Supporting Information for

Modulating Magnetic Anisotropy in Ln(III) Single-Ion Magnets using an External Electric Field

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Table S1: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition on the X-Ray structure of complex **1**.

Ab initio energies of KDs	g_x	g_y	g_z	Angle between g_z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.000	19.901	-	99% $\|\pm 15/2\rangle$
564	0.000	0.000	16.972	0.37	99%$\|\pm 13/2\rangle$
938	0.041	0.042	14.287	1.43	99%$\|\pm 11/2\rangle$
1138	0.062	0.316	11.437	5.82	96% $\|\pm 9/2\rangle$
1183	0.020	0.202	17.262	87.17	45% $\|\pm 1/2\rangle$, 15% $\|\pm 3/2\rangle$

Table S2: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition on the X-Ray structure of complex **2**.

Ab initio energies of KDs	g_X	g_Y	g_Z	Angle between g_Z axes	Wavefunction decomposition into M_J levels
0.0	0.014	0.019	17.830	-	99% $\|\pm 15/2\rangle$
37.6	0.181	0.196	15.511	7.046	80%$\|\pm 13/2\rangle$
83.5	0.136	0.229	12.807	4.975	90%$\|\pm 11/2\rangle$
135.2	0.930	1.019	9.957	4.208	41% $\|\pm 9/2\rangle$
181.1	5.393	5.759	7.461	91.559	56% $\|\pm 7/2\rangle$

Table S3: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition of complex **3**.

Ab initio energies of KDs	g_x	g_y	g_z	Angle between g_z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.026	0.050	19.488	-	92% $\|\pm 15/2\rangle$
210.8	1.285	3.342	14.089	1.92	61%$\|\pm 13/2\rangle$

Table S4: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition of complex $\mathbf{1_{opt}}$.

Ab initio energies of KDs	g_x	g_y	g_z	Angle between g_z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.000	19.996	-	99% $\|\pm15/2\rangle$
517	0.000	0.000	17.033	0.07	99%$\|\pm13/2\rangle$
870	0.025	0.025	14.333	0.12	99%$\|\pm11/2\rangle$
1064	0.040	0.156	11.623	0.47	98% $\|\pm9/2\rangle$
1118	13.048	7.550	1.116	90.00	54% $\|\pm1/2\rangle$, 2.0% $\|\pm3/2\rangle$

Table S5: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition of complex $\mathbf{2_{opt}}$.

Ab initio energies of KDs	g_X	g_Y	g_Z	Angle between g_Z axes	Wavefunction decomposition into M_J levels
0.0	0.009	0.009	17.766	-	99% $\|\pm15/2\rangle$
20.9	0.196	0.211	15.475	1.523	99%$\|\pm13/2\rangle$
57.7	0.157	0.231	12.832	1.043	97%$\|\pm11/2\rangle$
103.3	0.201	0.254	10.087	1.649	88% $\|\pm9/2\rangle$
143.7	6.825	6.374	5.535	90.3	58% $\|\pm7/2\rangle$

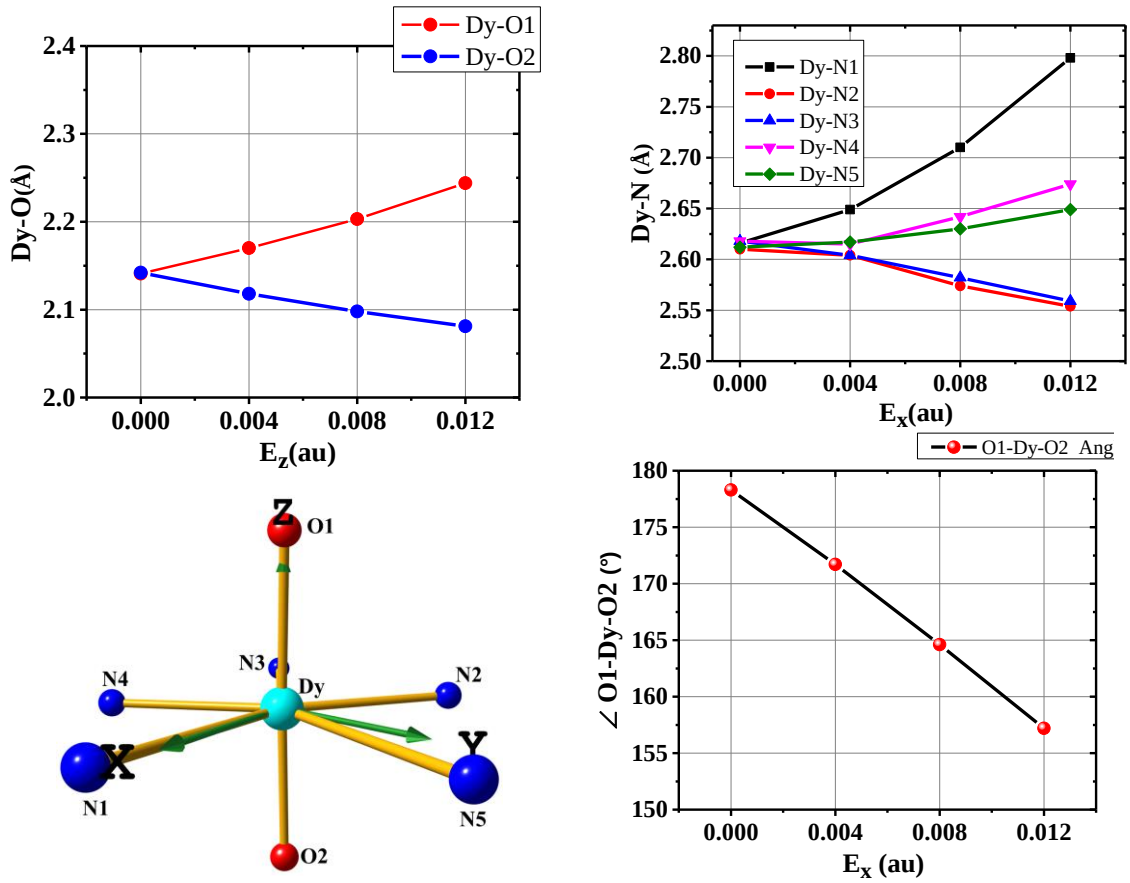

Figure S1: Variation of Dy-O bond length (top left), Dy-N bond length (top right) and change of the O-Dy-O axial angle (bottom) with respect to oriented external electric field. Orientation of complex **1** along with the atom numbering and axis orientation (bottom left).

Table S6: Details of electric field description along z-direction (along Dy-O(1) bond) and *ab initio* blocking barrier for complex **1**.

OEEF in DFT optimization (E_Z in au)	Magnitude of point charge on each Pt atoms on a single layer	Generated Electric field in ab initio method for the ground spin-free state (au)	U_{cal} (cm^{-1})	TA-QTM (Excited state)
0.0	0.0	0.0	1118	3.5 (4^{th})
0.004	0.03	E_Z = 0.0042 E_Y = 0.0000 E_X = 0.0001	1108	3.5 (4^{th})
0.008	0.06	E_Z = 0.0084 E_Y = -0.0001 E_X = -0.0000	1083	3.5 (4^{th})
0.012	0.09	E_Z = 0.0123 E_Y = -0.0004 E_X = -0.0000	1040	1.3 (4^{th})

Table S7: Details of electric field description along x-direction (along Dy-N1 bond) and *ab initio* blocking barrier for complex **1**.

OEEF in DFT optimization (E_X in au)	Magnitude of point charge on each Pt atoms on a single layer	Generated Electric field in ab initio method for the ground spin-free state (au)	U_{cal} (cm^{-1})	TA-QTM (Excited state)
0.0	0.0	0.0	1118	3.5 (4^{th})
0.004	0.08	E_Z = 0.0044 E_Y = -0.0001 E_X = -0.0000	1111	1.4 (4^{th})
0.008	0.14	E_Z = 0.0083 E_Y = -0.0002 E_X = -0.0000	1070	1.7 (4^{th})
0.012	0.20	E_Z = 0.0121 E_Y = -0.0002 E_X = -0.0000	939	0.25 (3^{rd})

Table S8: Variation of CASSCF computed LoProp charges in complex **1** (on the metal and first coordination sphere atoms) at different applied electric field.

LoProp Charges for ground state	Dy1	N1	N2	N3	N4	N5	O1	O2
0.00 Ez	2.442	-0.352	-0.352	-0.353	-0.351	-0.355	-1.055	-1.055
0.004Ez	2.442	-0.352	-0.354	-0.353	-0.351	-0.354	-1.047	-1.063
0.008Ez	2.441	-0.352	-0.354	-0.352	-0.351	-0.355	-1.038	-1.071
0.012Ez	2.440	-0.352	-0.355	-0.350	-0.351	-0.356	-1.029	-1.078
0.004Ex	2.442	-0.327	-0.370	-0.369	-0.350	-0.350	-1.055	-1.055
0.008Ex	2.444	-0.302	-0.384	-0.383	-0.347	-0.348	-1.054	-1.055
0.012Ex	2.446	-0.272	-0.398	-0.399	-0.344	-0.348	-1.051	-1.053

Table S9: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition of complex $^{4z}\mathbf{1}_{opt}$.

Ab initio energies of KDs	g_x	g_y	g_z	Angle between g_z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.000	19.996	-	99% $\|\pm15/2\rangle$
514	0.000	0.000	17.035	0.32	99%$\|\pm13/2\rangle$
865	0.025	0.027	14.335	0.48	99%$\|\pm11/2\rangle$
1057	0.104	0.256	11.600	0.63	98% $\|\pm9/2\rangle$
1108	12.583	7.864	1.162	90.4	32% $\|\pm1/2\rangle$, 3.7% $\|\pm3/2\rangle$

Table S10: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition of complex $^{8z}\mathbf{1}_{opt}$.

Ab initio energies of KDs	g_x	g_y	g_z	Angle between g_z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.000	19.996	-	99% $\|\pm15/2\rangle$
509	0.000	0.000	17.038	0.24	99%$\|\pm13/2\rangle$
855	0.030	0.032	14.337	0.32	99%$\|\pm11/2\rangle$
1041	0.060	0.334	11.478	1.17	98% $\|\pm9/2\rangle$
1083	12.561	7.840	1.199	90.86	58% $\|\pm1/2\rangle$, 3.5% $\|\pm3/2\rangle$

Table S11: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition of complex $^{12z}\mathbf{1}_{opt}$.

Ab initio energies of KDs	g_x	g_y	g_z	Angle between g_z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.000	19.996	-	99% $\|\pm15/2\rangle$
499	0.001	0.001	17.044	0.11	99%$\|\pm13/2\rangle$
831	0.032	0.035	14.345	0.03	99%$\|\pm11/2\rangle$
1007	0.006	0.432	11.305	2.21	95% $\|\pm9/2\rangle$
1040	1.083	6.504	13.354	89.06	27% $\|\pm1/2\rangle$, 3% $\|\pm3/2\rangle$

Table S12: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition of complex $^{4x}\mathbf{1}_{opt}$.

Ab initio energies of KDs	g_x	g_y	g_z	Angle between g_z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.000	19.996	-	99% $\|\pm15/2\rangle$
511	0.000	0.000	17.037	0.31	99%$\|\pm13/2\rangle$
864	0.017	0.017	14.335	1.46	99%$\|\pm11/2\rangle$
1060	0.032	0.105	11.657	6.54	98% $\|\pm9/2\rangle$
1111	1.149	6.523	14.145	93.49	64% $\|\pm1/2\rangle$, 4% $\|\pm3/2\rangle$

Table S13: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition of complex $^{8x}\mathbf{1}_{opt}$.

Ab initio energies of KDs	g_x	g_y	g_z	Angle between g_z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.000	19.996	-	99% $\|\pm15/2\rangle$
495	0.001	0.001	17.047	0.62	99%$\|\pm13/2\rangle$
833	0.005	0.007	14.349	2.38	99%$\|\pm11/2\rangle$
1020	0.035	0.113	11.608	8.64	96% $\|\pm9/2\rangle$
1070	1.354	6.490	13.580	85.51	55% $\|\pm1/2\rangle$, 15% $\|\pm3/2\rangle$

Table S14: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition of complex $^{12x}\mathbf{1}_{opt}$.

Ab initio energies of KDs	g_x	g_y	g_z	Angle between g_z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.000	19.994	-	99% $\|\pm15/2\rangle$
460	0.003	0.003	17.065	0.92	99%$\|\pm13/2\rangle$
769	0.047	0.052	14.355	3.19	98%$\|\pm11/2\rangle$
939	0.555	0.821	11.413	9.90	92% $\|\pm9/2\rangle$
991	11.295	6.871	2.000	95.21	23% $\|\pm1/2\rangle$, 20% $\|\pm7/2\rangle$, 9.5% $\|\pm3/2\rangle$

Table S15: *Ab initio* energies of KDs, corresponding g-tensor values and wavefunction decomposition of model complex $^{12x}\mathbf{1}_{opt}$.

Ab initio energies of KDs	g_x	g_y	g_z	Angle between g_z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.000	19.996	-	99% |±15/2⟩
528	0.001	0.001	17.024	0.73	99%|±13/2⟩
898	0.030	0.034	14.300	2.56	99%|±11/2⟩
1107	0.235	0.393	11.408	9.08	92% |±9/2⟩
1162	1.463	4.812	15.627	96.45	42% |±1/2⟩, 6.7% |±3/2⟩

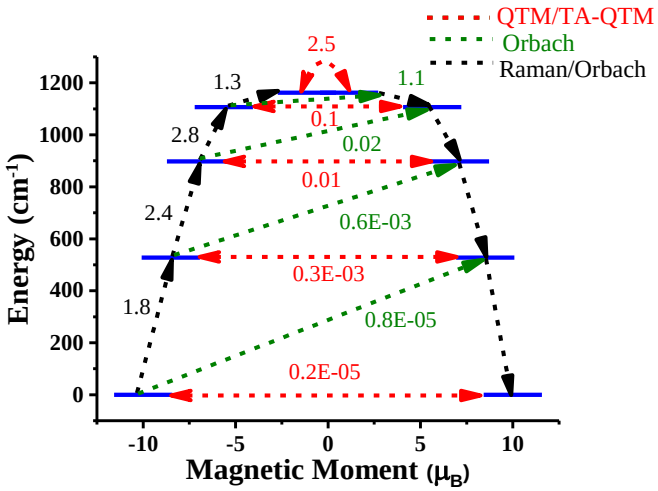

Figure S2: *Ab initio* blocking barrier diagram of the model $^{12x}\mathbf{1}_{opt}$.

Table S16: Crystal-field parameters (extended Stevens operators) obtained from SINGLE_ANISO calculations at different structures for complex **1**:

Structure	k	q	B(k,q)
$\mathbf{1}_{opt}$	2	-2	0.025
	2	-1	0.022
	2	0	-6.410
	2	1	-0.005
	2	2	-0.063
$^{4z}\mathbf{1}_{opt}$	2	-2	0.065
	2	-1	-0.006
	2	0	-6.356
	2	1	0.019
	2	2	0.060

$^{8z}\mathbf{1}_{opt}$	2	-2	0.092
	2	-1	-0.004
	2	0	-6.198
	2	1	0.000
	2	2	0.064
$^{12z}\mathbf{1}_{opt}$	2	-2	0.099
	2	-1	-0.023
	2	0	-5.926
	2	1	-0.042
	2	2	0.084
$^{4x}\mathbf{1}_{opt}$	2	-2	-0.025
	2	-1	0.038
	2	0	-6.401
	2	1	-0.372
	2	2	-0.078
$^{8x}\mathbf{1}_{opt}$	2	-2	0.042
	2	-1	-0.121
	2	0	-6.165
	2	1	0.534
	2	2	0.004
$^{12x}\mathbf{1}_{opt}$	2	-2	-0.049
	2	-1	-0.665
	2	0	-5.714
	2	1	0.073
	2	2	-0.122

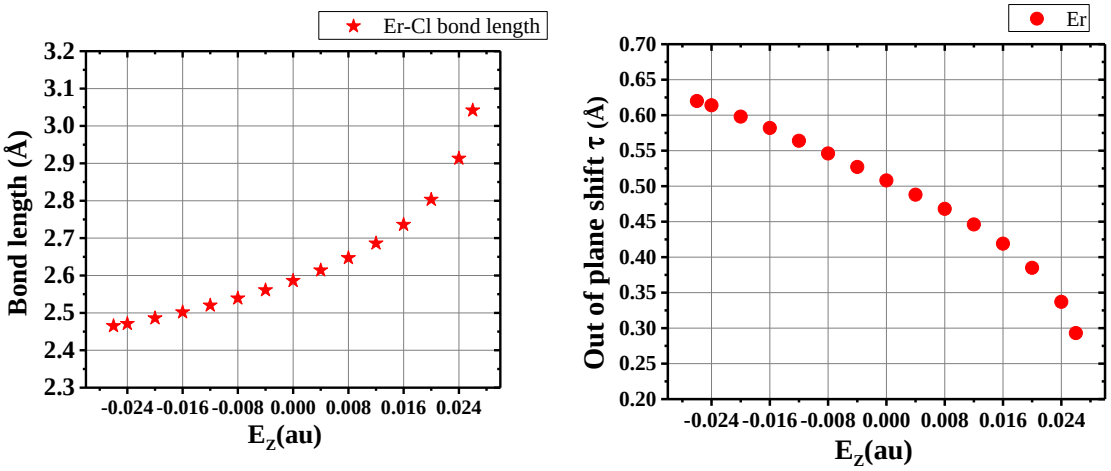

Figure S3: Variation of Er-Cl bond length (left) and Er(III) out-of-plane shift (right) with respect to oriented external electric field.

Table **S17**: Details of applying static electric field on Complex **2**.

OEEF in DFT optimisation (E_Z in au)	Magnitude of point charge on each Pt atoms on a single layer	Generated Electric field in *ab initio* method for the ground spin-free state (au)	U_{cal} (cm^{-1})	TA-QTM (Excited state)
0.0	0.0	0.0	143.7	2.2 (4^{th})
0.004	0.07	E_Z = 0.0043 E_Y = -0.0000 E_X = -0.0000	162.8	2.2 (4^{th})
0.008	0.12	E_Z = 0.0079 E_Y = -0.0000 E_X = -0.0000	178.1	2.4 (4^{th})
0.012	0.18	E_Z = 0.0121 E_Y = -0.0000 E_X = -0.0000	200.1	1.9 (4^{th})
0.016	0.24	E_Z = 0.0163 E_Y = -0.0000 E_X = -0.0000	223.2	1.8 (4^{th})
0.02	0.29	E_Z = 0.0199 E_Y = 0.0001 E_X = -0.0001	250.0	1.6 (4^{th})
0.024	0.35	E_Z = 0.0241 E_Y = 0.0002 E_X = -0.0001	285.4	1.5 (4^{th})
0.026	0.38	E_Z = 0.0262 E_Y = 0.0003 E_X = -0.0001	316.7	1.3 (4^{th})

Table S18: *Ab initio* computed energies of the KDs, g-factors, g_z angle and wavefunction of complex $^{4z}\mathbf{2}_{\mathbf{opt}}$.

Ab initio energies of KDs	g_X	g_Y	g_Z	Angle between g_Z axes	Wavefunction decomposition into M_J levels
0.0	0.002	0.004	17.797	-	99% |±15/2⟩
29.5	0.180	0.186	15.486	1.02	97%|±13/2⟩
69.6	0.121	0.227	12.874	0.90	96%|±11/2⟩
118.0	0.062	0.157	10.164	1.19	90% |±9/2⟩
162.8	6.435	6.191	5.815	90.91	69% |±7/2⟩

Table S19: *Ab initio* computed energies of the KDs, g-factors, g_z angle and wavefunction of complex $^{8z}\mathbf{2}_{\mathbf{opt}}$.

Ab initio energies of KDs	g_X	g_Y	g_Z	Angle between g_Z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.001	17.811	-	99% |±15/2⟩
34.8	0.174	0.174	15.492	0.81	99%|±13/2⟩
77.7	0.094	0.229	12.910	0.81	96%|±11/2⟩
129.3	0.010	0.135	10.228	1.07	91% |±9/2⟩
178.1	6.004	6.046	6.198	88.5	77% |±7/2⟩

Table S20: *Ab initio* computed energies of the KDs, g-factors, g_z angle and wavefunction of complex $^{12z}\mathbf{2}_{\mathbf{opt}}$.

Ab initio energies of KDs	g_X	g_Y	g_Z	Angle between g_Z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.001	17.830	-	99% |±15/2⟩
48.6	0.152	0.153	15.497	0.44	99%|±13/2⟩
94.1	0.077	0.208	12.941	0.57	98%|±11/2⟩
147.1	0.027	0.154	10.300	0.83	92% |±9/2⟩
200.1	5.641	5.819	6.317	0.80	81% |±7/2⟩

Table S21: *Ab initio* computed energies of the KDs, g-factors, g_z angle and wavefunction of complex $^{16z}\mathbf{2}_{opt}$.

Ab initio energies of KDs	g_X	g_Y	g_Z	Angle between g_Z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.001	17.844	-	99% $\|\pm 15/2\rangle$
61.1	0.132	0.133	15.502	0.39	99%$\|\pm 13/2\rangle$
110.1	0.058	0.188	12.972	0.37	98%$\|\pm 11/2\rangle$
165.5	0.036	0.161	10.367	0.67	94% $\|\pm 9/2\rangle$
223.2	5.255	5.448	6.595	0.44	84% $\|\pm 7/2\rangle$

Table S22: *Ab initio* computed energies of the KDs, g-factors, g_z angle and wavefunction of complex $^{20z}\mathbf{2}_{opt}$.

Ab initio energies of KDs	g_X	g_Y	g_Z	Angle between g_Z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.001	17.858	-	99% $\|\pm 15/2\rangle$
76.9	0.113	0.115	15.505	0.45	98%$\|\pm 13/2\rangle$
129.6	0.093	0.118	13.000	0.42	98%$\|\pm 11/2\rangle$
187.4	0.132	0.156	10.430	0.45	95% $\|\pm 9/2\rangle$
250.1	4.793	5.076	6.871	0.28	87% $\|\pm 7/2\rangle$

Table S23: *Ab initio* computed energies of the KDs, g-factors, g_z angle and wavefunction of complex $^{24z}\mathbf{2}_{opt}$.

Ab initio energies of KDs	g_X	g_Y	g_Z	Angle between g_Z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.001	17.872	-	99% $\|\pm 15/2\rangle$
98.7	0.095	0.097	15.505	0.53	99%$\|\pm 13/2\rangle$
156.0	0.067	0.109	13.030	0.16	98%$\|\pm 11/2\rangle$
216.3	0.058	0.098	10.499	0.33	97% $\|\pm 9/2\rangle$
285.4	4.350	4.506	7.174	0.19	88% $\|\pm 7/2\rangle$

Table S24: *Ab initio* computed energies of the KDs, g-factors, g_z angle and wavefunction of complex $^{26z}\mathbf{2}_{\mathbf{opt}}$.

Ab initio energies of KDs	g_X	g_Y	g_Z	Angle between g_Z axes (°)	Wavefunction decomposition into M_J levels
0.0	0.000	0.000	17.881	-	99% $\|\pm 15/2\rangle$
119.1	0.081	0.082	15.505	0.50	99%$\|\pm 13/2\rangle$
180.5	0.058	0.091	13.048	0.18	99%$\|\pm 11/2\rangle$
242.4	0.043	0.073	10.544	0.37	97% $\|\pm 9/2\rangle$
316.7	3.929	4.051	7.398	0.31	90% $\|\pm 7/2\rangle$

Table S25: Details of applying static electric field at the reverse z-direction on Complex **2**.

Electric Field at reverse Z-direction computed on ground spin-free state (au)	Magnitude of point charges on each Pt atom on a layer (au)	Er-Cl bond length (Å)	U_{cal} (cm^{-1})	TA-QTM	Relaxes Via
-0.0042	0.05	2.561	131.0	2.3	4^{th} ES
-0.0079	0.10	2.539	82.3	0.1	3^{rd} ES
-0.0122	0.16	2.520	70.6	0.2	3^{rd} ES
-0.0161	0.21	2.502	62.3	0.2	3^{rd} ES
-0.0198	0.26	2.486	56.8	0.2	3^{rd} ES
-0.0242	0.32	2.471	51.5	0.3	3^{rd} ES
-0.0263	0.35	2.465	50.9	0.1	GS

Table S26: Variation of CASSCF computed LoProp charges in complex **2** (on the metal and first coordination sphere atoms) at different applied electric field.

LoProp Charges for ground state	Er1	Cl1	N1	N2	N3
X-Ray	2.367	-0.820	-1.266	-1.261	-1.266
Optimised	2.358	-0.822	-1.242	-1.242	-1.242
0.004Ez	2.362	-0.834	-1.244	-1.244	-1.244
0.008Ez	2.366	-0.842	-1.246	-1.246	-1.245
0.012Ez	2.369	-0.852	-1.247	-1.248	-1.247
0.016Ez	2.373	-0.862	-1.249	-1.249	-1.248
0.020Ez	2.377	-0.872	-1.251	-1.251	-1.249
0.024Ez	2.383	-0.886	-1.253	-1.253	-1.251

0.026Ez	2.389	-0.898	-1.256	-1.255	-1.252
-0.004Ez	2.354	-0.814	-1.240	-1.240	-1.240
-0.008Ez	2.350	-0.805	-1.237	-1.238	-1.238
-0.012Ez	2.346	-0.795	-1.234	-1.235	-1.235
-0.016Ez	2.341	-0.786	-1.232	-1.232	-1.232
-0.020Ez	2.337	-0.776	-1.229	-1.229	-1.229
-0.024Ez	2.332	-0.766	-1.226	-1.226	-1.226
-0.026Ez	2.329	-0.760	-1.224	-1.224	-1.224

Table S27: Crystal-field parameters (extended Stevens operators) obtained from SINGLE_ANISO calculation at different structures for complex **2**:

Structure	k	q	B(k,q)
Optimised	2	-2	-0.027
	2	-1	-0.055
	2	0	-1.658
	2	1	-0.105
	2	2	0.009
0.004Ez	2	-2	-0.017
	2	-1	0.018
	2	0	-1.807
	2	1	0.082
	2	2	-0.004
0.008Ez	2	-2	-0.021
	2	-1	0.004
	2	0	-1.942
	2	1	0.076
	2	2	-0.014
0.012Ez	2	-2	-0.0002
	2	-1	-0.020
	2	0	-2.106
	2	1	0.038
	2	2	-0.033
0.016Ez	2	-2	0.019
	2	-1	0.005
	2	0	-2.283
	2	1	-0.026
	2	2	-0.034
0.02Ez	2	-2	0.028
	2	-1	0.025
	2	0	-2.488
	2	1	0.033
	2	2	-0.055
0.024z	2	-2	-0.029
	2	-1	0.045
	2	0	-2.760
	2	1	-0.001
	2	2	0.003
0.026Ez	2	-2	0.026
	2	-1	-0.029

	2	0	-2.997
	2	1	-0.029
	2	2	-0.026
-0.004Ez	2	-2	-0.028
	2	-1	-0.226
	2	0	-1.546
	2	1	0.001
	2	2	0.008
-0.008Ez	2	-2	-0.049
	2	-1	0.486
	2	0	-1.422
	2	1	0.0719
	2	2	0.030
-0.012Ez	2	-2	-0.082
	2	-1	1.217
	2	0	-1.253
	2	1	0.207
	2	2	0.090
-0.016Ez	2	-2	-0.044
	2	-1	1.623
	2	0	-1.090
	2	1	0.093
	2	2	0.172
-0.02Ez	2	-2	-0.058
	2	-1	0.807
	2	0	-1.055
	2	1	0.261
	2	2	0.081
-0.024Ez	2	-2	-0.061
	2	-1	0.457
	2	0	-0.959
	2	1	0.232
	2	2	0.053
-0.026Ez	2	-2	-0.069
	2	-1	0.288
	2	0	-0.913
	2	1	0.197
	2	2	0.040

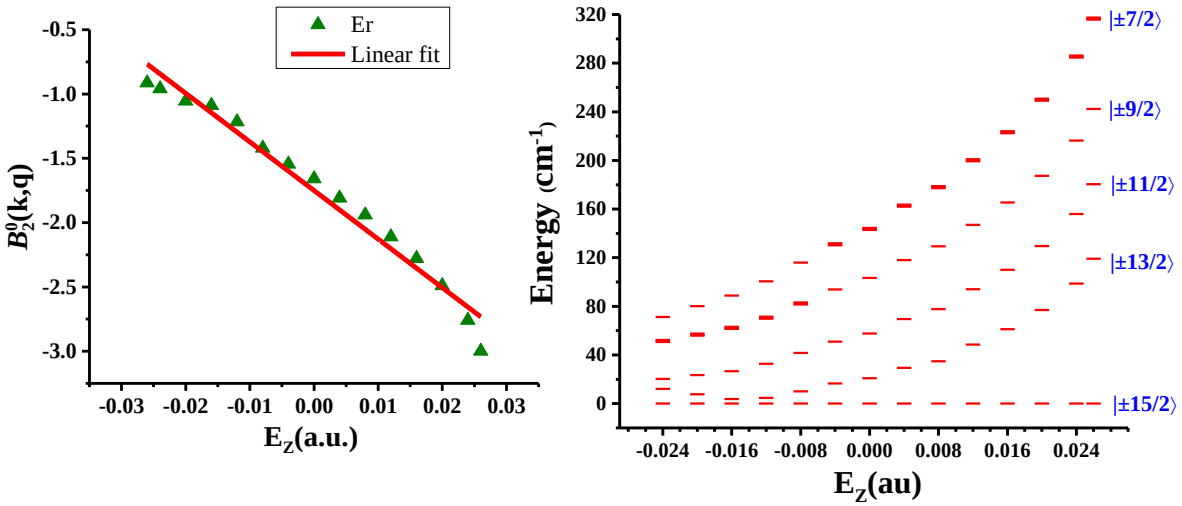

Figure S4. Variation of axial crystal field parameter for complex **2** with respect to applied external electric field (left). Increasing trend of U_{cal} vs. Z-component of the applied electric field for complex **2** (right). Bold bars indicate relaxing KD.

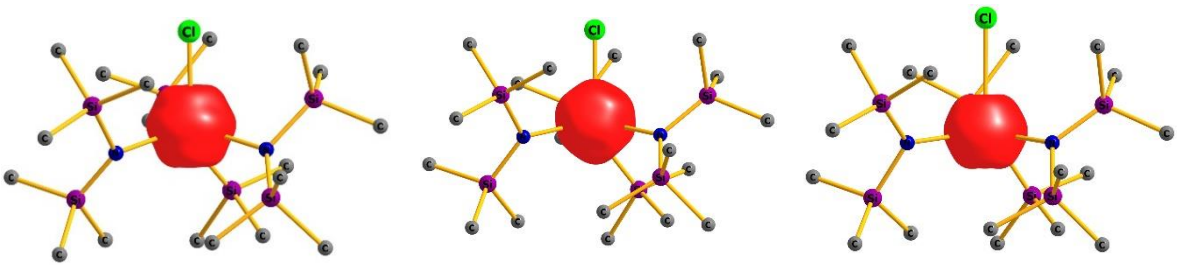

Figure S5. Beta electron density plot of complex $^{26\text{-}z}\mathbf{2}_{opt}$ (left), $\mathbf{2}_{opt}$ (middle) and $^{26z}\mathbf{2}_{opt}$(right).

Table S28: Selected structural parameters of complex **3** in the presence of an electric field. Bond lengths in Å unit, angles are in (°) and U_{cal} values in cm^{-1}.

	X-ray	$\mathbf{3}_{opt}$	$^{4z}\mathbf{3}_{opt}$	$^{8z}\mathbf{3}_{opt}$	$^{12z}\mathbf{3}_{opt}$	$^{16z}\mathbf{3}_{opt}$	$^{20z}\mathbf{3}_{opt}$	$^{22z}\mathbf{3}_{opt}$
Dy-Cl	2.540	2.555	2.590	2.631	2.681	2.753	2.853	2.940
Dy-C1	2.641	2.656	2.650	2.644	2.639	2.621	2.609	2.602
Dy-C2	2.666	2.648	2.641	2.634	2.626	2.615	2.600	2.594
Dy-C3	2.781	2.665	2.659	2.653	2.648	2.655	2.662	2.665
Dy-C4	2.754	2.666	2.663	2.661	2.662	2.687	2.715	2.723

Dy-C5	2.648	2.653	2.646	2.640	2.636	2.629	2.635	2.635
Dy-C6	2.641	2.656	2.650	2.644	2.639	2.621	2.609	2.602
Dy-C7	2.666	2.648	2.641	2.634	2.626	2.615	2.600	2.594
Dy-C8	2.781	2.665	2.659	2.653	2.648	2.655	2.662	2.665
Dy-C9	2.754	2.666	2.663	2.661	2.662	2.687	2.715	2.723
Dy-C10	2.648	2.653	2.646	2.640	2.636	2.629	2.635	2.635
∠Cp-Dy-Cp	147.6	134.4	134.4	134.2	134.2	135.8	139.3	139.6
U_{cal}	211	144	160	181	198	417	487	519

Table S29: Details of applying static external electric field on Complex **3**.

OEEF in DFT optimization (E_Z au)	OEEF optimized Dy^{III}-Cl bond length (Å)	Magnitude of point charge on each Pt atoms on the opposite layers	Generated Electric field in *ab initio* method for the ground spin-free state (au)	U_{cal} (cm^{-1})	TA-QTM (Excited state)
Model X-ray (**3**)	2.540	0.0	0.0	211.0	0.8 (1^{st})
0.0	2.555	0.0	0.0	144.1	1.2 (1^{st})
0.004	2.590	0.03	E_Z = 0.0042 E_Y = -0.0000 E_X = -0.0000	160.2	0.7 (1^{st})
0.008	2.631	0.08	E_Z = 0.0084 E_Y = -0.0000 E_X = -0.0000	180.5	0.3 (1^{st})
0.012	2.681	0.12	E_Z = 0.0125 E_Y = -0.0000 E_X = -0.0000	198.0	0.2 (1^{st})
0.016	2.753	0.16	E_Z = 0.0163 E_Y = -0.0001 E_X = -0.0001	417.2	3.0 (2^{nd})
0.02	2.853	0.20	E_Z = 0.0190 E_Y = 0.0001 E_X = -0.0001	487.2	0.6 (2^{nd})
0.022	2.940	0.23	E_Z = 0.022 E_Y = -0.0001 E_X = -0.0001	519.4	0.3 (2^{nd})

Coordinates

The coordinates are given in a column-wise manner for all the optimised geometries in xyz format (in Angstrom unit).

1$_{opt}$				**2**$_{opt}$				**3**$_{opt}$			
Dy	0.00000	0.00000	0.00000	Er	0.00000	0.00000	0.00000	Dy	0.00000	0.00000	0.00000
N	-1.08386	-2.37984	0.06013	C	-4.00842	-3.26490	-0.14127	Cl	0.00000	0.00000	2.55542
N	2.23392	1.34916	0.00629	H	-4.92500	-2.75388	-0.47752	C	1.77767	1.71818	-0.97083
N	-0.60515	2.54533	0.08111	H	-4.30452	-3.99345	0.63388	C	2.42056	1.06586	0.11968
N	-2.60144	0.24515	-0.15552	H	-3.60275	-3.83175	-0.99499	H	2.69358	1.52820	1.06142
N	1.94089	-1.74866	0.00281	Si	-3.09229	-0.26799	-1.78134	C	2.63930	-0.30021	-0.21524
O	-0.00000	0.00000	2.14243	C	-1.35192	-3.23233	1.26003	C	2.12113	-0.50902	-1.53244
O	0.06648	-0.00923	-2.13955	H	-1.78065	-3.91502	2.01443	C	1.59647	0.73790	-1.98611
C	-0.03877	-0.01033	3.54841	H	-0.52549	-2.69100	1.74461	H	1.15455	0.91321	-2.96085
C	1.02403	0.94511	4.13044	H	-0.93371	-3.84910	0.44780	C	1.46042	3.18969	-1.07170
H	2.03380	0.64516	3.81075	Cl	-0.00000	-0.00000	2.58570	C	3.37042	-1.30580	0.63726
H	1.00802	0.94365	5.23193	C	-3.56526	-1.28188	2.11261	C	2.24854	-1.76527	-2.35660
H	0.85434	1.98158	3.79879	H	-4.38448	-0.61367	1.79932	C	-1.77393	-1.72157	-0.97153
C	0.24635	-1.42828	4.08740	H	-2.84034	-0.68805	2.69077	C	-2.41828	-1.07098	0.11920
H	-0.46215	-2.15874	3.66704	H	-3.99020	-2.05128	2.78129	H	-2.69033	-1.53424	1.06077
H	0.16241	-1.46992	5.18513	Si	3.15428	-1.32803	0.60553	C	-2.63992	0.29472	-0.21522
H	1.26724	-1.74510	3.82254	C	-4.72657	0.47335	-1.13277	C	-2.12205	0.50513	-1.53231
C	-1.42979	0.43942	4.04037	H	-5.31634	0.90689	-1.95948	C	-1.59482	-0.74053	-1.98642
H	-1.65325	1.45760	3.68268	H	-4.53144	1.27060	-0.39703	H	-1.15233	-0.91441	-2.96116
H	-1.49207	0.44862	5.14016	H	-5.35626	-0.28466	-0.63823	C	-1.45360	-3.19235	-1.07291
H	-2.21328	-0.23856	3.66535	Si	-2.71351	-2.07749	0.61139	C	-3.37324	1.29837	0.63768
C	0.08201	0.00398	-3.54596	C	-3.58461	-1.53928	-3.11882	C	-2.25210	1.76126	-2.35625
C	-0.48404	-1.31966	-4.10051	H	-4.11915	-1.02081	-3.93459	H	2.11453	-2.67540	-1.76080
H	0.13608	-2.17033	-3.77546	H	-4.24381	-2.33565	-2.74246	H	1.51463	-1.78656	-3.16848
H	-0.50299	-1.32401	-5.20195	H	-2.69290	-2.01888	-3.55408	H	3.24360	-1.83277	-2.81612
H	-1.51323	-1.49019	-3.74616	Si	-0.43881	3.39185	0.61685	H	4.43908	-1.32828	0.38541
C	1.52210	0.17270	-4.07450	C	-2.23258	1.11249	-2.76134	H	3.28392	-1.05883	1.69944
H	1.98497	1.08391	-3.66616	H	-2.93424	1.51533	-3.51236	H	2.99181	-2.32516	0.50038
H	1.54359	0.24604	-5.17353	H	-1.35147	0.73946	-3.31123	H	2.32092	3.74602	-1.46522
H	2.14738	-0.68829	-3.79126	H	-1.89469	1.94089	-2.12265	H	0.61887	3.38121	-1.74624
C	-0.77200	1.17501	-4.07567	Si	1.77166	-2.51883	-1.81022	H	1.21991	3.62398	-0.09487
H	-1.80600	1.10410	-3.70205	Si	1.31186	2.81276	-1.77880	H	-1.51719	1.78495	-3.16716
H	-0.81171	1.18657	-5.17651	N	-2.06947	-0.88712	-0.50797	H	-3.24676	1.82589	-2.81707
H	-0.35056	2.13854	-3.74772	N	1.80065	-1.34870	-0.51396	H	-2.12167	2.67158	-1.75997
C	-0.87843	-3.27099	-0.92291	N	0.26753	2.23716	-0.50289	H	-3.28605	1.05124	1.69976
H	-0.23199	-2.94553	-1.74019	C	0.67647	3.73067	2.11821	H	-2.99701	2.31866	0.50112
C	-1.45380	-4.54264	-0.92651	H	0.22043	4.48112	2.78791	H	-4.44198	1.31851	0.38598
H	-1.25534	-5.22753	-1.75317	H	1.66308	4.10933	1.80389	H	-0.61157	-3.38176	-1.74741
C	-2.27828	-4.90879	0.13960	H	0.83280	2.80601	2.69542	H	-1.21222	-3.62645	-0.09620
H	-2.74451	-5.89666	0.17082	C	1.93378	-4.31856	-1.19728	H	-2.31290	-3.75035	-1.46669
C	-2.49503	-3.98508	1.16486	H	1.13208	-4.56663	-0.48257				
H	-3.13052	-4.22373	2.01989	H	2.89570	-4.49430	-0.68771				
C	-1.87935	-2.73559	1.08212	H	1.87076	-5.02800	-2.04109				
H	-2.02377	-1.98509	1.86235	C	2.08575	1.38142	-2.75607				
C	2.51120	2.24079	-0.95898	H	1.32138	0.77461	-3.27071				
H	1.75799	2.35453	-1.74167	H	2.67320	0.70066	-2.12410				
C	3.68807	2.98994	-0.98424	H	2.75024	1.79405	-3.53497				
H	3.86444	3.70024	-1.79434	C	2.76446	3.86921	-1.13452				
C	4.62114	2.80783	0.03922	H	3.43099	4.16836	-1.96244				
H	5.55332	3.37802	0.05219	H	3.36428	3.30795	-0.39955				
C	4.33746	1.88183	1.04555	H	2.41513	4.79097	-0.64059				
H	5.03325	1.70479	1.86795	C	0.44936	3.86426	-3.11910				
C	3.13430	1.17707	0.98728	H	1.16844	4.08792	-3.92723				
H	2.87247	0.44658	1.75547	H	0.06688	4.82316	-2.73959				
C	-1.22067	3.17515	-0.93311	H	-0.39673	3.31630	-3.56430				

H	-1.45225	2.56793	-1.80989	C	0.14916	-2.43408	-2.79212				
C	-1.55222	4.53033	-0.89452	H	0.02352	-1.46134	-3.29792				
H	-2.05092	4.99273	-1.74858	H	-0.73664	-2.59312	-2.16079				
C	-1.23435	5.26724	0.24875	H	0.16100	-3.20804	-3.57906				
H	-1.48048	6.32999	0.31408	C	3.12605	-2.29418	-3.13662				
C	-0.59581	4.61617	1.30657	H	2.94701	-3.00221	-3.96535				
H	-0.32771	5.14711	2.22209	H	4.14041	-2.47978	-2.75435				
C	-0.30138	3.25791	1.17834	H	3.10468	-1.27529	-3.55526				
H	0.19352	2.70773	1.98081	C	-0.81660	5.10841	-0.13493				
C	-3.33455	0.78354	0.83252	H	-1.52021	5.04575	-0.98111				
H	-2.78534	1.12124	1.71335	H	0.08272	5.64275	-0.48134				
C	-4.72291	0.91035	0.76431	H	-1.28728	5.73164	0.64573				
H	-5.27034	1.35357	1.59843	C	-2.12232	2.79523	1.26398				
C	-5.38242	0.46169	-0.38221	H	-2.85947	2.72505	0.44746				
H	-6.46842	0.54573	-0.47052	H	-2.50785	3.51950	2.00291				
C	-4.62391	-0.09688	-1.41350	H	-2.06810	1.81735	1.76578				
H	-5.09179	-0.46044	-2.33047	C	4.82832	-1.85746	-0.14966				
C	-3.24005	-0.18473	-1.25626	H	4.83836	-2.90219	-0.49979				
H	-2.60915	-0.61218	-2.03811	H	5.60475	-1.76526	0.63007				
C	2.82435	-1.78491	-1.00815	H	5.12392	-1.21298	-0.99346				
H	2.66919	-1.05627	-1.80576	C	3.48062	0.42262	1.26722				
C	3.88155	-2.69464	-1.05909	H	3.77670	1.10576	0.45441				
H	4.57080	-2.68113	-1.90568	H	4.30808	0.39095	1.99758				
C	4.03075	-3.60949	-0.01437	H	2.60892	0.85479	1.78148				
H	4.84734	-4.33574	-0.02055	C	2.88384	-2.47488	2.09708				
C	3.11342	-3.57651	1.03854	H	2.00332	-2.15017	2.67326				
H	3.18708	-4.26976	1.87870	H	3.75846	-2.46290	2.77135				
C	2.08686	-2.63154	1.00450	H	2.71766	-3.51603	1.77402				
H	1.35210	-2.57170	1.80924								
$^{4z}\mathbf{1}_{opt}$				$^{4z}\mathbf{2}_{opt}$				$^{4z}\mathbf{3}_{opt}$			
Dy	0.00000	0.00000	0.00000	Er	0.00000	0.00000	0.00000	Dy	0.00000	0.00000	0.00000
N	2.60355	0.01166	0.04512	C	-4.01542	-3.26029	-0.14236	Cl	0.00000	0.00000	2.58966
N	-2.15497	1.48297	0.00913	H	-4.92896	-2.74788	-0.48396	C	1.77054	1.72560	-0.95288
N	-2.05973	-1.62508	0.11135	H	-4.31586	-3.99048	0.63010	C	2.41567	1.05941	0.12817
N	0.87266	-2.45351	-0.10591	H	-3.60831	-3.82581	-0.99583	H	2.69411	1.51125	1.07363
N	0.80130	2.50298	-0.06587	Si	-3.08577	-0.26493	-1.78603	C	2.63241	-0.30323	-0.22572
O	0.00000	0.00000	2.17020	C	-1.36617	-3.23122	1.27408	C	2.11216	-0.49475	-1.54448
O	-0.03844	0.03849	-2.11755	H	-1.80289	-3.91953	2.01959	C	1.58513	0.75761	-1.97873
C	0.02211	0.06991	3.56620	H	-0.54564	-2.68859	1.76741	H	1.14676	0.94620	-2.95226
C	-1.36999	0.44590	4.12324	H	-0.93803	-3.84245	0.46305	C	1.45628	3.19848	-1.04022
H	-1.72029	1.39225	3.68395	Cl	0.00000	0.00000	2.61395	C	3.37226	-1.31998	0.60570
H	-1.35084	0.56534	5.21938	C	-3.57969	-1.28501	2.11850	C	2.23925	-1.73726	-2.38917
H	-2.11096	-0.33434	3.88961	H	-4.39558	-0.61456	1.80087	C	-1.76936	-1.72651	-0.95345
C	1.03151	1.14070	4.03799	H	-2.85326	-0.69319	2.69738	C	-2.41489	-1.06122	0.12792
H	2.04133	0.91657	3.65937	H	-4.00930	-2.05676	2.78274	H	-2.69299	-1.51364	1.07321
H	1.08695	1.19593	5.13812	Si	3.16018	-1.32617	0.60443	C	-2.63264	0.30141	-0.22539
H	0.73778	2.13420	3.66460	C	-4.72178	0.47835	-1.14145	C	-2.11258	0.49386	-1.54409
C	0.42952	-1.29431	4.16586	H	-5.30537	0.90939	-1.97336	C	-1.58474	-0.75796	-1.97891
H	-0.29393	-2.07158	3.87170	H	-4.53041	1.27828	-0.40725	H	-1.14628	-0.94583	-2.95254
H	0.46399	-1.26575	5.26778	H	-5.35571	-0.27911	-0.65093	C	-1.45411	-3.19913	-1.04144
H	1.42498	-1.59799	3.80430	Si	-2.72188	-2.07415	0.61006	C	-3.37319	1.31725	0.60652
C	-0.11889	0.02606	-3.53132	C	-3.56567	-1.54055	-3.11570	C	-2.24049	1.73669	-2.38821
C	1.29432	-0.01464	-4.14319	H	-4.08767	-1.02294	-3.93930	H	2.10059	-2.65804	-1.81080
H	1.86295	0.88708	-3.86387	H	-4.23405	-2.33300	-2.74788	H	1.51091	-1.74185	-3.20534
H	1.25732	-0.05201	-5.24263	H	-2.67344	-2.02520	-3.54316	H	3.23532	-1.79680	-2.84618
H	1.85453	-0.89885	-3.79872	Si	-0.43528	3.39701	0.61899	H	4.43679	-1.34423	0.33653
C	-0.83381	1.29102	-4.04592	C	-2.21392	1.11484	-2.74957	H	3.30188	-1.08325	1.67204
H	-1.82771	1.39770	-3.58529	H	-2.90208	1.50729	-3.51773	H	2.98841	-2.33662	0.46214
H	-0.97186	1.25707	-5.13749	H	-1.32124	0.74681	-3.28330	H	2.31127	3.75265	-1.44774
H	-0.24665	2.19488	-3.82178	H	-1.89600	1.95097	-2.11101	H	0.60520	3.39700	-1.70009
C	-0.90924	-1.21023	-4.00122	Si	1.76971	-2.52031	-1.80479	H	1.23399	3.62797	-0.05652

H	-0.42969	-2.13943	-3.65327	Si	1.30944	2.80751	-1.78012	H	-1.51196	1.74229	-3.20421
H	-0.97073	-1.25958	-5.09909	N	-2.07330	-0.87805	-0.49012	H	-3.23649	1.79565	-2.84541
H	-1.93946	-1.18331	-3.61173	N	1.79727	-1.35493	-0.49265	H	-2.10272	2.65727	-1.80932
C	3.29872	0.39035	-1.03998	N	0.27502	2.23772	-0.48245	H	-3.30250	1.08015	1.67275
H	2.70938	0.71804	-1.89826	C	0.67654	3.74552	2.12813	H	-2.99015	2.33426	0.46334
C	4.69371	0.36052	-1.09451	H	0.21997	4.50139	2.79268	H	-4.43777	1.34079	0.33748
H	5.20924	0.67387	-2.00434	H	1.66346	4.12049	1.80989	H	-0.60294	-3.39676	-1.70145
C	5.39889	-0.08082	0.02665	H	0.83046	2.82092	2.70668	H	-1.23145	-3.62889	-0.05794
H	6.49097	-0.12052	0.01674	C	1.93596	-4.31822	-1.18586	H	-2.30876	-3.75371	-1.44913
C	4.67873	-0.47492	1.15780	H	1.13583	-4.56827	-0.46973				
H	5.18515	-0.83039	2.05756	H	2.90106	-4.49294	-0.68139				
C	3.28566	-0.41272	1.12105	H	1.87167	-5.02597	-2.03048				
H	2.68201	-0.71354	1.98055	C	2.07082	1.36537	-2.74469				
C	-3.08981	1.31055	-0.93986	H	1.30223	0.75082	-3.24306				
H	-2.90158	0.51422	-1.66275	H	2.67245	0.69442	-2.11595				
C	-4.24023	2.09663	-1.02452	H	2.71987	1.76950	-3.54021				
H	-4.96366	1.91895	-1.82251	C	2.76708	3.86055	-1.13892				
C	-4.43063	3.10813	-0.08106	H	3.42894	4.15532	-1.97166				
H	-5.31660	3.74663	-0.12141	H	3.36990	3.29939	-0.40600				
C	-3.46261	3.28943	0.91020	H	2.42167	4.78569	-0.64792				
H	-3.56518	4.06851	1.66831	C	0.44010	3.85595	-3.11064				
C	-2.34375	2.45610	0.91459	H	1.15299	4.06559	-3.92718				
H	-1.56018	2.57193	1.66724	H	0.07126	4.82306	-2.73894				
C	-2.33692	-2.50508	-0.86506	H	-0.41396	3.31478	-3.54780				
H	-1.65863	-2.51127	-1.71937	C	0.14159	-2.43355	-2.77056				
C	-3.43370	-3.36791	-0.82105	H	0.00582	-1.45837	-3.26841				
H	-3.61555	-4.05828	-1.64693	H	-0.74093	-2.60870	-2.13934				
C	-4.28144	-3.31850	0.28718	H	0.15618	-3.19688	-3.56710				
H	-5.15163	-3.97646	0.35187	C	3.12028	-2.28764	-3.12588				
C	-3.99445	-2.40804	1.30735	H	2.93296	-2.98646	-3.95979				
H	-4.62739	-2.33010	2.19376	H	4.13624	-2.48403	-2.75388				
C	-2.87662	-1.58359	1.17620	H	3.10393	-1.26717	-3.53986				
H	-2.61378	-0.85771	1.94766	C	-0.81440	5.11186	-0.13164				
C	0.79103	-3.27722	0.95125	H	-1.51608	5.04638	-0.97878				
H	0.34647	-2.85402	1.85433	H	0.08435	5.64438	-0.48165				
C	1.24410	-4.59642	0.91967	H	-1.28652	5.73844	0.64600				
H	1.15229	-5.22535	1.80755	C	-2.11686	2.80433	1.28184				
C	1.80566	-5.08623	-0.26249	H	-2.85388	2.71819	0.46694				
H	2.16655	-6.11576	-0.32637	H	-2.50552	3.53886	2.00979				
C	1.89464	-4.23244	-1.36383	H	-2.05591	1.83253	1.79478				
H	2.32280	-4.56778	-2.31044	C	4.83378	-1.84635	-0.15364				
C	1.41652	-2.92670	-1.23974	H	4.84765	-2.89052	-0.50459				
H	1.46153	-2.22763	-2.07716	H	5.61568	-1.74810	0.62040				
C	0.42918	3.26497	-1.10812	H	5.11975	-1.20279	-1.00104				
H	-0.23163	2.79240	-1.83600	C	3.48345	0.42294	1.27886				
C	0.86097	4.58141	-1.28099	H	3.76009	1.11392	0.46610				
H	0.53247	5.15090	-2.15255	H	4.32400	0.39294	1.99505				
C	1.71824	5.13635	-0.32934	H	2.61400	0.84317	1.80687				
H	2.08056	6.16180	-0.43628	C	2.91013	-2.47324	2.10694				
C	2.10653	4.34920	0.75798	H	2.02967	-2.15134	2.68536				
H	2.77796	4.73540	1.52759	H	3.79090	-2.45504	2.77433				
C	1.62612	3.04237	0.84664	H	2.74767	-3.51506	1.78373				
H	1.91378	2.39866	1.67965								
$^{8z}\mathbf{1}_{opt}$				$^{8z}\mathbf{2}_{opt}$				$^{8z}\mathbf{3}_{opt}$			
Dy	0.00000	0.00000	0.00000	Er	0.00000	0.00000	0.00000	Dy	0.00000	0.00000	0.00000
N	2.60450	0.02556	0.05083	C	-4.02573	-3.25290	-0.13895	Cl	0.00000	0.00000	2.63068
N	-2.17851	1.44908	-0.01010	H	-4.93477	-2.73789	-0.48791	C	1.76403	1.74901	-0.90549
N	-2.03686	-1.65249	0.10957	H	-4.33280	-3.98290	0.63159	C	2.41588	1.03955	0.14359
N	0.88767	-2.44883	-0.12131	H	-3.61730	-3.81919	-0.99100	H	2.70895	1.45517	1.10141
N	0.77596	2.50933	-0.03397	Si	-3.07817	-0.26419	-1.79181	C	2.62174	-0.31078	-0.26531
O	0.00000	0.00000	2.20316	C	-1.38348	-3.22958	1.29293	C	2.08964	-0.44914	-1.58574

O	-0.03011	0.05647	-2.09710	H	-1.82890	-3.92245	2.03004	C	1.56190	0.82062	-1.96413
C	0.01080	0.05965	3.59144	H	-0.56845	-2.68619	1.79479	H	1.12103	1.04922	-2.92774
C	-1.35812	0.53071	4.14042	H	-0.94590	-3.83638	0.48372	C	1.45871	3.22581	-0.94043
H	-1.62099	1.51328	3.72018	Cl	0.00000	0.00000	2.64661	C	3.37312	-1.36152	0.51186
H	-1.35063	0.61901	5.24119	C	-3.59447	-1.28417	2.12791	C	2.20643	-1.65483	-2.48357
H	-2.15602	-0.17747	3.86779	H	-4.40832	-0.61291	1.80623	C	-1.76442	-1.74873	-0.90531
C	1.08613	1.05532	4.09086	H	-2.86624	-0.69307	2.70586	C	-2.41615	-1.03893	0.14361
H	2.08080	0.77180	3.71305	H	-4.02693	-2.05790	2.78956	H	-2.70940	-1.45431	1.10149
H	1.13628	1.09050	5.19365	Si	3.16555	-1.32593	0.60454	C	-2.62163	0.31139	-0.26552
H	0.86134	2.07104	3.72979	C	-4.71428	0.48540	-1.15299	C	-2.08944	0.44939	-1.58595
C	0.31757	-1.33434	4.19030	H	-5.29163	0.91125	-1.99155	C	-1.56199	-0.82057	-1.96409
H	-0.44428	-2.06207	3.86790	H	-4.52475	1.29086	-0.42394	H	-1.12113	-1.04945	-2.92763
H	0.32891	-1.31941	5.29466	H	-5.35320	-0.26843	-0.66276	C	-1.45949	-3.22561	-0.93997
H	1.29989	-1.69505	3.84562	Si	-2.73184	-2.06923	0.61213	C	-3.37278	1.36246	0.51144
C	-0.09952	0.06277	-3.52160	C	-3.54779	-1.54591	-3.11174	C	-2.20589	1.65494	-2.48399
C	1.31687	0.00298	-4.11962	H	-4.05698	-1.02953	-3.94364	H	2.05882	-2.59970	-1.94767
H	1.89768	0.89554	-3.83580	H	-4.22632	-2.33287	-2.75125	H	1.48156	-1.61623	-3.30100
H	1.28629	-0.02749	-5.21894	H	-2.65616	-2.03733	-3.53176	H	3.20200	-1.70042	-2.94209
H	1.86218	-0.89234	-3.77984	Si	-0.42756	3.40335	0.62431	H	4.43125	-1.38137	0.21784
C	-0.78515	1.34692	-4.02362	C	-2.19197	1.11171	-2.74140	H	3.32740	-1.16422	1.58838
H	-1.77755	1.47477	-3.56484	H	-2.86482	1.49060	-3.52932	H	2.98130	-2.37022	0.33651
H	-0.92388	1.32210	-5.11484	H	-1.28696	0.74753	-3.25606	H	2.30933	3.78515	-1.34952
H	-0.17628	2.23606	-3.79886	H	-1.89621	1.95785	-2.10561	H	0.59810	3.45119	-1.57866
C	-0.90903	-1.15245	-4.00779	Si	1.76790	-2.52188	-1.80030	H	1.25826	3.62591	0.06076
H	-0.45263	-2.09572	-3.66589	Si	1.30488	2.80121	-1.78372	H	-1.48107	1.61596	-3.30145
H	-0.95834	-1.19075	-5.10613	N	-2.07727	-0.86986	-0.47108	H	-3.20147	1.70077	-2.94248
H	-1.94480	-1.10734	-3.63431	N	1.79396	-1.36138	-0.47122	H	-2.05794	2.59988	-1.94828
C	3.28613	0.40652	-1.04246	N	0.28267	2.23887	-0.46115	H	-3.32731	1.16522	1.58798
H	2.68765	0.74580	-1.88965	C	0.68385	3.75917	2.14020	H	-2.98056	2.37101	0.33609
C	4.68012	0.35943	-1.12187	H	0.22788	4.51966	2.80153	H	-4.43085	1.38266	0.21725
H	5.18307	0.67113	-2.03939	H	1.67064	4.13074	1.81700	H	-0.59898	-3.45135	-1.57821
C	5.39801	-0.10198	-0.01769	H	0.83577	2.83384	2.71879	H	-1.25908	-3.62557	0.06128
H	6.48891	-0.15897	-0.05002	C	1.93703	-4.31795	-1.17537	H	-2.31028	-3.78481	-1.34890
C	4.69160	-0.49735	1.12259	H	1.13712	-4.56999	-0.45928				
H	5.20922	-0.87182	2.00858	H	2.90436	-4.49200	-0.67438				
C	3.29944	-0.41801	1.11040	H	1.87280	-5.02371	-2.02131				
H	2.70570	-0.72463	1.97533	C	2.04870	1.34654	-2.73698				
C	-3.07703	1.27015	-0.99304	H	1.27434	0.72349	-3.21504				
H	-2.86048	0.47258	-1.70598	H	2.66747	0.68657	-2.11354				
C	-4.22272	2.05687	-1.12903	H	2.67826	1.74078	-3.55248				
H	-4.91148	1.87698	-1.95676	C	2.77127	3.84784	-1.14968				
C	-4.44745	3.07632	-0.20244	H	3.42591	4.13739	-1.98958				
H	-5.32742	3.71874	-0.28739	H	3.37885	3.28561	-0.42118				
C	-3.51819	3.26329	0.82508	H	2.43310	4.77676	-0.66010				
H	-3.64650	4.05257	1.56897	C	0.42785	3.84877	-3.10273				
C	-2.40142	2.42959	0.87929	H	1.13344	4.04385	-3.92873				
H	-1.64415	2.55449	1.65749	H	0.07500	4.82427	-2.73783				
C	-2.33718	-2.46680	-0.91638	H	-0.43546	3.31631	-3.53137				
H	-1.68399	-2.41185	-1.78823	C	0.13459	-2.43231	-2.75070				
C	-3.43099	-3.33536	-0.90231	H	-0.00914	-1.45605	-3.24363				
H	-3.63408	-3.96696	-1.76938	H	-0.74516	-2.62034	-2.11964				
C	-4.24883	-3.36368	0.22820	H	0.15092	-3.18712	-3.55494				
H	-5.11714	-4.02611	0.26807	C	3.11536	-2.28184	-3.11614				
C	-3.93608	-2.52298	1.30035	H	2.91797	-2.96950	-3.95654				
H	-4.54788	-2.50598	2.20512	H	4.13226	-2.49238	-2.75501				
C	-2.82478	-1.68648	1.19592	H	3.10660	-1.25924	-3.52418				
H	-2.54370	-1.00979	2.00536	C	-0.80620	5.11727	-0.12436				
C	0.81962	-3.29236	0.92102	H	-1.50807	5.05000	-0.97090				
H	0.39266	-2.88367	1.83968	H	0.09230	5.64573	-0.48059				
C	1.25919	-4.61425	0.85469	H	-1.27651	5.74877	0.65097				
H	1.17667	-5.26097	1.73103	C	-2.10687	2.81718	1.30624				
C	1.79144	-5.08738	-0.34860	H	-2.84570	2.71668	0.49469				

H	2.13808	-6.11951	-0.44233	H	-2.49597	3.56202	2.02446				
C	1.86671	-4.21376	-1.43462	H	-2.03944	1.85131	1.82980				
H	2.26931	-4.53510	-2.39731	C	4.83857	-1.83532	-0.15758				
C	1.40417	-2.90558	-1.27511	H	4.85615	-2.87851	-0.51072				
H	1.43725	-2.19276	-2.10113	H	5.62664	-1.73170	0.61002				
C	0.41856	3.26447	-1.08677	H	5.11393	-1.19184	-1.00828				
H	-0.24037	2.79197	-1.81606	C	3.48470	0.42057	1.29522				
C	0.86923	4.57333	-1.27342	H	3.73969	1.12149	0.48407				
H	0.55693	5.13449	-2.15637	H	4.33911	0.39195	1.99593				
C	1.72934	5.12720	-0.32444	H	2.61800	0.82623	1.83920				
H	2.11004	6.14432	-0.44623	C	2.93620	-2.47529	2.11690				
C	2.10007	4.34773	0.77543	H	2.05490	-2.15798	2.69721				
H	2.77687	4.73299	1.54124	H	3.82247	-2.44956	2.77833				
C	1.60249	3.04875	0.87682	H	2.77975	-3.51780	1.79258				
H	1.88153	2.40726	1.71504								
$^{12z}\mathbf{1}_{opt}$				$^{12z}\mathbf{2}_{opt}$				$^{12z}\mathbf{3}_{opt}$			
Dy	0.00000	0.00000	0.00000	Er	0.00000	0.00000	0.00000	Dy	0.00000	0.00000	0.00000
N	2.60233	0.04390	0.06153	C	-4.03915	-3.24501	-0.12651	Cl	0.00000	0.00000	2.68113
N	-2.20013	1.42017	-0.04720	H	-4.94192	-2.72639	-0.48563	C	1.76155	1.75696	-0.87935
N	-2.02063	-1.68047	0.10748	H	-4.35543	-3.97056	0.64515	C	2.41331	1.02424	0.15402
N	0.90431	-2.44341	-0.13438	H	-3.63046	-3.81683	-0.97453	H	2.71550	1.42090	1.11748
N	0.75011	2.50896	0.01758	Si	-3.06660	-0.27391	-1.80181	C	2.61312	-0.31930	-0.28441
O	0.00000	-0.00000	2.24365	C	-1.40300	-3.22915	1.31937	C	2.07856	-0.42845	-1.60650
O	-0.01476	0.07420	-2.07960	H	-1.85743	-3.92208	2.05217	C	1.55116	0.85004	-1.95477
C	-0.04993	0.03685	3.62392	H	-0.59096	-2.68525	1.82598	H	1.11475	1.10077	-2.91491
C	-1.39090	0.63624	4.12351	H	-0.95941	-3.83632	0.51372	C	1.46454	3.23572	-0.89077
H	-1.51622	1.66124	3.74231	Cl	0.00000	0.00000	2.68590	C	3.37240	-1.38697	0.46159
H	-1.44407	0.67147	5.22802	C	-3.60740	-1.27953	2.14271	C	2.19456	-1.61119	-2.53440
H	-2.24365	0.04120	3.76172	H	-4.42084	-0.60922	1.81745	C	-1.76035	-1.75726	-0.88115
C	1.09377	0.91128	4.20254	H	-2.87659	-0.68727	2.71693	C	-2.41235	-1.02662	0.15356
H	2.07324	0.53456	3.86961	H	-4.04022	-2.05428	2.80487	H	-2.71386	-1.42496	1.11654
H	1.08819	0.92591	5.30892	Si	3.17305	-1.32028	0.60741	C	-2.61354	0.31737	-0.28283
H	0.99298	1.94926	3.84922	C	-4.70183	0.48883	-1.17550	C	-2.07955	0.42893	-1.60496
C	0.08924	-1.39103	4.21334	H	-5.27199	0.90462	-2.02370	C	-1.55122	-0.84859	-1.95533
H	-0.71396	-2.03872	3.82803	H	-4.51248	1.30458	-0.45741	H	-1.11495	-1.09751	-2.91600
H	0.03720	-1.39709	5.31862	H	-5.34720	-0.25661	-0.68026	C	-1.46206	-3.23574	-0.89484
H	1.05298	-1.83287	3.91424	Si	-2.74221	-2.06454	0.61959	C	-3.37350	1.38325	0.46504
C	-0.08153	0.09583	-3.51534	C	-3.52636	-1.56747	-3.10661	C	-2.19678	1.61298	-2.53104
C	1.33207	-0.00431	-4.11048	H	-4.02209	-1.05500	-3.94884	H	2.04575	-2.56992	-2.02404
H	1.93941	0.87198	-3.83121	H	-4.21606	-2.34660	-2.75077	H	1.47400	-1.55090	-3.35369
H	1.29846	-0.03151	-5.20960	H	-2.63597	-2.06804	-3.51749	H	3.19040	-1.64334	-2.99282
H	1.85290	-0.91661	-3.77752	Si	-0.42299	3.41007	0.63221	H	4.42677	-1.40122	0.15376
C	-0.72301	1.40608	-4.00419	C	-2.16136	1.09185	-2.74220	H	3.33952	-1.21283	1.54359
H	-1.70736	1.57172	-3.53996	H	-2.81356	1.45092	-3.55618	H	2.97856	-2.39139	0.26692
H	-0.87078	1.38872	-5.09419	H	-1.24085	0.72963	-3.22938	H	2.31001	3.79326	-1.31241
H	-0.07833	2.27171	-3.78775	H	-1.89342	1.95265	-2.11387	H	0.59434	3.47441	-1.51066
C	-0.92873	-1.08856	-4.00877	Si	1.77256	-2.52114	-1.79450	H	1.28621	3.62519	0.11944
H	-0.50202	-2.05038	-3.67958	Si	1.29591	2.79777	-1.78677	H	-1.47623	1.55465	-3.35048
H	-0.97827	-1.11514	-5.10720	N	-2.08039	-0.86559	-0.45038	H	-3.19269	1.64489	-2.98932
H	-1.96467	-1.01476	-3.63936	N	1.79341	-1.36461	-0.44816	H	-2.04884	2.57106	-2.01920
C	3.27265	0.37846	-1.05429	N	0.28766	2.24117	-0.43813	H	-3.33975	1.20772	1.54678
H	2.66577	0.67763	-1.91047	C	0.68835	3.77441	2.15514	H	-2.98084	2.38834	0.27146
C	4.66638	0.32760	-1.14667	H	0.23202	4.53891	2.81364	H	-4.42807	1.39678	0.15785
H	5.15901	0.59792	-2.08302	H	1.67470	4.14354	1.82731	H	-0.59160	-3.47271	-1.51501
C	5.39523	-0.08719	-0.03176	H	0.83882	2.84838	2.73379	H	-1.28349	-3.62660	0.11479
H	6.48556	-0.14772	-0.07570	C	1.94935	-4.31415	-1.16184	H	-2.30702	-3.79337	-1.31741
C	4.70002	-0.43393	1.13197	H	1.15016	-4.56892	-0.44538				
H	5.22755	-0.77363	2.02673	H	2.91924	-4.48453	-0.66391				
C	3.30812	-0.35525	1.13125	H	1.88690	-5.01925	-2.00818				
H	2.72103	-0.62697	2.01284	C	2.02452	1.33164	-2.72869				

C	-3.05169	1.23345	-1.07064	H	1.24636	0.69932	-3.18769				
H	-2.80100	0.43387	-1.76952	H	2.66082	0.68344	-2.11065				
C	-4.18875	2.02015	-1.26977	H	2.63457	1.71690	-3.56295				
H	-4.83351	1.83675	-2.13177	C	2.76984	3.83969	-1.16041				
C	-4.45619	3.04836	-0.36501	H	3.41614	4.12554	-2.00773				
H	-5.32701	3.69399	-0.50330	H	3.38360	3.27663	-0.43728				
C	-3.57745	3.24226	0.70571	H	2.43821	4.77156	-0.67118				
H	-3.73807	4.04215	1.43232	C	0.40962	3.84356	-3.09440				
C	-2.46548	2.40893	0.82118	H	1.10847	4.02644	-3.92872				
H	-1.74362	2.54463	1.63115	H	0.07007	4.82615	-2.73619				
C	-2.32817	-2.43999	-0.95827	H	-0.46077	3.31810	-3.51646				
H	-1.69145	-2.32801	-1.83693	C	0.13366	-2.43390	-2.72944				
C	-3.41297	-3.32085	-0.97790	H	-0.01901	-1.45850	-3.22082				
H	-3.62323	-3.90273	-1.87774	H	-0.74279	-2.63377	-2.09758				
C	-4.21239	-3.42230	0.16094	H	0.15206	-3.18280	-3.53901				
H	-5.07368	-4.09495	0.17365	C	3.11607	-2.27083	-3.10596				
C	-3.89173	-2.63893	1.27433	H	2.91026	-2.94908	-3.95180				
H	-4.49150	-2.67856	2.18705	H	4.13451	-2.49202	-2.75600				
C	-2.79197	-1.78451	1.20090	H	3.11162	-1.24683	-3.50980				
H	-2.50864	-1.14908	2.04296	C	-0.80319	5.12260	-0.11456				
C	0.87397	-3.29525	0.90296	H	-1.50626	5.05278	-0.95969				
H	0.47310	-2.89568	1.83787	H	0.09409	5.64766	-0.47831				
C	1.31455	-4.61485	0.81149	H	-1.27119	5.75874	0.65909				
H	1.26161	-5.26967	1.68467	C	-2.09875	2.82937	1.33558				
C	1.80723	-5.07837	-0.41318	H	-2.84086	2.71434	0.52896				
H	2.15185	-6.10896	-0.52872	H	-2.48728	3.58408	2.04508				
C	1.84340	-4.19698	-1.49435	H	-2.02321	1.86961	1.86961				
H	2.21231	-4.51005	-2.47346	C	4.84669	-1.81429	-0.15874				
C	1.38287	-2.89081	-1.30874	H	4.87086	-2.85619	-0.51475				
H	1.38510	-2.17339	-2.13126	H	5.64014	-1.70370	0.60299				
C	0.45235	3.25303	-1.06190	H	5.11034	-1.16987	-1.01224				
H	-0.17418	2.77725	-1.81712	C	3.48392	0.42318	1.31744				
C	0.92992	4.55339	-1.24606	H	3.71647	1.13593	0.50997				
H	0.67114	5.10358	-2.15317	H	4.35133	0.39653	2.00338				
C	1.75141	5.10922	-0.26515	H	2.61909	0.81122	1.87742				
H	2.15470	6.11761	-0.38720	C	2.96635	-2.47375	2.12894				
C	2.05700	4.34172	0.86390	H	2.08305	-2.16358	2.71086				
H	2.70512	4.72926	1.65361	H	3.85744	-2.43810	2.78536				
C	1.53838	3.05102	0.95989	H	2.81905	-3.51719	1.80294				
H	1.77131	2.41369	1.81612								
$^{4x}\mathbf{1}_{opt}$				**$^{16z}\mathbf{2}_{opt}$**				**$^{16z}\mathbf{3}_{opt}$**			
Dy	-0.00000	0.00000	0.00000	Er	0.00000	0.00000	0.00000	Dy	0.00000	0.00000	0.00000
N	-0.00000	0.00000	2.64853	C	-4.05972	-3.23128	-0.10403	Cl	0.00000	0.00000	2.75335
N	0.03958	1.50863	-2.12165	H	-4.95387	-2.70667	-0.47534	C	1.80904	1.86070	-0.36939
N	-0.03366	-1.50483	-2.12460	H	-4.38851	-3.94903	0.67040	C	2.48899	0.76673	0.23363
N	0.20163	-2.49288	0.76405	H	-3.65232	-3.81224	-0.94636	H	2.90637	0.75568	1.23529
N	-0.20621	2.49370	0.76704	Si	-3.05123	-0.28848	-1.81296	C	2.54147	-0.31701	-0.69877
O	-2.12654	-0.16926	0.14719	C	-1.42817	-3.22814	1.35435	C	1.89718	0.10943	-1.90030
O	2.12859	0.14918	0.16288	H	-1.89227	-3.91772	2.08573	C	1.42576	1.43883	-1.67608
C	-3.53160	-0.21041	0.15773	H	-0.61677	-2.68470	1.86305	H	0.93865	2.05506	-2.42409
C	-4.09661	0.87575	-0.77959	H	-0.98172	-3.83921	0.55312	C	1.62884	3.24178	0.20898
H	-3.76487	1.87571	-0.45611	Cl	0.00000	0.00000	2.73561	C	3.29178	-1.61209	-0.51169
H	-5.19808	0.87407	-0.79493	C	-3.61951	-1.26684	2.16505	C	1.88153	-0.62459	-3.21584
H	-3.74766	0.71636	-1.81175	H	-4.43105	-0.59558	1.83627	C	-1.80935	-1.86042	-0.36940
C	-4.07221	0.03401	1.58390	H	-2.88363	-0.67511	2.73410	C	-2.48908	-0.76642	0.23379
H	-3.72360	-0.75065	2.27394	H	-4.05417	-2.04049	2.82958	H	-2.90633	-0.75541	1.23550
H	-5.17392	0.03045	1.60304	Si	3.17861	-1.31872	0.61968	C	-2.54148	0.31743	-0.69849
H	-3.73460	1.00636	1.97700	C	-4.68202	0.49815	-1.20518	C	-1.89740	-0.10899	-1.90014
C	-4.03379	-1.59092	-0.31396	H	-5.24199	0.90287	-2.06526	C	-1.42615	-1.43849	-1.67609
H	-3.64001	-1.83046	-1.31329	H	-4.48921	1.32609	-0.50156	H	-0.93920	-2.05472	-2.42422

H	-5.13344	-1.62774	-0.36771	H	-5.33806	-0.23333	-0.70243	C	-1.62928	-3.24158	0.20883
H	-3.70906	-2.37925	0.38403	Si	-2.75552	-2.05699	0.63435	C	-3.29156	1.61261	-0.51118
C	3.53413	0.19224	0.17232	C	-3.50616	-1.59751	-3.09755	C	-1.88177	0.62512	-3.21562
C	4.07823	-0.07257	1.59372	H	-3.98302	-1.08943	-3.95344	H	1.70308	-1.69883	-3.10553
H	3.71936	0.69342	2.29907	H	-4.21326	-2.36215	-2.74484	H	1.12939	-0.22458	-3.89836
H	5.17979	-0.05428	1.61230	H	-2.61973	-2.11478	-3.49538	H	2.84882	-0.51173	-3.72032
H	3.75596	-1.05745	1.96818	Si	-0.41650	3.41730	0.64739	H	4.28835	-1.55033	-0.96758
C	4.03293	1.58015	-0.28024	C	-2.11841	1.05810	-2.74883	H	3.42665	-1.84700	0.55208
H	3.63663	1.83238	-1.27543	H	-2.74649	1.39648	-3.59033	H	2.78964	-2.46010	-0.98954
H	5.13240	1.61995	-0.33528	H	-1.18441	0.69191	-3.20598	H	2.49586	3.87290	-0.02656
H	3.70769	2.35804	0.42914	H	-1.87534	1.93509	-2.13293	H	0.75311	3.74830	-0.21150
C	4.09987	-0.88005	-0.78047	Si	1.78004	-2.51874	-1.78631	H	1.52065	3.21354	1.30163
H	3.76592	-1.88418	-0.47235	Si	1.28942	2.79640	-1.78343	H	-1.12956	0.22525	-3.89814
H	5.20136	-0.87985	-0.79268	N	-2.08399	-0.86289	-0.42601	H	-2.84903	0.51217	-3.72015
H	3.75464	-0.70494	-1.81129	N	1.79387	-1.36789	-0.42019	H	-1.70347	1.69938	-3.10521
C	0.89279	0.73359	3.32856	N	0.29335	2.24458	-0.40971	H	-3.42614	1.84749	0.55264
H	1.60319	1.30317	2.72597	C	0.69564	3.78861	2.17786	H	-2.78940	2.46057	-0.98910
C	0.93395	0.77561	4.72373	H	0.23938	4.55666	2.83468	H	-4.28825	1.55102	-0.96685
H	1.68343	1.38959	5.22721	H	1.68178	4.15503	1.84586	H	-0.75347	-3.74807	-0.21153
C	0.00692	0.01929	5.44366	H	0.84377	2.86121	2.75578	H	-1.52130	-3.21346	1.30150
H	0.00940	0.02705	6.53692	C	1.96440	-4.30938	-1.14822	H	-2.49625	-3.87267	-0.02697
C	-0.92343	-0.74714	4.73863	H	1.16495	-4.56761	-0.43269				
H	-1.67037	-1.35410	5.25433	H	2.93606	-4.47694	-0.65218				
C	-0.88896	-0.72463	3.34280	H	1.90467	-5.01273	-1.99604				
H	-1.60173	-1.30353	2.75212	C	2.00714	1.32001	-2.71260				
C	1.09985	1.44804	-2.94691	H	1.22802	0.67928	-3.15785				
H	1.91344	0.78791	-2.63803	H	2.65867	0.68276	-2.09904				
C	1.18022	2.17145	-4.13686	H	2.60103	1.69823	-3.56182				
H	2.06477	2.08335	-4.77061	C	2.76876	3.83447	-1.16171				
C	0.11078	2.99633	-4.49474	H	3.40801	4.11756	-2.01513				
H	0.13639	3.57224	-5.42304	H	3.38758	3.26998	-0.44347				
C	-0.99331	3.06481	-3.64125	H	2.44263	4.76867	-0.67245				
H	-1.85500	3.69162	-3.87886	C	0.39469	3.83868	-3.08202				
C	-0.98391	2.30825	-2.46912	H	1.08882	4.01215	-3.92243				
H	-1.83298	2.33671	-1.78273	H	0.06395	4.82683	-2.73113				
C	0.99578	-2.29503	-2.47546	H	-0.47945	3.31744	-3.50087				
H	1.84470	-2.31929	-1.78886	C	0.13567	-2.43406	-2.70622				
C	1.01136	-3.04541	-3.65157	H	-0.02799	-1.45907	-3.19433				
H	1.87785	-3.66443	-3.89216	H	-0.73711	-2.64926	-2.07435				
C	-0.09200	-2.97889	-4.50607	H	0.15800	-3.17519	-3.52298				
H	-0.11223	-3.54846	-5.43841	C	3.11963	-2.25514	-3.09312				
C	-1.16764	-2.16383	-4.14442	H	2.91023	-2.92865	-3.94204				
H	-2.05159	-2.07722	-4.77924	H	4.14054	-2.47918	-2.75260				
C	-1.09391	-1.44726	-2.94993	H	3.11347	-1.23140	-3.49702				
H	-1.91221	-0.79484	-2.63739	C	-0.79812	5.12854	-0.09734				
C	-0.76503	-3.37767	0.47047	H	-1.50401	5.05579	-0.93980				
H	-1.64699	-2.97572	-0.03139	H	0.09755	5.64912	-0.47089				
C	-0.66519	-4.73630	0.77488	H	-1.26187	5.77044	0.67486				
H	-1.47722	-5.41484	0.50639	C	-2.08801	2.84232	1.37390				
C	0.48980	-5.19835	1.40992	H	-2.83468	2.71399	0.57342				
H	0.60616	-6.25762	1.65270	H	-2.47440	3.60625	2.07618				
C	1.49605	-4.28033	1.71931	H	-2.00369	1.88843	1.91758				
H	2.42085	-4.59340	2.20808	C	4.85279	-1.80252	-0.14719				
C	1.30870	-2.93989	1.37741	H	4.87968	-2.84175	-0.51020				
H	2.07150	-2.18785	1.58846	H	5.65006	-1.69147	0.61116				
C	0.76604	3.37404	0.47666	H	5.10996	-1.15506	-1.00034				
H	1.64636	2.96942	-0.02595	C	3.48513	0.42064	1.35013				
C	0.67463	4.73236	0.78498	H	3.70431	1.14348	0.54786				
H	1.49133	5.40636	0.51926	H	4.36044	0.39220	2.02742				
C	-0.47787	5.20012	1.42026	H	2.62070	0.79525	1.92021				
H	-0.58762	6.25937	1.66606	C	2.98626	-2.47544	2.15014				
C	-1.49017	4.28749	1.72569	H	2.10150	-2.16773	2.73201				

H	-2.41349	4.60507	2.21434	H	3.88093	-2.43441	2.80362				
C	-1.31096	2.94682	1.38060	H	2.84350	-3.51891	1.82180				
H	-2.08021	2.20105	1.59052								
$^{8x}\mathbf{1}_{opt}$				$^{20z}\mathbf{2}_{opt}$				$^{20z}\mathbf{3}_{opt}$			
Dy	-0.00000	0.00000	0.00000	Er	0.00000	0.00000	0.00000	Dy	0.00000	0.00000	0.00000
N	0.00000	0.00000	2.71024	C	-4.07923	-3.21916	-0.07377	Cl	0.00000	0.00000	2.85261
N	0.04587	1.46922	-2.11290	H	-4.96479	-2.68936	-0.45770	C	1.87182	1.81644	-0.06164
N	-0.07253	-1.48998	-2.10739	H	-4.42031	-3.92904	0.70336	C	2.52099	0.58815	0.24652
N	0.15731	-2.52917	0.74693	H	-3.67258	-3.80895	-0.91037	H	2.98191	0.33810	1.19789
N	-0.14104	2.52476	0.72335	Si	-3.03476	-0.30692	-1.82036	C	2.48849	-0.25836	-0.90853
O	-2.11467	-0.11705	0.29320	C	-1.45322	-3.22547	1.40042	C	1.82810	0.45761	-1.95409
O	2.11774	0.11380	0.27834	H	-1.92734	-3.91125	2.13064	C	1.41870	1.71496	-1.41113
C	-3.51392	-0.16009	0.40342	H	-0.64432	-2.68061	1.91226	H	0.94650	2.50555	-1.98585
C	-4.15233	0.86573	-0.55400	H	-1.00158	-3.84084	0.60523	C	1.78981	3.03944	0.81682
H	-3.80304	1.88441	-0.32063	Cl	-0.00000	-0.00000	2.80275	C	3.19195	-1.58362	-1.06312
H	-5.25203	0.86180	-0.48966	C	-3.63198	-1.25152	2.19363	C	1.76260	0.05760	-3.40330
H	-3.88050	0.64266	-1.59692	H	-4.43838	-0.57644	1.85940	C	-1.87174	-1.81656	-0.06178
C	-3.95429	0.16663	1.84944	H	-2.88983	-0.66298	2.75875	C	-2.52092	-0.58839	0.24687
H	-3.53737	-0.56597	2.55883	H	-4.07250	-2.02224	2.86033	H	-2.98161	-0.33863	1.19842
H	-5.05188	0.14785	1.94939	Si	3.18254	-1.31990	0.64241	C	-2.48869	0.25846	-0.90793
H	-3.60758	1.16731	2.15370	C	-4.65793	0.50886	-1.23201	C	-1.82848	-0.45716	-1.95384
C	-4.03627	-1.56815	0.05095	H	-5.20624	0.90400	-2.10394	C	-1.41892	-1.71466	-1.41134
H	-3.72707	-1.85432	-0.96586	H	-4.45969	1.34779	-0.54244	H	-0.94677	-2.50504	-1.98638
H	-5.13616	-1.61840	0.09104	H	-5.32672	-0.20695	-0.72276	C	-1.78949	-3.03981	0.81630
H	-3.63852	-2.31548	0.75716	Si	-2.76859	-2.05004	0.65658	C	-3.19218	1.58377	-1.06196
C	3.51871	0.11255	0.38620	C	-3.49025	-1.63255	-3.08174	C	-1.76319	-0.05668	-3.40293
C	3.94940	-0.14618	1.84898	H	-3.94191	-1.12851	-3.95409	H	1.52103	-0.99915	-3.54925
H	3.55523	0.63850	2.51437	H	-4.22154	-2.37556	-2.73238	H	1.04192	0.65525	-3.96320
H	5.04704	-0.15408	1.94928	H	-2.61113	-2.17415	-3.46246	H	2.73851	0.22459	-3.87603
H	3.57430	-1.11719	2.21129	Si	-0.40885	3.42539	0.67260	H	4.17044	-1.44648	-1.54034
C	4.09386	1.47742	-0.04447	C	-2.07007	1.01486	-2.75495	H	3.36090	-2.06668	-0.09147
H	3.77831	1.72774	-1.06835	H	-2.67832	1.33893	-3.61692	H	2.63909	-2.27941	-1.70161
H	5.19521	1.48098	-0.02461	H	-1.13056	0.63851	-3.19198	H	2.68434	3.66533	0.68989
H	3.74491	2.27578	0.63069	H	-1.83935	1.90504	-2.15338	H	0.93038	3.66798	0.55494
C	4.11670	-0.98870	-0.51153	Si	1.79039	-2.51434	-1.77441	H	1.70824	2.76831	1.87882
H	3.72466	-1.97820	-0.22581	Si	1.28317	2.79817	-1.77194	H	-1.04259	-0.65414	-3.96312
H	5.21548	-1.02600	-0.44253	N	-2.08716	-0.86285	-0.39649	H	-2.73917	-0.22350	-3.87559
H	3.85684	-0.80955	-1.56579	N	1.79533	-1.37084	-0.38579	H	-1.52163	1.00012	-3.54856
C	0.78191	0.84235	3.39653	N	0.29827	2.24935	-0.37348	H	-3.36089	2.06655	-0.09013
H	1.41544	1.50176	2.80011	C	0.70599	3.80284	2.21025	H	-2.63945	2.27974	-1.70038
C	0.80509	0.88942	4.79334	H	0.25077	4.57468	2.86614	H	-4.17078	1.44680	-1.53900
H	1.46287	1.59784	5.30153	H	1.69221	4.16553	1.87394	H	-0.93013	-3.66827	0.55401
C	-0.01912	0.01591	5.50515	H	0.85052	2.87369	2.78724	H	-1.70764	-2.76900	1.87836
H	-0.02681	0.02250	6.59923	C	1.98293	-4.30326	-1.13352	H	-2.68405	-3.66567	0.68942
C	-0.83358	-0.86563	4.79205	H	1.18237	-4.56656	-0.42041				
H	-1.49918	-1.56758	5.29917	H	2.95573	-4.46845	-0.63829				
C	-0.79152	-0.83436	3.39540	H	1.92736	-5.00351	-1.98416				
H	-1.41783	-1.50034	2.79837	C	1.99522	1.31265	-2.68643				
C	1.14021	1.47267	-2.89784	H	1.21840	0.66152	-3.12023				
H	2.00109	0.90920	-2.52941	H	2.66274	0.68826	-2.07676				
C	1.19711	2.13749	-4.12237	H	2.57341	1.68565	-3.54917				
H	2.10825	2.10209	-4.72301	C	2.76500	3.83479	-1.15259				
C	0.06708	2.83189	-4.56384	H	3.39843	4.11559	-2.01105				
H	0.07222	3.35376	-5.52416	H	3.38808	3.26950	-0.43800				
C	-1.07140	2.83608	-3.75263	H	2.44260	4.77108	-0.66408				
H	-1.97968	3.35922	-4.05819	C	0.37922	3.83387	-3.06363				
C	-1.03623	2.14638	-2.54090	H	1.07076	4.00250	-3.90761				
H	-1.91334	2.12318	-1.88944	H	0.05061	4.82533	-2.72028				
C	1.00309	-2.18313	-2.52570	H	-0.49425	3.31249	-3.48324				
H	1.87083	-2.18106	-1.86158	C	0.14020	-2.43230	-2.67904				

C	1.04292	-2.86505	-3.74178	H	-0.03875	-1.45608	-3.15869				
H	1.94668	-3.40055	-4.03923	H	-0.72791	-2.66995	-2.04870				
C	-0.08425	-2.83584	-4.56787	H	0.16931	-3.16083	-3.50731				
H	-0.08496	-3.34955	-5.53259	C	3.12563	-2.23390	-3.07646				
C	-1.20876	-2.12689	-4.13558	H	2.91761	-2.90759	-3.92608				
H	-2.11131	-2.07212	-4.74763	H	4.15022	-2.45256	-2.74383				
C	-1.15693	-1.47128	-2.90587	H	3.11127	-1.21219	-3.48485				
H	-2.01401	-0.89642	-2.54627	C	-0.79286	5.13510	-0.07026				
C	-0.78573	-3.40043	0.35264	H	-1.50383	5.05883	-0.90819				
H	-1.64920	-2.97583	-0.16149	H	0.10032	5.65025	-0.45670				
C	-0.68281	-4.77674	0.56373	H	-1.24994	5.78396	0.70093				
H	-1.47173	-5.44149	0.20655	C	-2.07475	2.85678	1.42591				
C	0.45124	-5.27277	1.21018	H	-2.82805	2.71588	0.63365				
H	0.57427	-6.34673	1.37196	H	-2.45654	3.63010	2.12221				
C	1.43166	-4.36943	1.62721	H	-1.98030	1.90902	1.97923				
H	2.34393	-4.70852	2.12253	C	4.85762	-1.79723	-0.12200				
C	1.24229	-3.00966	1.37308	H	4.88449	-2.83261	-0.49547				
H	1.99007	-2.26928	1.66315	H	5.65724	-1.69098	0.63530				
C	0.85567	3.36034	0.38637	H	5.11267	-1.14487	-0.97212				
H	1.74536	2.89723	-0.04325	C	3.48718	0.41454	1.39444				
C	0.77387	4.74396	0.55223	H	3.70118	1.14621	0.59866				
H	1.60693	5.37856	0.24365	H	4.36573	0.38108	2.06908				
C	-0.39537	5.28700	1.08937	H	2.62117	0.77914	1.96917				
H	-0.50175	6.36787	1.21184	C	2.99740	-2.47896	2.18214				
C	-1.43159	4.42113	1.44675	H	2.11174	-2.16910	2.76245				
H	-2.37158	4.79779	1.85545	H	3.89476	-2.43617	2.83445				
C	-1.26062	3.05038	1.24408	H	2.85500	-3.52191	1.85154				
H	-2.05090	2.33779	1.48729								
$^{12x}\mathbf{1}_{opt}$				$^{24z}\mathbf{2}_{opt}$				$^{22z}\mathbf{3}_{opt}$			
Dy	-0.00000	0.00000	0.00000	Er	0.00000	0.00000	0.00000	Dy	0.00000	0.00000	0.00000
N	-0.00000	0.00000	2.79807	C	-4.10003	-3.20348	-0.02711	Cl	0.00000	0.00000	2.93981
N	0.04656	1.46515	-2.09192	H	-4.97801	-2.66921	-0.42201	C	1.88677	1.79222	-0.00006
N	-0.07362	-1.45661	-2.10218	H	-4.45185	-3.90720	0.75163	C	2.52640	0.54013	0.23024
N	0.11037	-2.57118	0.72738	H	-3.69424	-3.79989	-0.85961	H	3.00410	0.23368	1.15715
N	-0.10456	2.55114	0.70431	Si	-3.01645	-0.32540	-1.81696	C	2.47018	-0.23888	-0.97098
O	-2.09385	-0.08752	0.42624	C	-1.48228	-3.21401	1.47115	C	1.80415	0.54287	-1.96588
O	2.09620	0.07812	0.41768	H	-1.96866	-3.89643	2.19833	C	1.41334	1.77060	-1.34546
C	-3.47827	-0.14039	0.63928	H	-0.68116	-2.66419	1.99073	H	0.94527	2.59839	-1.86908
C	-4.20125	0.83632	-0.30915	H	-1.01881	-3.83313	0.68553	C	1.83536	2.96740	0.94414
H	-3.85302	1.86880	-0.14693	Cl	0.00000	0.00000	2.91340	C	3.16193	-1.55689	-1.21470
H	-5.29351	0.82014	-0.16563	C	-3.64913	-1.22430	2.23458	C	1.72449	0.23311	-3.43574
H	-4.00143	0.57348	-1.35861	H	-4.44337	-0.53964	1.89032	C	-1.88731	-1.79273	0.00006
C	-3.81597	0.24129	2.10251	H	-2.89900	-0.64432	2.79903	C	-2.52627	-0.54179	0.23072
H	-3.34853	-0.46576	2.80744	H	-4.10445	-1.98800	2.90237	H	-3.00397	-0.23581	1.15780
H	-4.90455	0.22846	2.27944	Si	3.18063	-1.32821	0.68396	C	-2.46986	0.23749	-0.97046
H	-3.44801	1.25164	2.34445	C	-4.62369	0.53534	-1.25228	C	-1.80393	-0.54392	-1.96558
C	-4.00460	-1.56790	0.38578	H	-5.15878	0.91840	-2.13783	C	-1.41318	-1.77179	-1.34534
H	-3.79072	-1.88022	-0.64757	H	-4.41424	1.38780	-0.58228	H	-0.94487	-2.59900	-1.86963
H	-5.09477	-1.63511	0.53310	H	-5.30883	-0.15741	-0.73214	C	-1.83597	-2.96830	0.94366
H	-3.52124	-2.28419	1.07131	Si	-2.78436	-2.03842	0.69574	C	-3.16180	1.55569	-1.21304
C	3.48563	0.04998	0.61111	C	-3.48642	-1.67007	-3.04740	C	-1.72408	-0.23326	-3.43525
C	3.81908	-0.22715	2.09827	H	-3.88779	-1.17040	-3.94739	H	1.51151	-0.81845	-3.64605
H	3.39324	0.55839	2.74392	H	-4.26538	-2.36599	-2.70420	H	0.98127	0.84465	-3.94935
H	4.90868	-0.25239	2.26652	H	-2.62542	-2.26226	-3.39205	H	2.68937	0.45628	-3.90881
H	3.40666	-1.19544	2.42655	Si	-0.39043	3.43567	0.72061	H	4.12783	-1.39672	-1.70971
C	4.11132	1.40762	0.23126	C	-2.00666	0.95582	-2.75712	H	3.35356	-2.09275	-0.27535
H	3.86504	1.67066	-0.80817	H	-2.60244	1.28135	-3.62811	H	2.59087	-2.21515	-1.87608
H	5.20950	1.39053	0.31716	H	-1.07834	0.55113	-3.19261	H	2.74895	3.57294	0.85567
H	3.73432	2.20716	0.89054	H	-1.76004	1.85271	-2.17188	H	0.99620	3.63349	0.71022
C	4.12132	-1.05345	-0.25726	Si	1.79932	-2.51832	-1.74758	H	1.73688	2.64173	1.98987

H	3.68437	-2.03656	-0.01994	Si	1.28097	2.80023	-1.74388	H	-0.98028	-0.84388	-3.94908
H	5.21126	-1.11879	-0.10998	N	-2.09093	-0.86231	-0.35382	H	-2.68867	-0.45686	-3.90871
H	3.94505	-0.85155	-1.32425	N	1.79360	-1.37923	-0.33721	H	-1.51183	0.81861	-3.64479
C	0.67125	0.93903	3.47234	N	0.30655	2.25581	-0.31948	H	-3.35319	2.09084	-0.27324
H	1.21332	1.66837	2.86644	C	0.73435	3.81573	2.26160	H	-2.59097	2.21450	-1.87408
C	0.69083	1.00334	4.87013	H	0.28574	4.59422	2.91736	H	-4.12784	1.39587	-1.70790
H	1.25406	1.79591	5.36854	H	1.72163	4.16925	1.91832	H	-0.99682	-3.63425	0.70949
C	-0.01248	0.03786	5.59258	H	0.87144	2.88475	2.83842	H	-1.73755	-2.64304	1.98955
H	-0.01770	0.05314	6.68790	C	2.00286	-4.30385	-1.10092	H	-2.74958	-3.57378	0.85490
C	-0.71004	-0.94671	4.89015	H	1.20061	-4.57250	-0.39097				
H	-1.27969	-1.72423	5.40503	H	2.97629	-4.46450	-0.60490				
C	-0.67822	-0.91981	3.49146	H	1.95365	-5.00226	-1.95356				
H	-1.21776	-1.66347	2.90056	C	1.98237	1.30201	-2.64241				
C	1.15555	1.52655	-2.85695	H	1.20656	0.63924	-3.06008				
H	2.04958	1.03957	-2.45767	H	2.66971	0.69244	-2.03959				
C	1.18931	2.15089	-4.10322	H	2.53997	1.66739	-3.52266				
H	2.11190	2.16176	-4.68761	C	2.76832	3.83159	-1.12930				
C	0.01978	2.74122	-4.59320	H	3.39611	4.10689	-1.99376				
H	0.00589	3.22373	-5.57441	H	3.39442	3.26477	-0.41793				
C	-1.13278	2.68989	-3.80228	H	2.45260	4.77166	-0.64296				
H	-2.07018	3.13158	-4.14665	C	0.36880	3.83020	-3.02903				
C	-1.07330	2.04715	-2.56629	H	1.05908	3.99578	-3.87545				
H	-1.96225	1.98101	-1.93261	H	0.04072	4.82411	-2.69238				
C	1.04129	-2.04203	-2.58387	H	-0.50273	3.30842	-3.45192				
H	1.92456	-2.00939	-1.94021	C	0.14298	-2.44372	-2.63729				
C	1.10247	-2.64747	-3.83866	H	-0.05135	-1.46954	-3.11441				
H	2.03654	-3.09199	-4.18837	H	-0.72072	-2.70112	-2.00847				
C	-0.04329	-2.65683	-4.64074	H	0.17994	-3.16369	-3.47350				
H	-0.02727	-3.10813	-5.63664	C	3.12829	-2.21914	-3.04654				
C	-1.20867	-2.06466	-4.14267	H	2.92750	-2.90073	-3.89245				
H	-2.12587	-2.04339	-4.73517	H	4.15842	-2.42072	-2.72053				
C	-1.17670	-1.47846	-2.87814	H	3.09653	-1.20268	-3.46675				
H	-2.06648	-0.98876	-2.47259	C	-0.77611	5.14449	-0.01969				
C	-0.80387	-3.42239	0.23381	H	-1.49560	5.06564	-0.85029				
H	-1.65373	-2.97383	-0.28169	H	0.11407	5.65159	-0.42312				
C	-0.68719	-4.81007	0.33975	H	-1.22175	5.80228	0.75151				
H	-1.44785	-5.45419	-0.10569	C	-2.04789	2.87734	1.50927				
C	0.42996	-5.34070	0.98733	H	-2.81280	2.72597	0.72998				
H	0.56826	-6.42256	1.05994	H	-2.41873	3.66117	2.20183				
C	1.37774	-4.45928	1.51374	H	-1.94157	1.93612	2.07231				
H	2.28022	-4.82413	2.00929	C	4.85739	-1.80041	-0.07551				
C	1.17739	-3.08649	1.35629	H	4.88319	-2.83093	-0.46193				
H	1.90621	-2.36256	1.72509	H	5.65830	-1.70208	0.68227				
C	0.91021	3.35598	0.34568	H	5.11281	-1.14154	-0.92070				
H	1.82170	2.85862	0.01094	C	3.48286	0.40051	1.45929				
C	0.81868	4.74879	0.36575	H	3.69764	1.14124	0.67196				
H	1.66467	5.35417	0.03432	H	4.36081	0.35942	2.13631				
C	-0.38064	5.33602	0.77519	H	2.61330	0.75598	2.03497				
H	-0.49768	6.42271	0.77082	C	2.99585	-2.48875	2.23306				
C	-1.43452	4.50356	1.15999	H	2.11069	-2.17072	2.81071				
H	-2.39977	4.91368	1.46474	H	3.89546	-2.44830	2.88534				
C	-1.25198	3.12042	1.10459	H	2.84841	-3.53065	1.90097				
H	-2.05740	2.42991	1.36048								
$^{12x}1_{opt}$ model				**$^{26z}2_{opt}$**							
Dy	0.00000	0.00000	0.00000	Er	0.00000	0.00000	0.00000				
N	0.00000	0.00000	2.79807	C	-4.09073	-3.21204	0.00970				
N	0.04656	1.46515	-2.09192	H	-4.96647	-2.68303	-0.39706				
N	-0.07362	-1.45661	-2.10218	H	-4.44758	-3.91433	0.78777				
N	0.11037	-2.57118	0.72738	H	-3.67575	-3.80980	-0.81747				
N	-0.10456	2.55114	0.70431	Si	-3.00975	-0.33740	-1.79516				

O	-2.13692	-0.08447	0.00439	C	-1.48513	-3.19572	1.53946
O	2.13716	0.08448	-0.00439	H	-1.97942	-3.89000	2.25079
C	-3.53623	-0.13482	-0.06009	H	-0.70956	-2.63169	2.08275
C	-4.05663	0.85120	-1.12458	H	-0.98871	-3.80262	0.76445
H	-3.74573	1.88138	-0.88864	Cl	0.00000	0.00000	3.04189
H	-5.15577	0.83721	-1.19934	C	-3.66444	-1.21501	2.26669
H	-3.65421	0.59571	-2.11614	H	-4.45203	-0.52758	1.91276
C	-4.15523	0.23679	1.31086	H	-2.91465	-0.63766	2.83494
H	-3.83697	-0.47697	2.08841	H	-4.12898	-1.97552	2.93330
H	-5.25735	0.22588	1.26960	Si	3.17544	-1.33378	0.72957
H	-3.84074	1.24417	1.62867	C	-4.61323	0.53448	-1.23975
C	-4.00431	-1.55879	-0.42381	H	-5.14250	0.91352	-2.13062
H	-3.59135	-1.86392	-1.39718	H	-4.40259	1.39092	-0.57487
H	-5.10223	-1.62384	-0.49484	H	-5.30379	-0.15257	-0.71893
H	-3.66663	-2.28169	0.33780	Si	-2.78667	-2.03697	0.73454
C	3.53754	0.05990	-0.08848	C	-3.47690	-1.68798	-3.01733
C	4.15844	-0.20483	1.30580	H	-3.86352	-1.19005	-3.92529
H	3.86589	0.58525	2.01677	H	-4.26813	-2.37260	-2.67947
H	5.25989	-0.22715	1.25612	H	-2.61986	-2.29142	-3.35191
H	3.82173	-1.17105	1.71627	Si	-0.38534	3.43798	0.77019
C	4.07200	1.41536	-0.59449	C	-1.98355	0.93420	-2.72987
H	3.62486	1.66970	-1.56693	H	-2.57337	1.25845	-3.60606
H	5.16561	1.40054	-0.72667	H	-1.05682	0.52512	-3.16467
H	3.82998	2.21961	0.12010	H	-1.73791	1.83489	-2.14984
C	3.99286	-1.04953	-1.05676	Si	1.80890	-2.51775	-1.71893
H	3.61421	-2.03134	-0.73052	Si	1.27601	2.80510	-1.70753
H	5.09064	-1.11212	-1.12677	N	-2.09104	-0.86502	-0.31497
H	3.60911	-0.85644	-2.06955	N	1.79304	-1.38369	-0.29477
C	0.67125	0.93903	3.47234	N	0.30811	2.25951	-0.27032
H	1.21332	1.66837	2.86644	C	0.74829	3.82409	2.30835
C	0.69083	1.00334	4.87013	H	0.30354	4.60691	2.96324
H	1.25406	1.79591	5.36854	H	1.73481	4.17343	1.95857
C	-0.01248	0.03786	5.59258	H	0.88371	2.89399	2.88742
H	-0.01770	0.05314	6.68790	C	2.01259	-4.30348	-1.07419
C	-0.71004	-0.94671	4.89015	H	1.20551	-4.57676	-0.37120
H	-1.27969	-1.72423	5.40503	H	2.98350	-4.46407	-0.57298
C	-0.67822	-0.91981	3.49146	H	1.97058	-4.99803	-1.93047
H	-1.21776	-1.66347	2.90056	C	1.97073	1.29978	-2.59887
C	1.15555	1.52655	-2.85695	H	1.19668	0.62967	-3.00839
H	2.04958	1.03957	-2.45767	H	2.67073	0.69899	-2.00163
C	1.18931	2.15089	-4.10322	H	2.51555	1.66183	-3.48905
H	2.11190	2.16176	-4.68761	C	2.76694	3.83231	-1.09635
C	0.01978	2.74122	-4.59320	H	3.39164	4.10441	-1.96416
H	0.00589	3.22373	-5.57441	H	3.39440	3.26448	-0.38669
C	-1.13278	2.68989	-3.80228	H	2.45494	4.77444	-0.61131
H	-2.07018	3.13158	-4.14665	C	0.35852	3.83312	-2.98780
C	-1.07330	2.04715	-2.56629	H	1.04578	3.99364	-3.83818
H	-1.96225	1.98101	-1.93261	H	0.03620	4.82998	-2.65422
C	1.04129	-2.04203	-2.58387	H	-0.51580	3.31441	-3.40860
H	1.92456	-2.00939	-1.94021	C	0.15271	-2.44073	-2.60720
C	1.10247	-2.64747	-3.83866	H	-0.04679	-1.46648	-3.08193
H	2.03654	-3.09199	-4.18837	H	-0.71155	-2.70991	-1.98396
C	-0.04329	-2.65683	-4.64074	H	0.19598	-3.15371	-3.44969
H	-0.02727	-3.10813	-5.63664	C	3.14030	-2.20673	-3.01019
C	-1.20867	-2.06466	-4.14267	H	2.94417	-2.88758	-3.85834
H	-2.12587	-2.04339	-4.73517	H	4.17125	-2.40472	-2.68452
C	-1.17670	-1.47846	-2.87814	H	3.10461	-1.19089	-3.43160
H	-2.06648	-0.98876	-2.47259	C	-0.78140	5.14398	0.03075
C	-0.80387	-3.42239	0.23381	H	-1.50543	5.06035	-0.79558
H	-1.65373	-2.97383	-0.28169	H	0.10446	5.65125	-0.38187
C	-0.68719	-4.81007	0.33975	H	-1.22371	5.80438	0.80207
H	-1.44785	-5.45419	-0.10569	C	-2.03214	2.87582	1.58264

C	0.42996	-5.34070	0.98733	H	-2.80376	2.70829	0.81322	
H	0.56826	-6.42256	1.05994	H	-2.40207	3.66587	2.26965	
C	1.37774	-4.45928	1.51374	H	-1.90984	1.94266	2.15637	
H	2.28022	-4.82413	2.00929	C	4.85611	-1.80020	-0.02279	
C	1.17739	-3.08649	1.35629	H	4.88357	-2.82783	-0.41671	
H	1.90621	-2.36256	1.72509	H	5.65498	-1.70609	0.73809	
C	0.91021	3.35598	0.34568	H	5.11386	-1.13689	-0.86393	
H	1.82170	2.85862	0.01094	C	3.46873	0.39082	1.52137	
C	0.81868	4.74879	0.36575	H	3.68245	1.13967	0.74135	
H	1.66467	5.35417	0.03432	H	4.34474	0.34755	2.20181	
C	-0.38064	5.33602	0.77519	H	2.59461	0.73540	2.09726	
H	-0.49768	6.42271	0.77082	C	2.98471	-2.49806	2.27989	
C	-1.43452	4.50356	1.15999	H	2.10220	-2.17160	2.85739	
H	-2.39977	4.91368	1.46474	H	3.88591	-2.46521	2.93199	
C	-1.25198	3.12042	1.10459	H	2.82870	-3.53784	1.94494	
H	-2.05740	2.42991	1.36048					
				$^{4-z}\mathbf{2}_{\mathbf{opt}}$				
				Er	0.00000	0.00000	0.00000	
				C	-4.01542	-3.26029	-0.14236	
				H	-4.92896	-2.74788	-0.48396	
				H	-4.31586	-3.99048	0.63010	
				H	-3.60831	-3.82581	-0.99583	
				Si	-3.08577	-0.26493	-1.78603	
				C	-1.36617	-3.23122	1.27408	
				H	-1.80289	-3.91953	2.01959	
				H	-0.54564	-2.68859	1.76741	
				H	-0.93803	-3.84245	0.46305	
				Cl	0.00000	0.00000	2.61395	
				C	-3.57969	-1.28501	2.11850	
				H	-4.39558	-0.61456	1.80087	
				H	-2.85326	-0.69319	2.69738	
				H	-4.00930	-2.05676	2.78274	
				Si	3.16018	-1.32617	0.60443	
				C	-4.72178	0.47835	-1.14145	
				H	-5.30537	0.90939	-1.97336	
				H	-4.53041	1.27828	-0.40725	
				H	-5.35571	-0.27911	-0.65093	
				Si	-2.72188	-2.07415	0.61006	
				C	-3.56567	-1.54055	-3.11570	
				H	-4.08767	-1.02294	-3.93930	
				H	-4.23405	-2.33300	-2.74788	
				H	-2.67344	-2.02520	-3.54316	
				Si	-0.43528	3.39701	0.61899	
				C	-2.21392	1.11484	-2.74957	
				H	-2.90208	1.50729	-3.51773	
				H	-1.32124	0.74681	-3.28330	
				H	-1.89600	1.95097	-2.11101	
				Si	1.76971	-2.52031	-1.80479	
				Si	1.30944	2.80751	-1.78012	
				N	-2.07330	-0.87805	-0.49012	
				N	1.79727	-1.35493	-0.49265	
				N	0.27502	2.23772	-0.48245	
				C	0.67654	3.74552	2.12813	
				H	0.21997	4.50139	2.79268	
				H	1.66346	4.12049	1.80989	
				H	0.83046	2.82092	2.70668	
				C	1.93596	-4.31822	-1.18586	
				H	1.13583	-4.56827	-0.46973	
				H	2.90106	-4.49294	-0.68139	
				H	1.87167	-5.02597	-2.03048	
				C	2.07082	1.36537	-2.74469	

	H	1.30223	0.75082	-3.24306	
	H	2.67245	0.69442	-2.11595	
	H	2.71987	1.76950	-3.54021	
	C	2.76708	3.86055	-1.13892	
	H	3.42894	4.15532	-1.97166	
	H	3.36990	3.29939	-0.40600	
	H	2.42167	4.78569	-0.64792	
	C	0.44010	3.85595	-3.11064	
	H	1.15299	4.06559	-3.92718	
	H	0.07126	4.82306	-2.73894	
	H	-0.41396	3.31478	-3.54780	
	C	0.14159	-2.43355	-2.77056	
	H	0.00582	-1.45837	-3.26841	
	H	-0.74093	-2.60870	-2.13934	
	H	0.15618	-3.19688	-3.56710	
	C	3.12028	-2.28764	-3.12588	
	H	2.93296	-2.98646	-3.95979	
	H	4.13624	-2.48403	-2.75388	
	H	3.10393	-1.26717	-3.53986	
	C	-0.81440	5.11186	-0.13164	
	H	-1.51608	5.04638	-0.97878	
	H	0.08435	5.64438	-0.48165	
	H	-1.28652	5.73844	0.64600	
	C	-2.11686	2.80433	1.28184	
	H	-2.85388	2.71819	0.46694	
	H	-2.50552	3.53886	2.00979	
	H	-2.05591	1.83253	1.79478	
	C	4.83378	-1.84635	-0.15364	
	H	4.84765	-2.89052	-0.50459	
	H	5.61568	-1.74810	0.62040	
	H	5.11975	-1.20279	-1.00104	
	C	3.48345	0.42294	1.27886	
	H	3.76009	1.11392	0.46610	
	H	4.32400	0.39294	1.99505	
	H	2.61400	0.84317	1.80687	
	C	2.91013	-2.47324	2.10694	
	H	2.02967	-2.15134	2.68536	
	H	3.79090	-2.45504	2.77433	
	H	2.74767	-3.51506	1.78373	
	$^{8\text{-}z}\mathbf{2}_{\mathbf{opt}}$				
	Er	0.00000	0.00000	0.00000	
	C	-3.99627	-3.27491	-0.12984	
	H	-4.91662	-2.76590	-0.46049	
	H	-4.28789	-3.99653	0.65268	
	H	-3.59198	-3.84857	-0.98087	
	Si	-3.10417	-0.28274	-1.77351	
	C	-1.32732	-3.23435	1.24759	
	H	-1.74253	-3.90003	2.02342	
	H	-0.48927	-2.69468	1.71333	
	H	-0.92855	-3.86828	0.43819	
	Cl	0.00000	0.00000	2.53946	
	C	-3.53758	-1.27101	2.10761	
	H	-4.36754	-0.61244	1.80313	
	H	-2.81613	-0.66813	2.68000	
	H	-3.94737	-2.03456	2.79072	
	Si	3.14345	-1.33437	0.61163	
	C	-4.73214	0.46106	-1.11786	
	H	-5.33488	0.89750	-1.93484	
	H	-4.52544	1.25581	-0.38299	
	H	-5.35417	-0.29388	-0.61004	
	Si	-2.69813	-2.08512	0.62195	

	C	-3.62645	-1.54746	-3.12466	
	H	-4.18991	-1.02722	-3.92214	
	H	-4.26536	-2.35120	-2.72845	
	H	-2.73862	-2.01670	-3.58122	
	Si	-0.44159	3.38344	0.62267	
	C	-2.26695	1.09494	-2.79098	
	H	-2.99236	1.51311	-3.51246	
	H	-1.40784	0.70994	-3.36810	
	H	-1.89337	1.91210	-2.15656	
	Si	1.78065	-2.50599	-1.82980	
	Si	1.30933	2.82550	-1.77821	
	N	-2.06164	-0.91088	-0.54158	
	N	1.81023	-1.33441	-0.55604	
	N	0.25091	2.23860	-0.53961	
	C	0.68544	3.69805	2.10749	
	H	0.23249	4.43669	2.79062	
	H	1.67149	4.08343	1.80053	
	H	0.84546	2.77177	2.68024	
	C	1.92194	-4.31296	-1.23717	
	H	1.10793	-4.55779	-0.53579	
	H	2.87049	-4.49557	-0.70627	
	H	1.86970	-5.02192	-2.08342	
	C	2.10092	1.41510	-2.78622	
	H	1.34267	0.82719	-3.33233	
	H	2.66123	0.71256	-2.15227	
	H	2.79340	1.84370	-3.53353	
	C	2.75774	3.88354	-1.13285	
	H	3.42812	4.19578	-1.95402	
	H	3.35604	3.31641	-0.40143	
	H	2.40575	4.79559	-0.62408	
	C	0.45733	3.88711	-3.13493	
	H	1.18574	4.13549	-3.92980	
	H	0.05394	4.83092	-2.73865	
	H	-0.37659	3.32926	-3.59320	
	C	0.17511	-2.41038	-2.85272	
	H	0.08720	-1.44554	-3.38263	
	H	-0.72185	-2.52025	-2.22522	
	H	0.17368	-3.21053	-3.61523	
	C	3.15015	-2.29831	-3.16154	
	H	2.98377	-3.01782	-3.98553	
	H	4.15839	-2.47369	-2.75768	
	H	3.12799	-1.27995	-3.58390	
	C	-0.81494	5.10442	-0.12956	
	H	-1.52648	5.04827	-0.97074	
	H	0.08524	5.63966	-0.47385	
	H	-1.27744	5.72295	0.65891	
	C	-2.12778	2.78178	1.24473	
	H	-2.87098	2.75318	0.43054	
	H	-2.49884	3.48078	2.01371	
	H	-2.08805	1.78868	1.71690	
	C	4.81707	-1.88379	-0.13843	
	H	4.81597	-2.92799	-0.49191	
	H	5.58188	-1.80998	0.65385	
	H	5.13518	-1.23523	-0.97198	
	C	3.47593	0.41673	1.25518	
	H	3.81435	1.08690	0.44733	
	H	4.27326	0.37868	2.01699	
	H	2.59902	0.87104	1.74047	
	C	2.83086	-2.48363	2.07978	
	H	1.95042	-2.15418	2.65248	
	H	3.69295	-2.48346	2.76849	
	H	2.65850	-3.52341	1.75613	

	$^{12\text{-}z}2_{opt}$			
	Er	0.00000	0.00000	0.00000
	C	-3.99509	-3.27587	-0.11894
	H	-4.91585	-2.76642	-0.44869
	H	-4.28678	-3.99172	0.66859
	H	-3.59220	-3.85565	-0.96725
	Si	-3.10904	-0.29329	-1.77242
	C	-1.31974	-3.23439	1.24736
	H	-1.72851	-3.88660	2.03770
	H	-0.47338	-2.69642	1.69975
	H	-0.93429	-3.88192	0.44185
	Cl	0.00000	0.00000	2.51994
	C	-3.52448	-1.25926	2.10821
	H	-4.36026	-0.60612	1.80836
	H	-2.80385	-0.65124	2.67598
	H	-3.92560	-2.01869	2.80069
	Si	3.13934	-1.33656	0.61676
	C	-4.73345	0.45490	-1.11601
	H	-5.34284	0.88954	-1.92975
	H	-4.52032	1.25146	-0.38498
	H	-5.35161	-0.29597	-0.59791
	Si	-2.69298	-2.08655	0.63073
	C	-3.64641	-1.55745	-3.12878
	H	-4.22350	-1.03783	-3.91862
	H	-4.27566	-2.36353	-2.72144
	H	-2.76082	-2.02285	-3.59499
	Si	-0.44013	3.38038	0.62865
	C	-2.28180	1.08046	-2.81110
	H	-3.01703	1.50204	-3.52198
	H	-1.43158	0.68886	-3.39758
	H	-1.89444	1.89510	-2.18093
	Si	1.78845	-2.49820	-1.84038
	Si	1.30209	2.83102	-1.78332
	N	-2.05836	-0.92359	-0.55809
	N	1.81656	-1.32685	-0.57603
	N	0.24151	2.24017	-0.55783
	C	0.69604	3.68078	2.10381
	H	0.24578	4.41280	2.79546
	H	1.68132	4.06983	1.79936
	H	0.85840	2.75313	2.67345
	C	1.91654	-4.30886	-1.25823
	H	1.09309	-4.55164	-0.56727
	H	2.85557	-4.49502	-0.71220
	H	1.87359	-5.01763	-2.10599
	C	2.09319	1.42919	-2.81175
	H	1.33356	0.85421	-3.37042
	H	2.64088	0.71363	-2.18054
	H	2.79693	1.86354	-3.54651
	C	2.75459	3.88493	-1.14331
	H	3.42338	4.20393	-1.96393
	H	3.35445	3.31187	-0.41783
	H	2.40611	4.79167	-0.62315
	C	0.45284	3.90136	-3.14501
	H	1.18319	4.15829	-3.93707
	H	0.04537	4.83957	-2.73915
	H	-0.37939	3.34215	-3.60613
	C	0.19299	-2.39540	-2.88630
	H	0.12736	-1.43632	-3.43057
	H	-0.70958	-2.47722	-2.26157
	H	0.18298	-3.20988	-3.63487
	C	3.16750	-2.29993	-3.17405

	H	3.00496	-3.02231	-3.99806	
	H	4.17180	-2.47521	-2.75978	
	H	3.14868	-1.28076	-3.59611	
	C	-0.80980	5.10409	-0.12308	
	H	-1.52762	5.05219	-0.95994	
	H	0.09094	5.63779	-0.46916	
	H	-1.26482	5.72158	0.67027	
	C	-2.12695	2.77801	1.24217	
	H	-2.87522	2.77064	0.43171	
	H	-2.48824	3.46424	2.02693	
	H	-2.09414	1.77779	1.69956	
	C	4.81230	-1.89499	-0.13190	
	H	4.80569	-2.93892	-0.48709	
	H	5.57196	-1.82999	0.66582	
	H	5.14060	-1.24466	-0.96081	
	C	3.47306	0.41453	1.25307	
	H	3.83332	1.07916	0.44965	
	H	4.25364	0.37329	2.03166	
	H	2.59300	0.87868	1.72311	
	C	2.80762	-2.48704	2.07415	
	H	1.92707	-2.15641	2.64568	
	H	3.66383	-2.48963	2.76983	
	H	2.63464	-3.52704	1.75176	
	$^{16\text{-}z}2_{opt}$				
	Er	0.00000	0.00000	0.00000	
	C	-3.99820	-3.27268	-0.10284	
	H	-4.91816	-2.76170	-0.43347	
	H	-4.29176	-3.98046	0.69107	
	H	-3.59751	-3.86115	-0.94704	
	Si	-3.11288	-0.30679	-1.77387	
	C	-1.31574	-3.23281	1.25147	
	H	-1.71810	-3.86957	2.05755	
	H	-0.45990	-2.69745	1.68884	
	H	-0.94556	-3.89568	0.45079	
	Cl	0.00000	0.00000	2.50224	
	C	-3.51182	-1.24154	2.11175	
	H	-4.35331	-0.59374	1.81656	
	H	-2.79126	-0.62840	2.67396	
	H	-3.90409	-1.99592	2.81477	
	Si	3.13662	-1.33656	0.62496	
	C	-4.73492	0.44673	-1.12060	
	H	-5.35099	0.87571	-1.93316	
	H	-4.51643	1.24820	-0.39644	
	H	-5.34864	-0.29846	-0.58949	
	Si	-2.68996	-2.08498	0.64287	
	C	-3.66203	-1.57383	-3.13436	
	H	-4.25075	-1.05740	-3.91978	
	H	-4.28211	-2.38150	-2.71560	
	H	-2.77717	-2.03594	-3.60674	
	Si	-0.43707	3.37815	0.63635	
	C	-2.29541	1.06166	-2.83553	
	H	-3.03899	1.48244	-3.53987	
	H	-1.45123	0.66396	-3.42742	
	H	-1.89874	1.87666	-2.21069	
	Si	1.79987	-2.49184	-1.84806	
	Si	1.28617	2.83462	-1.79598	
	N	-2.05583	-0.93597	-0.57374	
	N	1.82480	-1.31892	-0.59428	
	N	0.22925	2.24234	-0.57723	
	C	0.71168	3.66174	2.09991	
	H	0.26610	4.38740	2.80125	

	H	1.69617	4.05345	1.79651	
	H	0.87590	2.73239	2.66608	
	C	1.91580	-4.30511	-1.27390	
	H	1.08237	-4.54535	-0.59406	
	H	2.84455	-4.49347	-0.71155	
	H	1.88362	-5.01480	-2.12232	
	C	2.06114	1.43831	-2.85300	
	H	1.29246	0.88683	-3.42386	
	H	2.59117	0.70224	-2.22936	
	H	2.77772	1.87400	-3.57608	
	C	2.75229	3.87555	-1.16884	
	H	3.41548	4.20032	-1.99258	
	H	3.35552	3.29196	-0.45455	
	H	2.41486	4.77703	-0.63275	
	C	0.43749	3.92020	-3.15702	
	H	1.16608	4.18003	-3.95182	
	H	0.03552	4.85592	-2.73947	
	H	-0.39996	3.36529	-3.61539	
	C	0.21488	-2.38523	-2.91799	
	H	0.16738	-1.43045	-3.47248	
	H	-0.69286	-2.44638	-2.29739	
	H	0.20059	-3.21058	-3.65622	
	C	3.18876	-2.30348	-3.18430	
	H	3.03063	-3.02928	-4.00827	
	H	4.18911	-2.47794	-2.75950	
	H	3.17278	-1.28395	-3.60719	
	C	-0.80125	5.10551	-0.11332	
	H	-1.52667	5.05968	-0.94480	
	H	0.10059	5.63603	-0.46241	
	H	-1.24629	5.72244	0.68595	
	C	-2.12390	2.77660	1.24478	
	H	-2.87843	2.78937	0.43966	
	H	-2.47415	3.45057	2.04502	
	H	-2.09751	1.76995	1.68832	
	C	4.80926	-1.90283	-0.12216	
	H	4.79822	-2.94679	-0.47822	
	H	5.56405	-1.84498	0.68055	
	H	5.14653	-1.25127	-0.94730	
	C	3.47005	0.41477	1.25437	
	H	3.85760	1.07250	0.45750	
	H	4.22919	0.37009	2.05371	
	H	2.58567	0.89071	1.70413	
	C	2.78699	-2.48760	2.07276	
	H	1.90619	-2.15630	2.64335	
	H	3.63769	-2.49035	2.77519	
	H	2.61507	-3.52865	1.75344	
	$^{20\text{-}z}\mathbf{2}_{opt}$				
	Er	0.00000	0.00000	0.00000	
	C	-4.00532	-3.26569	-0.08090	
	H	-4.92295	-2.75216	-0.41511	
	H	-4.30338	-3.96300	0.72050	
	H	-3.60684	-3.86560	-0.91900	
	Si	-3.11471	-0.32495	-1.77837	
	C	-1.31568	-3.22899	1.26250	
	H	-1.71259	-3.84976	2.08385	
	H	-0.45102	-2.69646	1.68579	
	H	-0.95995	-3.90734	0.46771	
	Cl	0.00000	0.00000	2.48609	
	C	-3.50099	-1.21734	2.11843	
	H	-4.34673	-0.57362	1.82667	
	H	-2.77964	-0.60012	2.67515	

	H	-3.88624	-1.96517	2.83260	
	Si	3.13476	-1.33658	0.63718	
	C	-4.73578	0.43628	-1.13406	
	H	-5.35830	0.85475	-1.94814	
	H	-4.51304	1.24653	-0.42079	
	H	-5.34470	-0.30065	-0.58635	
	Si	-2.68950	-2.08070	0.65974	
	C	-3.67236	-1.59927	-3.14120	
	H	-4.27021	-1.08862	-3.92598	
	H	-4.28441	-2.40705	-2.71031	
	H	-2.78672	-2.05943	-3.61570	
	Si	-0.43178	3.37732	0.64660	
	C	-2.30536	1.03505	-2.86587	
	H	-3.05512	1.44977	-3.56932	
	H	-1.46370	0.63061	-3.45765	
	H	-1.90430	1.85430	-2.24841	
	Si	1.81383	-2.48813	-1.85213	
	Si	1.26092	2.83724	-1.81625	
	N	-2.05408	-0.94860	-0.58750	
	N	1.83403	-1.31169	-0.61016	
	N	0.21457	2.24533	-0.59726	
	C	0.73329	3.64115	2.09617	
	H	0.29532	4.36183	2.80775	
	H	1.71723	4.03335	1.79161	
	H	0.89801	2.71013	2.65936	
	C	1.92118	-4.30282	-1.28311	
	H	1.07947	-4.54009	-0.61231	
	H	2.84061	-4.49113	-0.70582	
	H	1.89907	-5.01521	-2.13062	
	C	2.00285	1.44460	-2.91141	
	H	1.21617	0.92417	-3.48809	
	H	2.51619	0.68443	-2.30185	
	H	2.72815	1.87841	-3.62883	
	C	2.75053	3.85598	-1.21096	
	H	3.40480	4.18420	-2.04141	
	H	3.35780	3.25778	-0.51216	
	H	2.43236	4.75283	-0.65580	
	C	0.40981	3.94424	-3.17043	
	H	1.13373	4.20479	-3.97167	
	H	0.01900	4.87843	-2.73855	
	H	-0.43679	3.39696	-3.62276	
	C	0.23879	-2.38309	-2.94594	
	H	0.20273	-1.42991	-3.50481	
	H	-0.67400	-2.43427	-2.33088	
	H	0.22692	-3.21482	-3.67914	
	C	3.21131	-2.30912	-3.19310	
	H	3.06130	-3.04343	-4.01350	
	H	4.20858	-2.47526	-2.75710	
	H	3.19275	-1.29165	-3.62262	
	C	-0.78774	5.10926	-0.09938	
	H	-1.52318	5.07201	-0.92335	
	H	0.11576	5.63415	-0.45379	
	H	-1.21870	5.72658	0.70722	
	C	-2.11818	2.77846	1.25303	
	H	-2.88026	2.81202	0.45503	
	H	-2.45526	3.44013	2.06928	
	H	-2.09858	1.76558	1.68257	
	C	4.80709	-1.90801	-0.11004	
	H	4.79295	-2.95149	-0.46849	
	H	5.55780	-1.85718	0.69688	
	H	5.15138	-1.25360	-0.93096	
	C	3.46632	0.41415	1.26258	

	H 3.87977 1.06677 0.47417 H 4.20451 0.36492 2.08132 H 2.57837 0.90006 1.69432 C 2.76836 -2.48944 2.07503 H 1.88645 -2.15918 2.64448 H 3.61334 -2.48966 2.78471 H 2.60048 -3.53221 1.75941	
	$^{24\text{-}z}2_{opt}$ Er 0.00000 0.00000 0.00000 C -4.01989 -3.25170 -0.05463 H -4.93284 -2.73354 -0.39555 H -4.32614 -3.93466 0.75604 H -3.62473 -3.86726 -0.88386 Si -3.11070 -0.34932 -1.79176 C -1.32343 -3.22249 1.28063 H -1.71756 -3.82619 2.11639 H -0.45083 -2.69350 1.69196 H -0.98051 -3.91691 0.49353 Cl 0.00000 0.00000 2.47139 C -3.49354 -1.18286 2.12495 H -4.33974 -0.53929 1.83429 H -2.76968 -0.56510 2.67793 H -3.87697 -1.92194 2.84985 Si 3.13239 -1.33742 0.65383 C -4.73104 0.42788 -1.16665 H -5.35839 0.82910 -1.98678 H -4.50452 1.25248 -0.47088 H -5.33650 -0.29521 -0.59716 Si -2.69354 -2.07212 0.67935 C -3.67648 -1.63722 -3.15216 H -4.27750 -1.13497 -3.94283 H -4.28611 -2.43934 -2.70678 H -2.79002 -2.10235 -3.62197 Si -0.42818 3.37696 0.65752 C -2.30142 0.99312 -2.91076 H -3.05348 1.40055 -3.61843 H -1.46215 0.57538 -3.49763 H -1.89485 1.81866 -2.30427 Si 1.83019 -2.48442 -1.85525 Si 1.24093 2.84278 -1.83183 N -2.05245 -0.96194 -0.60194 N 1.84280 -1.30663 -0.62293 N 0.20141 2.24888 -0.61644 C 0.75055 3.62332 2.09478 H 0.31810 4.34017 2.81435 H 1.73470 4.01558 1.79119 H 0.91388 2.69156 2.65723 C 1.93091 -4.30109 -1.29312 H 1.08064 -4.53694 -0.63236 H 2.84037 -4.48836 -0.70003 H 1.92081 -5.01580 -2.14005 C 1.96776 1.45676 -2.95605 H 1.17004 0.94695 -3.52811 H 2.48257 0.68844 -2.35704 H 2.68878 1.89561 -3.67709 C 2.74343 3.85162 -1.24409 H 3.39061 4.18501 -2.07906 H 3.35522 3.24544 -0.55588 H 2.43612 4.74333 -0.67480 C 0.38648 3.96038 -3.18834 H 1.10808 4.22811 -3.99205	

	H	-0.00568	4.88951	-2.74614	
	H	-0.46042	3.41116	-3.63955	
	C	0.26613	-2.38345	-2.97510	
	H	0.23760	-1.42969	-3.53423	
	H	-0.65266	-2.43254	-2.36790	
	H	0.26273	-3.21809	-3.70760	
	C	3.23642	-2.31062	-3.20131	
	H	3.09572	-3.05144	-4.02039	
	H	4.23078	-2.46803	-2.75471	
	H	3.21374	-1.29423	-3.63508	
	C	-0.77728	5.11161	-0.08804	
	H	-1.52273	5.08055	-0.90422	
	H	0.12724	5.63076	-0.44936	
	H	-1.19452	5.73081	0.72437	
	C	-2.11333	2.77854	1.26181	
	H	-2.88272	2.82928	0.47119	
	H	-2.43868	3.42900	2.09219	
	H	-2.09894	1.76084	1.68008	
	C	4.80445	-1.91307	-0.09405	
	H	4.78772	-2.95573	-0.45595	
	H	5.55122	-1.86955	0.71700	
	H	5.15516	-1.25491	-0.91022	
	C	3.46072	0.41338	1.27420	
	H	3.88957	1.06374	0.49177	
	H	4.18543	0.36171	2.10527	
	H	2.57125	0.90452	1.69684	
	C	2.75016	-2.49094	2.08308	
	H	1.86599	-2.16255	2.65019	
	H	3.58887	-2.48502	2.80091	
	H	2.58932	-3.53646	1.77314	
	$^{26\text{-}z}2_{opt}$				
	Er	0.00000	0.00000	0.00000	
	C	-4.02651	-3.24738	-0.03697	
	H	-4.93671	-2.72724	-0.38283	
	H	-4.33740	-3.92116	0.77963	
	H	-3.63299	-3.87264	-0.86019	
	Si	-3.10502	-0.37115	-1.80268	
	C	-1.32669	-3.22010	1.29497	
	H	-1.71971	-3.81454	2.13817	
	H	-0.45070	-2.69207	1.70034	
	H	-0.98932	-3.92308	0.51276	
	Cl	0.00000	0.00000	2.46456	
	C	-3.48948	-1.16448	2.12857	
	H	-4.33657	-0.52255	1.83683	
	H	-2.76511	-0.54464	2.67858	
	H	-3.87140	-1.89800	2.86039	
	Si	3.13343	-1.33277	0.66576	
	C	-4.72465	0.41895	-1.19273	
	H	-5.35388	0.80707	-2.01830	
	H	-4.49589	1.25429	-0.51043	
	H	-5.32896	-0.29342	-0.60865	
	Si	-2.69468	-2.06977	0.69179	
	C	-3.67494	-1.67125	-3.15691	
	H	-4.27458	-1.17594	-3.95466	
	H	-4.28615	-2.46692	-2.70187	
	H	-2.78809	-2.14298	-3.62020	
	Si	-0.43078	3.37695	0.66466	
	C	-2.29277	0.95607	-2.94320	
	H	-3.04527	1.35867	-3.65453	
	H	-1.45596	0.52739	-3.52614	
	H	-1.88167	1.78625	-2.34555	

	Si	1.84431	-2.48087	-1.85410
	Si	1.22684	2.84816	-1.83876
	N	-2.05005	-0.97324	-0.60904
	N	1.84981	-1.30207	-0.62677
	N	0.19129	2.25150	-0.62541
	C	0.75496	3.61548	2.09551
	H	0.32504	4.33146	2.81801
	H	1.73941	4.00723	1.79235
	H	0.91705	2.68404	2.65891
	C	1.94514	-4.29805	-1.29450
	H	1.09061	-4.53457	-0.63929
	H	2.84948	-4.48269	-0.69285
	H	1.94308	-5.01428	-2.14082
	C	1.95037	1.46666	-2.97645
	H	1.14847	0.95670	-3.54297
	H	2.47158	0.69834	-2.38247
	H	2.66491	1.91044	-3.70229
	C	2.73319	3.85562	-1.25963
	H	3.37582	4.19314	-2.09700
	H	3.34871	3.24683	-0.57689
	H	2.42937	4.74399	-0.68331
	C	0.36876	3.96844	-3.19782
	H	1.08873	4.24103	-4.00292
	H	-0.02638	4.89443	-2.75124
	H	-0.47673	3.41607	-3.64874
	C	0.28640	-2.38638	-2.98851
	H	0.25871	-1.43198	-3.54696
	H	-0.63589	-2.43858	-2.38640
	H	0.29123	-3.22169	-3.72167
	C	3.25536	-2.30668	-3.20231
	H	3.12093	-3.05017	-4.02170
	H	4.24836	-2.45842	-2.75031
	H	3.22902	-1.29057	-3.63752
	C	-0.77806	5.11240	-0.08088
	H	-1.52889	5.08330	-0.89270
	H	0.12623	5.62931	-0.44649
	H	-1.18858	5.73243	0.73437
	C	-2.11445	2.77699	1.26846
	H	-2.88782	2.83667	0.48210
	H	-2.43394	3.42078	2.10661
	H	-2.10204	1.75654	1.68004
	C	4.80642	-1.90837	-0.08172
	H	4.79009	-2.95055	-0.44561
	H	5.55088	-1.86736	0.73164
	H	5.15940	-1.24765	-0.89539
	C	3.45724	0.41909	1.28235
	H	3.89294	1.06823	0.50248
	H	4.17496	0.36825	2.11984
	H	2.56609	0.91181	1.69963
	C	2.74467	-2.48628	2.09147
	H	1.85867	-2.15998	2.65702
	H	3.58019	-2.47508	2.81347
	H	2.58939	-3.53372	1.78529