168	3.5176	N	4.9214	4.8480	3.5054

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N	5.0432	3.5320	1.3902	N	4.9810	3.5579	1.3770
N	5.5364	2.3447	3.5168	N	5.4932	2.3852	3.5063
N	6.4447	1.4353	1.3897	N	6.4603	1.5245	1.3819
N	7.6322	0.9449	3.5169	N	7.6493	1.0840	3.5172
N	8.9181	0.9420	1.3904	N	8.9375	1.0479	1.3967
N	10.1033	1.4371	3.5176	N	10.1437	1.4922	3.5265
N	11.0162	2.3426	1.3909	N	11.1047	2.3311	1.3945
N	11.5041	3.5313	3.5174	N	11.6594	3.5057	3.5169
N	11.4593	4.8075	5.6534	N	11.6858	4.7982	5.6510
N	11.0292	6.0135	7.7867	N	11.0284	5.9179	7.7850
N	10.0796	6.8736	5.6536	N	10.0340	6.6972	5.6574
N	8.9231	7.4222	7.7874	N	8.8668	7.2116	7.7789
N	7.6430	7.3588	5.6542	N	7.5903	7.2860	5.6496
N	6.4378	6.9279	7.7879	N	6.3443	6.9807	7.7826
N	5.5771	5.9786	5.6541	N	5.3858	6.0747	5.6425
N	5.0290	4.8219	7.7873	N	4.8854	4.9019	7.7849
N	5.0937	3.5424	5.6535	N	5.0490	3.5830	5.6356
N	5.5253	2.3369	7.7866	N	5.4789	2.3218	7.7850
N	6.4736	1.4778	5.6532	N	6.4122	1.4702	5.6428
N	7.6311	0.9270	7.7869	N	7.6341	0.9708	7.7800
N	8.9088	0.9909	5.6538	N	8.9082	1.1822	5.6551
N	10.1171	1.4204	7.7873	N	10.0993	1.5653	7.7793
N	10.9740	2.3712	5.6538	N	11.1407	2.3395	5.6544
N	11.5238	3.5282	7.7869	N	11.6906	3.5031	7.7937
N	11.5025	4.8160	9.9155	N	11.6183	4.7974	9.9226
N	11.0133	6.0028	12.0443	N	11.0418	5.9582	12.0461
N	10.1046	6.9105	9.9156	N	10.0757	6.7892	9.9096
N	8.9190	7.4033	12.0448	N	8.9010	7.2877	12.0414
N	7.6346	7.4014	9.9164	N	7.6073	7.3091	9.9095
N	6.4487	6.9098	12.0453	N	6.4130	6.8942	12.0397
N	5.5395	6.0035	9.9163	N	5.4222	6.0594	9.9134
N	5.0479	4.8168	12.0445	N	4.9550	4.8451	12.0274
N	5.0483	3.5332	9.9149	N	5.0014	3.5671	9.8930
N	5.5393	2.3467	12.0433	N	5.5248	2.3955	12.0282
N	6.4479	1.4388	9.9146	N	6.4489	1.4935	9.9124
N	7.6336	0.9477	12.0437	N	7.6610	1.0601	12.0413
N	8.9182	0.9471	9.9156	N	8.9300	1.0580	9.9089
N	10.1042	1.4379	12.0448	N	10.1443	1.4766	12.0438
N	11.0122	2.3461	9.9160	N	11.1036	2.3386	9.9168
N	11.5047	3.5317	12.0447	N	11.6248	3.5100	12.0481
N	8.2570	4.1702	7.3490	N	7.0815	4.0356	7.0234
B	11.4350	4.8020	2.8122	B	11.5382	4.7782	2.8117
B	10.9548	5.9640	0.6864	B	10.9818	5.9178	0.6934
B	10.0657	6.8526	2.8122	B	10.0471	6.7533	2.8233
B	8.9049	7.3343	0.6867	B	8.8821	7.2275	0.6909

B	7.6475	7.3334	2.8128	B	7.6087	7.2412	2.8171
B	6.4867	6.8523	0.6874	B	6.4462	6.8212	0.6826
B	5.5962	5.9643	2.8128	B	5.5038	5.9689	2.8058
B	5.1163	4.8034	0.6865	B	5.0338	4.8231	0.6687
B	5.1144	3.5458	2.8120	B	5.0414	3.5785	2.8090
B	5.5976	2.3859	0.6853	B	5.5749	2.4412	0.6709
B	6.4846	1.4955	2.8115	B	6.4717	1.5903	2.8084
B	7.6471	1.0162	0.6856	B	7.6625	1.1273	0.6869
B	8.9031	1.0143	2.8121	B	8.9115	1.1232	2.8213
B	10.0652	1.4958	0.6868	B	10.1030	1.5346	0.6916
B	10.9539	2.3837	2.8126	B	11.0489	2.3760	2.8148
B	11.4355	3.5452	0.6868	B	11.5419	3.5243	0.6920
B	11.3931	4.7941	7.0956	B	11.6037	4.7770	7.0852
B	10.9492	5.9607	4.9429	B	11.0128	5.8938	4.9416
B	10.0420	6.8167	7.0957	B	10.0288	6.7247	7.0917
B	8.9035	7.3290	4.9434	B	8.8378	7.1758	4.9469
B	7.6571	7.2907	7.0966	B	7.5709	7.2334	7.0839
B	6.4892	6.8492	4.9439	B	6.3873	6.8263	4.9440
B	5.6361	5.9401	7.0966	B	5.4645	6.0192	7.0868
B	5.1201	4.8032	4.9433	B	5.0101	4.8286	4.9479
B	5.1637	3.5568	7.0960	B	5.5474	3.6995	7.0720
B	5.6006	2.3878	4.9426	B	5.5478	2.4471	4.9479
B	6.5137	1.5359	7.0958	B	6.4515	1.5367	7.0883
B	7.6480	1.0195	4.9427	B	7.6156	1.1552	4.9425
B	8.8968	1.0582	7.0963	B	8.8796	1.1241	7.0925
B	10.0621	1.5002	4.9433	B	10.1078	1.5672	4.9440
B	10.9188	2.4085	7.0961	B	11.0853	2.3741	7.0888
B	11.4294	3.5468	4.9430	B	11.6309	3.5177	4.9363
B	11.4309	4.8015	11.3387	B	11.5223	4.7798	11.3521
B	10.9476	5.9595	9.2119	B	10.9760	5.8949	9.2266
B	10.0637	6.8492	11.3388	B	10.0474	6.7559	11.3431
B	8.9032	7.3260	9.2124	B	8.8561	7.1828	9.2153
B	7.6492	7.3287	11.3394	B	7.6211	7.2484	11.3370
B	6.4914	6.8460	9.2129	B	6.4005	6.8536	9.2061
B	5.6018	5.9616	11.3392	B	5.5124	5.9867	11.3274
B	5.1246	4.8023	9.2120	B	4.9859	4.8522	9.1802
B	5.1207	3.5475	11.3379	B	5.0646	3.5809	11.3061
B	5.6054	2.3907	9.2111	B	5.5480	2.4103	9.1821
B	6.4887	1.5008	11.3375	B	6.4928	1.5787	11.3293
B	7.6495	1.0233	9.2116	B	7.6403	1.0962	9.2098
B	8.9033	1.0203	11.3385	B	8.9190	1.1118	11.3399
B	10.0618	1.5023	9.2124	B	10.0800	1.5744	9.2233
B	10.9507	2.3870	11.3390	B	11.0342	2.3798	11.3482
B	11.4273	3.5472	9.2120	B	11.5716	3.5237	9.2296
Tb	8.2631	4.1677	5.4692	Tb	8.9106	4.0764	6.4901

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9Tb$_{\|\|}$				9Tb$_{\perp}$			
B	12.3535	5.7330	0.6475	B	12.3923	5.7309	0.6469
B	11.1145	7.8700	0.6482	B	11.1365	7.8628	0.6449
B	11.9305	6.9096	2.7744	B	11.9696	6.9169	2.7670
B	8.7938	8.7158	0.6479	B	8.8043	8.6964	0.6427
B	10.0290	8.4959	2.7746	B	10.0444	8.4809	2.7736
B	6.4734	7.8715	0.6479	B	6.4798	7.8530	0.6386
B	7.5599	8.4975	2.7750	B	7.5644	8.4723	2.7720
B	5.2390	5.7325	0.6483	B	5.2473	5.7130	0.6342
B	5.6716	6.9092	2.7763	B	5.6717	6.8844	2.7689
B	5.6689	3.3008	0.6479	B	5.6659	3.2815	0.6337
B	5.2431	4.4785	2.7763	B	5.2376	4.4581	2.7669
B	7.5622	1.7150	0.6481	B	7.5561	1.6974	0.6378
B	6.4763	2.3414	2.7751	B	6.4642	2.3245	2.7673
B	10.0323	1.7161	0.6484	B	10.0282	1.7134	0.6420
B	8.7986	1.4985	2.7749	B	8.7864	1.4927	2.7716
B	11.9268	3.3006	0.6476	B	11.9316	3.2977	0.6449
B	11.1297	2.3369	2.7740	B	11.1128	2.3447	2.7757
B	12.3802	4.4738	2.7711	B	12.3864	4.4747	2.7693
B	12.3213	5.7327	4.8759	B	12.4427	5.7448	4.8845
B	11.0757	7.8593	4.8899	B	11.1550	7.8607	4.8959
B	11.9157	6.9060	7.0437	B	12.0191	6.9084	7.0383
B	8.7789	8.7219	4.8968	B	8.7913	8.6696	4.8999
B	10.0235	8.5097	7.0362	B	10.0402	8.4589	7.0369
B	6.4682	7.8733	4.9000	B	6.4667	7.8339	4.9005
B	7.5497	8.5127	7.0343	B	7.5574	8.4565	7.0274
B	5.2409	5.7325	4.9005	B	5.2315	5.7000	4.9016
B	5.6615	6.9144	7.0338	B	5.6792	6.8707	7.0232
B	5.6611	3.3016	4.8992	B	5.6425	3.2744	4.9013
B	5.2304	4.4776	7.0335	B	5.2720	4.4603	7.0183
B	7.5449	1.7209	4.8957	B	7.5320	1.6988	4.9014
B	6.4603	2.3312	7.0343	B	6.4694	2.3405	7.0202
B	9.9986	1.7451	4.8869	B	9.9981	1.7286	4.9012
B	8.7889	1.4936	7.0372	B	8.7698	1.4984	7.0262
B	11.8979	3.3154	4.8735	B	11.9304	3.3129	4.8981
B	11.1183	2.3469	7.0455	B	11.0819	2.3710	7.0358
B	12.3688	4.4760	7.0478	B	12.4293	4.5087	7.0397
B	12.3757	5.7354	9.1732	B	12.4753	5.7495	9.1782
B	11.1162	7.8738	9.1707	B	11.1482	7.8458	9.1772
B	11.9220	6.9116	11.2980	B	11.9699	6.9110	11.3023
B	8.7919	8.7220	9.1689	B	8.8040	8.6764	9.1642
B	10.0287	8.4997	11.2984	B	10.0432	8.4717	11.2956
B	6.4688	7.8763	9.1673	B	6.4746	7.8484	9.1535
B	7.5577	8.5013	11.2978	B	7.5681	8.4769	11.2896

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B	5.2343	5.7335	9.1665	B	5.2381	5.7105	9.1476
B	5.6656	6.9120	11.2973	B	5.6738	6.8918	11.2836
B	5.6626	3.2981	9.1677	B	5.6508	3.2730	9.1469
B	5.2373	4.4784	11.2973	B	5.2427	4.4592	11.2800
B	7.5578	1.7108	9.1693	B	7.5451	1.6921	9.1522
B	6.4731	2.3385	11.2982	B	6.4660	2.3158	11.2822
B	10.0338	1.7105	9.1714	B	10.0152	1.7288	9.1620
B	8.7963	1.4964	11.2982	B	8.7924	1.4873	11.2885
B	11.9501	3.2892	9.1737	B	11.9137	3.3330	9.1757
B	11.1183	2.3412	11.2981	B	11.1138	2.3502	11.2942
B	12.3564	4.4793	11.2987	B	12.3921	4.4761	11.3021
N	11.9821	6.9450	1.3478	N	12.0162	6.9447	1.3453
N	12.4727	5.7502	3.4672	N	12.4806	5.7488	3.4660
N	10.0523	8.5612	1.3483	N	10.0680	8.5409	1.3474
N	11.1689	7.9312	3.4748	N	11.1919	7.9163	3.4747
N	7.5362	8.5624	1.3483	N	7.5498	8.5431	1.3440
N	8.7940	8.7963	3.4758	N	8.8102	8.7491	3.4768
N	5.6097	6.9445	1.3491	N	5.6208	6.9258	1.3393
N	6.4256	7.9300	3.4773	N	6.4388	7.8993	3.4711
N	5.1734	4.4667	1.3490	N	5.1776	4.4495	1.3364
N	5.1689	5.7447	3.4778	N	5.1758	5.7234	3.4679
N	6.4322	2.2885	1.3482	N	6.4293	2.2696	1.3379
N	5.6027	3.2615	3.4770	N	5.5971	3.2438	3.4669
N	8.7975	1.4295	1.3484	N	8.7981	1.4249	1.3431
N	7.5348	1.6398	3.4758	N	7.5327	1.6370	3.4704
N	11.1643	2.2877	1.3476	N	11.1600	2.2962	1.3485
N	10.0649	1.6353	3.4738	N	10.0496	1.6629	3.4768
N	12.4298	4.4661	1.3451	N	12.4418	4.4628	1.3470
N	12.0392	3.2392	3.4660	N	11.9906	3.2739	3.4774
N	11.8988	6.9052	5.6125	N	12.0512	6.9487	5.6013
N	12.4552	5.7487	7.7429	N	12.6089	5.7741	7.7524
N	10.0329	8.5567	5.6098	N	10.0588	8.4852	5.6085
N	11.1537	7.9208	7.7401	N	11.1720	7.8605	7.7391
N	7.5269	8.5691	5.6085	N	7.5426	8.5280	5.6021
N	8.7902	8.7890	7.7401	N	8.8090	8.7274	7.7334
N	5.6117	6.9428	5.6084	N	5.5931	6.9254	5.5976
N	6.4275	7.9260	7.7393	N	6.4298	7.9047	7.7299
N	5.1733	4.4678	5.6084	N	5.1238	4.4354	5.5928
N	5.1739	5.7438	7.7384	N	5.1599	5.7251	7.7294
N	6.4186	2.2866	5.6088	N	6.3895	2.2384	5.5946
N	5.6057	3.2652	7.7391	N	5.5770	3.2308	7.7305
N	8.7806	1.4553	5.6102	N	8.7803	1.4159	5.6011
N	7.5338	1.6500	7.7399	N	7.5216	1.6188	7.7303
N	11.0956	2.3623	5.6129	N	11.1227	2.3454	5.6090
N	10.0543	1.6525	7.7403	N	10.0384	1.6713	7.7339

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N	12.3510	4.4806	5.6121	N	12.4601	4.4800	5.6039
N	12.0258	3.2462	7.7435	N	11.9204	3.3417	7.7364
N	11.9830	6.9445	9.8675	N	12.0493	6.9516	9.8748
N	12.4181	5.7456	11.9979	N	12.4699	5.7436	12.0024
N	10.0521	8.5626	9.8683	N	10.0699	8.5174	9.8641
N	11.1580	7.9228	11.9983	N	11.1791	7.9051	11.9976
N	7.5349	8.5649	9.8687	N	7.5508	8.5349	9.8614
N	8.7940	8.7846	11.9987	N	8.8106	8.7570	11.9937
N	5.6077	6.9456	9.8684	N	5.6169	6.9257	9.8592
N	6.4297	7.9238	11.9987	N	6.4408	7.9069	11.9908
N	5.1709	4.4668	9.8683	N	5.1768	4.4474	9.8579
N	5.1723	5.7443	11.9989	N	5.1859	5.7265	11.9874
N	6.4295	2.2868	9.8689	N	6.4199	2.2610	9.8591
N	5.6100	3.2666	11.9990	N	5.6095	3.2465	11.9877
N	8.7970	1.4296	9.8681	N	8.7929	1.4265	9.8617
N	7.5385	1.6501	11.9990	N	7.5373	1.6297	11.9907
N	11.1660	2.2879	9.8678	N	11.1465	2.3240	9.8624
N	10.0545	1.6525	11.9984	N	10.0565	1.6563	11.9921
N	12.4326	4.4656	9.8691	N	12.4712	4.4725	9.8729
N	11.9826	3.2679	11.9979	N	11.9900	3.2705	11.9965
N	9.2996	4.9696	4.1496	N	7.9683	4.7916	6.5215
Tb	9.6196	4.8925	5.9999	Tb	9.7491	5.2830	6.7228

Cluster Models

SUPPORTING INFORMATION

8Dy‖				**8Dy⊥**			
Dy	0.0000	0.0000	0.0000	Dy	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.8764	N	0.0000	0.0000	1.9012
N	0.0534	3.3327	-1.9257	N	-2.7743	-0.7450	-2.9146
N	-2.2868	2.3888	-1.9400	N	-4.2306	-0.4685	-0.8679
N	-3.2745	0.0663	-1.9567	N	-4.3759	-1.2516	1.5210
N	-2.3309	-2.2753	-1.9660	N	-2.9713	-2.7626	2.9573
N	-0.0071	-3.2627	-1.9626	N	-0.8586	-4.0627	2.4745
N	2.3338	-2.3170	-1.9486	N	0.5970	-4.3242	0.4367
N	3.3202	0.0060	-1.9321	N	0.7039	-3.5186	-1.9567
N	2.3757	2.3455	-1.9226	N	-0.6739	-2.0270	-3.4515
N	1.2857	3.0133	0.2134	N	-0.5513	0.4028	-2.8943
N	0.0377	3.3255	2.3431	N	-0.4148	2.5756	-1.6664
N	-1.1993	3.0358	0.2043	N	-2.3917	1.1316	-1.3410
N	-2.3140	2.3778	2.3292	N	-1.8944	2.8669	0.3567
N	-2.9710	1.2945	0.1881	N	-3.3343	0.9368	0.9779
N	-3.3075	0.0440	2.3128	N	-2.1185	2.1475	2.7761
N	-2.9926	-1.1884	0.1745	N	-2.7173	-0.2720	3.0986
N	-2.3588	-2.3091	2.3037	N	-0.6767	0.6240	4.2091
N	-1.2530	-2.9588	0.1716	N	-0.7468	-1.7930	3.4747
N	-0.0231	-3.3009	2.3071	N	1.5355	-0.7328	3.6955
N	1.2293	-2.9822	0.1806	N	1.2331	-2.7128	2.2237
N	2.3295	-2.3511	2.3209	N	3.0326	-1.0486	1.6676
N	3.0031	-1.2442	0.1965	N	1.9049	-2.3000	-0.1617
N	3.3208	-0.0168	2.3369	N	2.9704	-0.1447	-0.7016
N	3.0272	1.2403	0.2101	N	1.3573	-1.1344	-2.3207
N	2.3711	2.3338	2.3462	N	1.6808	1.3399	-2.2574
N	1.2862	3.0295	4.4730	N	1.7768	3.7423	-1.6020
N	-1.2314	3.0530	4.4638	N	-0.1384	4.5457	-0.1748
N	-3.0281	1.2888	4.4474	N	-1.0121	4.3024	2.1770
N	-3.0518	-1.2292	4.4336	N	-0.3557	3.0830	4.2788
N	-1.2876	-3.0258	4.4305	N	1.5919	1.5373	4.7203
N	1.2303	-3.0482	4.4398	N	3.5676	0.6615	3.4050
N	3.0275	-1.2848	4.4560	N	4.3608	0.9643	1.0326
N	3.0509	1.2333	4.4697	N	3.6870	2.2049	-1.0589
B	1.2863	3.0054	-2.6283	B	-2.1225	-1.8732	-3.5616
B	-1.1799	3.0285	-2.6375	B	-3.9965	-1.0556	-2.1682
B	-2.9399	1.3005	-2.6540	B	-4.8363	-1.3207	0.1573
B	-2.9634	-1.1663	-2.6677	B	-4.1715	-2.5353	2.1891
B	-1.2351	-2.9273	-2.6708	B	-2.2984	-4.0187	2.6781
B	1.2321	-2.9491	-2.6615	B	-0.4163	-4.8531	1.3542
B	2.9919	-1.2202	-2.6455	B	0.4044	-4.5643	-0.9714
B	3.0143	1.2459	-2.6319	B	-0.2479	-3.3666	-3.0416
B	1.2534	2.9424	1.6554	B	0.2364	1.4989	-2.4006
B	0.0478	3.2460	-0.4999	B	-1.9560	0.3267	-2.4710

B	-1.1795	2.9646	1.6465	B	-1.6407	2.2838	-0.9306
B	-2.2360	2.3254	-0.5138	B	-3.3967	0.5907	-0.4136
B	-2.9145	1.2599	1.6312	B	-2.5097	2.0321	1.4014
B	-3.2004	0.0589	-0.5303	B	-3.5443	-0.1592	1.9337
B	-2.9361	-1.1713	1.6183	B	-1.8676	0.8494	3.4345
B	-2.2792	-2.2259	-0.5394	B	-2.1473	-1.6210	3.2839
B	-1.2324	-2.9052	1.6156	B	0.0329	-0.4844	3.3939
B	-0.0111	-3.1893	-0.5361	B	-0.1055	-2.8823	2.8308
B	1.1985	-2.9278	1.6242	B	1.9766	-1.5274	2.5917
B	2.2733	-2.2669	-0.5224	B	1.3155	-3.1711	0.8748
B	2.9350	-1.2258	1.6392	B	2.7407	-1.2137	0.2769
B	3.2362	0.0000	-0.5061	B	1.4149	-2.3697	-1.5207
B	2.9584	1.2066	1.6520	B	2.1082	0.0000	-1.8587
B	2.3140	2.2829	-0.4968	B	0.0911	-0.9107	-3.0214
B	0.0317	3.2194	3.7671	B	0.3830	3.6871	-1.2078
B	-2.2497	2.2994	3.7536	B	-1.0741	3.9667	0.7825
B	-3.2126	0.0353	3.7376	B	-1.2265	3.2071	3.1325
B	-2.2921	-2.2465	3.7288	B	0.1489	1.7136	4.5078
B	-0.0276	-3.2083	3.7321	B	2.2467	0.4274	4.0283
B	2.2538	-2.2876	3.7454	B	3.7187	0.1459	2.0690
B	3.2164	-0.0237	3.7612	B	3.7553	0.9881	-0.2688
B	2.2955	2.2572	3.7702	B	2.4283	2.4525	-1.7289
H	-3.0577	1.3596	-3.8593	H	-0.1498	-5.5744	-1.3493
H	-3.0837	-1.2097	-3.8734	H	-0.9881	-5.8830	1.0590
H	-1.2830	-3.0432	-3.8767	H	-0.8193	-4.3363	-3.4890
H	-1.2258	3.1610	-3.8419	H	-2.7887	-2.7687	-4.0320
H	1.3435	3.1354	-3.8325	H	-4.7337	-1.9224	-2.5849
H	3.1446	1.3031	-3.8360	H	-5.6098	-2.1894	-0.1880
H	3.1191	-1.2661	-3.8504	H	-4.9284	-3.4534	1.9442
H	1.2869	-3.0674	-3.8670	H	-2.9602	-5.0122	2.4478
H	-1.2336	-2.8946	5.4427	H	4.0424	1.5395	3.6273
H	1.1703	-2.9144	5.4513	H	4.8225	1.8198	1.3487
H	2.8875	-1.2326	5.4672	H	4.1737	3.0196	-0.6780
H	-2.9161	-1.1782	5.4454	H	2.3335	4.4929	-1.1866
H	-2.8956	1.2255	5.4588	H	0.4737	5.2875	0.1716
H	-1.1792	2.9089	5.4743	H	-0.3476	5.0269	2.4569
H	1.2251	2.8884	5.4835	H	0.2932	3.8538	4.4544
H	2.9087	1.1717	5.4799	H	2.1406	2.3929	4.8300
9Dy‖				**9Dy⊥**			
Dy	0.0000	0.0000	0.0000	Dy	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.8782	N	0.0000	0.0000	1.8566
B	3.1957	-1.0536	2.8827	B	0.6858	4.2479	-2.1491
B	1.8363	-3.0921	3.2532	B	2.6911	4.2375	-0.6896
B	-0.5070	-3.7654	3.6463	B	3.3317	4.0521	1.6998

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B	-2.7471	-2.7562	3.8778	B	2.3069	3.7669	3.9274
B	-3.8388	-0.5422	3.8429	B	0.0869	3.5120	4.9669
B	-3.2683	1.8416	3.5568	B	-2.2885	3.4072	4.3305
B	-1.3004	3.2806	3.1508	B	-3.6948	3.5046	2.3068
B	1.1492	3.1113	2.8159	B	-3.4836	3.7549	-0.1503
B	2.9397	1.4035	2.7104	B	-1.7725	4.0529	-1.9247
B	2.9361	0.0000	0.7000	B	-0.4182	2.0725	-2.5088
B	2.3505	-2.3791	0.9738	B	1.9505	2.1576	-1.8064
B	2.5727	-1.4215	-1.3247	B	0.9554	0.0086	-2.6035
B	0.4138	-3.8312	1.3686	B	3.3435	2.0482	0.2666
B	1.2298	-3.4734	-0.9473	B	2.9616	0.0000	-1.0851
B	-2.0184	-3.6440	1.6969	B	3.1570	1.7962	2.7135
B	-1.1161	-4.1504	-0.5511	B	3.6132	-0.1765	1.3025
B	-3.7853	-1.9253	1.7999	B	1.4346	1.5063	4.4493
B	-3.3589	-3.1287	-0.3181	B	2.5856	-0.4590	3.5132
B	-4.0726	0.5191	1.6316	B	-1.0049	1.3156	4.6636
B	-4.4549	-0.9091	-0.3536	B	0.3741	-0.7074	4.5194
B	-2.7313	2.5477	1.2683	B	-3.0148	1.3132	3.2475
B	-3.8934	1.4839	-0.6412	B	-1.9824	-0.8152	3.9141
B	-0.3928	3.1860	0.8886	B	-3.6370	1.5027	0.8717
B	-1.9180	2.9176	-1.0509	B	-3.3873	-0.7222	1.9098
B	1.8556	2.1989	0.6672	B	-2.6182	1.7951	-1.3855
B	0.5321	2.7298	-1.3941	B	-3.1531	-0.4766	-0.5354
B	2.3227	1.0321	-1.5059	B	-1.4521	-0.1826	-2.3806
B	2.3763	-0.3566	-3.5474	B	-0.1292	-2.1880	-2.9618
B	1.7844	-2.7476	-3.2529	B	2.2310	-2.0960	-2.2056
B	-0.1812	-4.1925	-2.8447	B	3.6435	-2.1846	-0.1602
B	-2.6235	-4.0115	-2.5094	B	3.4616	-2.4250	2.2933
B	-4.3980	-2.2941	-2.4033	B	1.7322	-2.7088	4.0332
B	-4.6774	0.1566	-2.5763	B	-0.7218	-2.9005	4.2568
B	-3.3267	2.1930	-2.9473	B	-2.7386	-2.9081	2.8361
B	-0.9766	2.8629	-3.3437	B	-3.3473	-2.7271	0.4482
B	1.2855	1.8714	-3.5849	B	-2.3005	-2.4506	-1.7895
N	3.2916	0.1461	2.0632	N	-0.5240	3.4843	-2.4115
N	2.6606	-2.2999	2.3569	N	1.8974	3.5762	-1.7189
N	0.6491	-3.7750	2.7711	N	3.3173	3.4703	0.3630
N	-1.8424	-3.5880	3.1096	N	3.1260	3.2194	2.8600
N	-3.6493	-1.8354	3.2157	N	1.3700	2.9281	4.6362
N	-3.9374	0.6625	3.0422	N	-1.1268	2.7323	4.8598
N	-2.5605	2.7424	2.6670	N	-3.1792	2.7275	3.4075
N	-0.1583	3.4347	2.2653	N	-3.8103	2.9152	0.9790
N	2.1723	2.4378	2.0268	N	-2.7702	3.2075	-1.2996
N	2.7578	-1.3006	0.0895	N	0.8926	1.4421	-2.5138
N	2.6584	-0.2253	-2.1490	N	-0.2390	-0.7601	-2.9586
N	1.4570	-3.3942	0.4594	N	2.8779	1.4214	-0.9718

N	2.0357	-2.6600	-1.8456	N	2.1346	-0.6661	-2.0863
N	-0.9188	-4.0881	0.8605	N	3.5890	1.2441	1.4343
N	0.0390	-4.1373	-1.4323	N	3.5932	-0.7593	-0.0392
N	-3.1945	-3.0468	1.0958	N	2.5663	0.9552	3.7215
N	-2.4468	-3.9503	-1.0919	N	3.4319	-1.0104	2.4597
N	-4.3078	-0.7926	1.0602	N	0.2933	0.6950	4.8039
N	-4.2505	-2.1987	-0.9847	N	1.6705	-1.3053	4.2406
N	-3.7427	1.6389	0.7692	N	-2.1458	0.5881	4.1378
N	-4.5397	0.2950	-1.1597	N	-0.8414	-1.5035	4.4755
N	-1.7328	3.0745	0.3561	N	-3.5660	0.6863	2.0534
N	-3.1661	2.3688	-1.5362	N	-2.9017	-1.5051	3.0148
N	0.7177	2.8256	0.0237	N	-3.2918	0.9401	-0.4347
N	-0.7712	3.0466	-1.9380	N	-3.5070	-1.3132	0.5776
N	2.5132	1.1459	-0.0872	N	-1.5853	1.2414	-2.2584
N	1.5483	2.0555	-2.1879	N	-2.3868	-1.0198	-1.6546
N	2.2481	-1.6812	-4.1184	N	1.1891	-2.8026	-2.9232
N	0.8714	-3.7576	-3.7423	N	3.2055	-2.7983	-1.4051
N	-1.5172	-4.4427	-3.3419	N	3.8853	-2.9839	1.0134
N	-3.8028	-3.4150	-3.1031	N	2.8497	-3.2750	3.2873
N	-4.9151	-1.1570	-3.1392	N	0.5814	-3.5347	4.3467
N	-4.3335	1.2744	-3.4333	N	-1.8491	-3.6430	3.7074
N	-2.3277	2.7393	-3.8460	N	-3.2715	-3.5426	1.6339
N	0.1617	2.5592	-4.1870	N	-3.0200	-3.2829	-0.8586
N	1.9773	0.8168	-4.2973	N	-1.3084	-2.9961	-2.6926
H	0.6645	-3.7594	-4.7432	H	3.8468	-4.0001	0.9129
H	-1.6551	-4.4217	-4.3543	H	2.8317	-4.2806	3.1074
H	-3.8740	-3.4255	-4.1225	H	0.6388	-4.5302	4.1247
H	-4.9540	-1.2336	-4.1576	H	-1.7051	-4.6353	3.5108
H	-4.3873	1.1256	-4.4430	H	-3.0895	-4.5410	1.5145
H	-2.4424	2.5500	-4.8438	H	-2.8871	-4.2941	-0.9221
H	-0.0271	2.3689	-5.1734	H	-1.1900	-4.0114	-2.6919
H	1.7266	0.6778	-5.2786	H	1.2267	-3.8239	-2.9058
H	1.9966	-1.7416	-5.1073	H	3.2121	-3.8191	-1.4537
H	2.0792	-3.0926	4.4415	H	0.6367	5.4592	-2.1452
H	-0.3460	-3.7851	4.8485	H	2.7076	5.4493	-0.6464
H	-2.6637	-2.7431	5.0881	H	-1.9128	5.2571	-1.9122
H	-3.7924	-0.4534	5.0519	H	-3.6794	4.9504	-0.0939
H	-3.2001	2.0115	4.7560	H	-3.9048	4.6921	2.4453
H	-1.1681	3.5031	4.3357	H	-2.4485	4.5923	4.5449
H	3.2130	1.5552	3.8824	H	0.0154	4.7025	5.2004
H	1.3600	3.3249	3.9911	H	2.3137	4.9656	4.1244
H	3.4796	-0.9866	4.0600	H	3.3782	5.2591	1.8171

SUPPORTING INFORMATION

Reference

1 L. Chkhartishvili, *J. Phys.: Conf. Ser.*, 2009, 176, 012014.
2 L. Zhao, M. von Hopffgarten, D. M. Andrada and G. Frenking, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 2018, 8, e1345.
3 S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, 32, 1456–1465.

Input files

PEDA-NOCV calculations

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# dependency: /home/netweb/KK/Project_DyN/new/903/par/8pardos.Region_1 8pardos.Region_1.results/band.rkf Region_1.rkf
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"$AMSBIN/ams" << eor

Task SinglePoint
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N 1.42054264 1.46698506 2.97255098 region=Region_2
N -0.7121837600000001 0.21314163 3.23620878 region=Region_2
N 1.42067044 -1.06464761 3.13953099 region=Region_2
N -0.71205596 -2.13694443 2.43768551 region=Region_2
N 1.42067044 -2.97216073 1.46600505 region=Region_2
N -0.7121837600000001 -3.23573448 0.21174306 region=Region_2
N 1.42041484 -3.1379133 -1.06565886 region=Region_2
N -0.71243936 -2.4400882 -2.14078259 region=Region_2
N 1.42003144 -1.46544274 -2.97215278 region=Region_2
N -0.71243936 -0.21244846 -3.24120335 region=Region_2
N 1.42015924 1.06449164 -3.13717177 region=Region_2
N 3.54726244 2.16905587 -2.47415429 region=Region_2
N 5.67577144 2.95043655 -1.45589985 region=Region_2
N 3.54739024 3.28330031 -0.21634543 region=Region_2
N 5.67564364 3.11533998 1.05625201 region=Region_2
N 3.54726244 2.47406776 2.16814468 region=Region_2
N 5.67538804 1.45543673 2.94941107 region=Region_2
N 3.54726244 0.21602872 3.28278277 region=Region_2
N 5.67526024 -1.05700533 3.11511641 region=Region_2
N 3.54726244 -2.16836269 2.47347394 region=Region_2
N 5.67538804 -2.95008303 1.4548273 region=Region_2
N 3.54726244 -3.28175799 0.21497872 region=Region_2
N 5.67538804 -3.1146468 -1.05752067 region=Region_2
N 3.54713464 -2.47337458 -2.16960944 region=Region_2
N 5.67538804 -1.45508321 -2.95126802 region=Region_2
N 3.54700684 -0.21516571 -3.28395337 region=Region_2
N 5.67538804 1.05735885 -3.11599286 region=Region_2
N 0.97196464 -0.01001295 0.01466155 region=Region_1
B -3.55381676 2.12422116 -2.42297193 region=Region_2
B -5.68181456 2.88454312 -1.42315098 region=Region_2
B -3.55381676 3.21570859 -0.2112468 region=Region_2
B -5.68194236 3.04571031 1.03271989 region=Region_2
B -3.55432796 2.42311922 2.12441416 region=Region_2
B -5.68258136 1.42265984 2.88342308 region=Region_2
B -3.55458356 0.21110369 3.21659868 region=Region_2
B -5.68245356 -1.033569 3.04569666 region=Region_2
B -3.55458356 -2.12556592 2.42425259 region=Region_2
B -5.68232576 -2.88452925 1.42266673 region=Region_2
B -3.55445576 -3.21637404 0.21115475 region=Region_2
B -5.68232576 -3.04518696 -1.03369439 region=Region_2
B -3.55445576 -2.42293553 -2.12480036 region=Region_2
B -5.68232576 -1.42247615 -2.88498589 region=Region_2
B -3.55432796 -0.21108983 -3.21571022 region=Region_2
B -5.68219796 1.03375269 -3.04608286 region=Region_2
B 0.73029484 2.09568998 -2.39061526 region=Region_2
B -1.42211276 2.88556209 -1.42393538 region=Region_2
B 0.73042264 3.17189285 -0.20850139 region=Region_2
B -1.42236836 3.04774825 1.03311209 region=Region_2
B 0.7309338399999999 2.38949319 2.09460681 region=Region_2
B -1.42300736 1.42469778 2.88597239 region=Region_2
B 0.73131724 0.20872609 3.16953444 region=Region_2
B -1.42313516 -1.033569 3.04804987 region=Region_2
B 0.73157284 -2.09295886 2.3875817 region=Region_2
B -1.42313516 -2.88605771 1.42315698 region=Region_2
B 0.73118944 -3.16865225 0.20752688 region=Region_2
B -1.42300736 -3.04688525 -1.0352632 region=Region_2

```
    B 0.73042264 -2.3893095 -2.09577741 region=Region_2
    B -1.42262396 -1.4228158 -2.8869469 region=Region_2
    B 0.72991144 -0.20820275 -3.17286215 region=Region_2
    B -1.42224056 1.03409235 -3.04725946 region=Region_2
    B 4.97018764 2.11929613 -2.41738305 region=Region_2
    B 2.84500144 2.88250517 -1.42236658 region=Region_2
    B 4.97031544 3.20772665 -0.21134485 region=Region_2
    B 2.84512924 3.04418186 1.03222964 region=Region_2
    B 4.97005984 2.41683557 2.11804088 region=Region_2
    B 2.84500144 1.42265984 2.88263868 region=Region_2
    B 4.96993204 0.21093386 3.20689168 region=Region_2
    B 2.84512924 -1.03255003 3.04412785 region=Region_2
    B 4.97005984 -2.11877278 2.41660465 region=Region_2
    B 2.84512924 -2.88215165 1.42168623 region=Region_2
    B 4.97005984 -3.20652399 0.20997815 region=Region_2
    B 2.84487364 -3.04314902 -1.03330219 region=Region_2
    B 4.96993204 -2.41614239 -2.11950563 region=Region_2
    B 2.84474584 -1.421627 -2.88331903 region=Region_2
    B 4.96993204 -0.21024069 -3.20816033 region=Region_2
    B 2.84487364 1.03290355 -3.0440238 region=Region_2
    Dy -0.90439496 -0.01612677 0.02544711 region=Region_1
  End
  Lattice
    12.78 0.0 0.0
  End
End

Engine BAND
  Basis
    Type TZP
    Core None
    PerAtomType Symbol=Dy File=TZ2P/Dy
  End
  DOS
    CalcPDOS Yes
  End
  EnforcedSpinPolarization 5
  Fragment
    FileName Region_1.rkf
    AtomMapping
      1 49
      2 98
    End
  End
  Fragment
    FileName Region_2.rkf
\End
    KSpace
    Quality GammaOnly
  End
  NumericalQuality Good
  PEDA
  PEDANOCV
    Enabled Yes
  End
  Save TAPE10
  SCF
```

```
    Iterations 1000
    Method DIIS
  End
  UseSymmetry No
  Unrestricted Yes
  XC
    GGA PBE
    DISPERSION GRIMME3 BJDAMP
  End
EndEngine
Eor
```

Molcas input
Guess orbitals

```
&GATEWAY
Basis set
Dy.ANO-RCC-VTZP
Dy1        0.000000    0.000000    0.0000000    angstrom
End of basis
Basis set
N.ANO-RCC-VDZP
N2         0.000000    0.000000    1.875137     angstrom
End of basis
Basis set
N.ANO-RCC-VDZ
N50        -3.466709   0.638359    -3.744983    angstrom
End of basis
Basis set
B.ANO-RCC-VDZ
B98        -3.205039   0.813194    -0.931753    angstrom
………..
End of basis
Basis set
H.ANO-RCC-VDZ
H114       2.827594    0.993059    -5.124873    angstrom
…..
End of basis
RICD
AMFI
Doughlas-Kroll
SDIPolar
ANGM
0.0000000    0.0000000    0.0000000
&SEWARD
&GUESSORB
PRMO
 3
PRPOpulation
```

Rasscf

```
&RASSCF
  LUMORB
  Spin
   6
  Inactive
```

```
  328
 Nactel
   9 0 0
 Ras2
   7
 Ras1
   0
 Ras3
   0
 CIRoot
   21 21 1
>>COPY $Project.JobIph RAS-6.JobIph
>>COPY $Project.RasOrb RAS-6.RasOrb
```

RASSI

```
>>COPY RAS-6.JobIph JOB001
 &RASSI
  Nr of JobIph
    1 21
    1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
  Spin
  MEES
  Properties
    3
  'AngMom' 1 'AngMom' 2 'AngMom' 3
  SOProperties
    3
  'AngMom' 1 'AngMom' 2 'AngMom' 3
```

SINGLE_ANISO

```
&SINGLE_ANISO
MLTP
8
2 2 2 2 2 2 2 2
TINT
0.0 300 80
HINT
0.0 12.0 20
TMAG
3 2.0 3.0 5.0
CRYS
Dy
UBAR
PLOT
```