Supplementary Material (ESI) for Dalton Transactions

Curious matrix effects: A computational, electron diffraction, and vibrational spectroscopic study of dysprosium triiodide

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Electronic supplementary information (ESI)

Table S1 Electron diffraction molecular intensities for DyI_3 at the two camera ranges

Camera range= 19 cm

s_{min} = 8.75 Å^{-1} s_{max} = 27.25 Å^{-1} step size = 0.25 Å^{-1}

			-115.1	89.9	262.1	300.8	163.2
1.1	-154.2	-243.7	-223.9	-84.8	81.3	183.3	219.8
135.8	16.9	-126.0	-187.9	-185.8	-49.9	47.1	146.5
154.9	98.3	30.4	-90.3	-145.4	-121.1	-23.1	48.0
90.0	93.5	74.6	8.4	-51.1	-88.1	-89.1	-31.9
11.2	54.9	92.8	59.0	20.5	-28.1	-83.1	-76.9
-24.7	-32.4	22.8	49.3	45.8	3.8	-19.8	-21.0
-39.7	-30.4	-20.3	-30.1	50.2	-1.3	41.8	-4.1
-19.7	-49.0	-33.8	-30.2	7.4	16.4	18.1	10.0
2.1	-4.3	-25.8	3.1	-7.2	4.4		

Camera range= 50 cm

s_{min} = 2.00 Å^{-1} s_{max} = 14.00 Å^{-1} step size = 0.125 Å^{-1}

-307.3	-251.8	-124.0	57.3	258.8	449.9	575.4	610.6
530.5	375.0	121.7	-128.5	-350.0	-500.9	-552.5	-536.2
-449.1	-305.1	-151.4	13.5	156.9	264.5	354.4	426.2
443.1	404.1	318.3	194.3	43.7	-109.8	-255.5	-361.9
-427.8	-431.2	-374.1	-284.1	-153.2	-15.1	127.6	248.1
343.4	372.4	381.8	332.0	236.6	144.5	28.7	-102.5
-225.1	-301.3	-338.9	-342.3	-303.0	-224.1	-127.4	-18.4
103.6	191.7	266.9	314.1	290.5	281.0	221.9	110.9
11.8	-89.8	-164.3	-232.4	-263.9	-272.6	-257.5	-184.0
-102.4	-12.1	72.8	154.3	196.2	250.1	214.0	193.3
165.5	81.7	2.8	-64.2	-140.0	-160.4	-193.6	-190.4
-194.7	-126.5	-64.8	-25.9	43.4	91.3	132.0	156.9
188.6							

Table S2 Calculated and experimental harmonic vibrational frequencies (cm^{-1}), with IR intensities (km mol^{-1}) in parentheses for Dy_2I_6

symmetry	mode	character[a]	MP2(FC)(Cundari)	IR (gas)
A_g	ν_1	ν_s Dy-I_t	184.4 (0)	
	ν_2	ν_s Dy-I_b	120.7 (0)	
	ν_3	β_s I_b-Dy-I_b	56.5 (0)	
	ν_4	β_s I_t-Dy-I_t	25.8 (0)	
A_u	ν_5	δ_{as} I_t-Dy-I_t	22.1 (0)	
B_{1g}	ν_6	ν_{as} Dy-I_t	199.9 (0)	
	ν_7	β_{as} I_t-Dy-I_t	23.3 (0)	
B_{1u}	ν_8	ν_{as} Dy-I_b	144.9 (23)	
	ν_9	δ_s I_t-Dy-I_t	24.8 (4)	
B_{2g}	ν_{10}	ν_{as} Dy-I_b	112.2 (0)	
	ν_{11}	δ_{as} I_t-Dy-I_t	33.3 (0)	
B_{2u}	ν_{12}	ν_{as} Dy-I_t	202.1 (86)	
	ν_{13}	ring puckering	37.7 (0)	
	ν_{14}	Θ Dy-I_b-Dy-I_b	3.8 (0)	
B_{3g}	ν_{15}	ring twist	27.5 (0)	
B_{3u}	ν_{16}	ν_s Dy-I_t	173.8 (86)	171
	ν_{17}	ν_{as} Dy-I_b	114.5 (16)	
	ν_{18}	β_{as} I_t-Dy-I_t	33.9 (1)	

[a] The symbols or abbreviations ν, β, δ, Θ, 's', and 'as' mean stretch, in-plane bend, out-of-plane bend, torsion, symmetric and asymmetric, respectively.

Table S3 Calculated vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) in parentheses of $DyI_3 \cdot Ng_{a,b}$ (Ng = Ar, Kr, Xe; a and b = 0, 1, 3) matrices at MP2 (Stuttgart LC) level of theory.[a]

	DyI_3	$DyI_3.Ar_{1,0}$	$DyI_3.Ar_{1,1}$	$DyI_3.Ar_{3,0}$	$DyI_3.Ar_{3,1}$
	D_{3h}	C_{3v}	D_{3h}	C_{3v}	C_{3v}
1	*26.0 (12)*	29.8 (0)	29.3 (1)	24.5 (0)	19.0 (0)
2	*35.2 (1)*	29.8 (0)	29.3 (1)	24.5 (0)	19.0 (0)
3	*35.2 (1)*	*33.8 (9)*	39.7 (0)	32.2 (0)	19.5 (4)
4	*142.0 (0)*	*36.8 (0)*	39.7 (0)	*35.0 (1)*	23.3 (1)
5	*199.5 (46)*	*36.8 (0)*	*41.2 (0)*	*35.0 (1)*	23.3 (1)
6	*199.5 (46)*	96.1 (6)	*41.2 (0)*	*40.5 (9)*	32.9 (0)
7		*142.8 (1)*	*41.3 (12)*	47.4 (0)	*34.2 (1)*
8		*197.2 (44)*	77.4 (0)	47.4 (0)	*34.2 (1)*
9		*197.2 (44)*	84.5 (11)	50.4 (2)	*39.7 (9)*
10			*139.7 (0)*	54.5 (0)	47.1 (0)
11			*195.5 (44)*	54.5 (0)	47.1 (0)
12			*195.5 (44)*	66.7 (2)	49.0 (0)
13				*150.2 (6)*	54.2 (0)
14				*191.4 (45)*	54.2 (0)
15				*191.4 (45)*	64.9 (1)
16					*148.4 (5)*
17					*191.7 (45)*
18					*191.7 (45)*

[a] Italic style: normal vibrations of DyI_3 units

Table S3 continued

	DyI_3	$DyI_3.Kr_{1,0}$	$DyI_3.Kr_{1,1}$	$DyI_3.Kr_{3,0}$	$DyI_3.Kr_{3,1}$
	D_{3h}	C_{3v}	D_{3h}	C_{3v}	C_{3v}
1	*26.0 (12)*	24.7 (0)	24.1 (0)	24.3 (0)	16.2 (0)
2	*35.2 (1)*	24.7 (0)	24.1 (0)	24.3 (0)	16.2 (0)
3	*35.2 (1)*	*32.9 (8)*	34.1 (0)	26.9 (0)	17.6 (2)
4	*142.0 (0)*	*36.0 (0)*	34.1 (0)	*33.6 (0)*	24.9 (1)
5	*199.5 (46)*	*36.0 (0)*	*38.4 (0)*	*33.6 (0)*	24.9 (1)
6	*199.5 (46)*	81.3 (8)	*38.4 (0)*	*39.8 (5)*	27.8 (0)
7		*142.5 (2)*	*41.2 (9)*	40.3 (0)	32.4 (1)
8		*196.7 (43)*	59.6 (0)	40.3 (0)	32.4 (1)
9		*196.7 (43)*	74.3 (17)	44.2 (5)	*40.7 (0)*
10			*139.0 (0)*	45.3 (0)	*40.7 (0)*
11			*194.5 (42)*	45.3 (0)	41.1 (1)
12			*194.5 (42)*	54.4 (6)	*42.4 (10)*
13				*151.4 (8)*	45.7 (0)
14				*189.4 (45)*	45.7 (0)
15				*189.4 (45)*	51.6 (3)
16					*149.3 (7)*
17					*189.6 (44)*
18					*189.6 (44)*

Table S3 continued

	DyI_3	$DyI_3.Xe_{1,0}$	$DyI_3.Xe_{1,1}$	$DyI_3.Xe_{3,0}$	$DyI_3.Xe_{3,1}$
	D_{3h}	C_{3v}	D_{3h}	C_{3v}	C_{3v}
1	*26.0 (12)*	22.4 (0)	21.1 (1)	23.3 (0)	13.6 (0)
2	*35.2 (1)*	22.4 (0)	21.1 (1)	23.3 (0)	13.6 (0)
3	*35.2 (1)*	*32.0 (7)*	32.8 (0)	25.0 (0)	17.8 (1)
4	*142.0 (0)*	*35.7 (0)*	32.8 (0)	31.2 (1)	24.6 (1)
5	*199.5 (46)*	*35.7 (0)*	*37.7 (0)*	31.2 (1)	24.6 (1)
6	*199.5 (46)*	76.7 (10)	*37.7 (0)*	35.4 (0)	25.7 (0)
7		*142.4 (2)*	*41.3 (7)*	38.2 (0)	30.3 (1)
8		*195.8 (42)*	51.1 (0)	38.2 (0)	30.3 (1)
9		*195.8 (42)*	71.9 (24)	*42.6 (0)*	36.2 (0)
10			*137.8 (0)*	*42.6 (0)*	39.0 (0)
11			*192.8 (40)*	*42.6 (2)*	39.0 (0)
12			*192.8 (40)*	52.4 (8)	*43.0 (0)*
13				*152.2 (11)*	*43.0 (0)*
14				*186.6 (45)*	*43.1 (5)*
15				*186.6 (45)*	48.8 (9)
16					*150.5 (10)*
17					*186.7 (43)*
18					*186.7 (43)*

Table S4 Computed geometrical and vibrational parameters, and relative energies of the bending potential of DyI_3 at MP2(FC)(Cundari) level of theory

I–Dy–I (deg)	*r* (Å)	ΔE (cm^{-1})	frequencies (cm^{-1})					
			ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
120.0	2.826	0.0	142.1	25.0	201.6	201.6	35.3	35.3
119.0	2.824	88.5	144.1	26.5	201.2	201.2	35.5	35.5
117.5	2.822	233.2	147.1	28.7	200.4	200.4	36.0	35.8
115.0	2.819	508.3	151.7	32.4	198.9	198.8	37.0	36.8
112.5	2.816	832.7	156.3	35.5	197.2	197.1	38.2	38.0
110.0	2.813	1210.4	160.7	38.6	195.6	195.4	39.5	39.4
105.0	2.809	2155.7	168.8	44.8	191.5	191.4	42.9	42.9
100.0	2.808	3418.9	175.8	52.2	186.4	186.4	47.5	47.5
90.0	2.816	7361.4	185.0	72.9	172.1	172.1	60.7	60.7