

Ab initio prediction of key parameters and magneto-structural correlation of tetracoordinated lanthanide singleion magnet.

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Table S1 *ab initio* results of DUXGUB

DUXGUB		E (K)	g_x	g_y	g_z	θ (°)	wave functions
KD ₀	this work	0	0.0001	0.0002	19.9921	0	99.96% $ \pm 15/2\rangle$
	Ref	0	0.0001	0.0001	19.8830		
KD ₁	this work	487	0.0091	0.0100	17.1396	0.2	99.89% $ \pm 13/2\rangle$
	Ref	485	0.0106	0.0094	17.0716		
KD ₂	this work	969	0.0096	0.0108	14.2757	0.9	98.99% $ \pm 11/2\rangle$
	Ref	954	0.0365	0.0279	14.2201		
KD ₃	this work	1337	1.1384	1.4331	11.2571	3.7	94.01% $ \pm 9/2\rangle$
	Ref	1304	1.6501	1.3082	11.1331		
KD ₄	this work	1479	0.1910	0.3524	19.2834	88.7	51.55% $ \pm 1/2\rangle$ +33.54% $ \pm 3/2\rangle$
	Ref	1479	2.4631	3.5013	12.3088		
KD ₅	this work	1534	5.6322	6.4175	7.7325	80.7	72.04% $ \pm 7/2\rangle$
	Ref	1512	0.9453	3.7841	10.8352		
KD ₆	this work	1624	0.9388	2.1746	15.4244	89.2	44.56% $ \pm 5/2\rangle$ +27.38% $ \pm 3/2\rangle$

	Ref	1567	1.9997	6.1477	12.1487		
KD ₇	this work	1733	0.3624	0.6479	18.9808	88.2	30.77% ±3/2> +30.67% ±1/2> +27.43% ±5/2>
	Ref	1688	0.3807	0.2456	18.7140		

Ref—*Inorg. Chem. Front.*, 2020, 7, 4805–4812

Table S2 *ab initio* results of ABIKUV

ABIKUV		E (K)	g _x	g _y	g _z	θ (°)	wave functions
KD ₀	this work	0	0.0006	0.0007	19.8409	0	97.5% ±15/2>
	Ref	0	0.00	0.00	19.72	0	97% ±15/2>
KD ₁	this work	299	0.0118	0.0157	16.8121	7.2	90.1% ±13/2>
	Ref	288	0.01	0.01	16.74	6.7	90% ±13/2>
KD ₂	this work	541	0.0423	0.0603	13.8981	10.0	77.1% ±11/2>
	Ref	526	0.05	0.07	13.92	9.5	78% ±11/2>
KD ₃	this work	754	0.9583	1.0635	11.2031	13.0	61.5% ±9/2>
	Ref	736	0.66	0.77	11.39	14.3	64% ±9/2>
KD ₄	this work	927	2.3959	3.5276	8.6282	26.2	44.6% ±7/2> +23.7% ±5/2>
	Ref	906	1.27	2.24	9.19	26.0	47% ±7/2> +28% ±5/2>

KD ₅	this work	1052	3.0744	4.2161	9.2166	74.4	42.5% ±3/2> +26.7% ±5/2>
	Ref	1030	1.35	4.91	7.03	45.2	52% ±3/2> +26% ±5/2>
KD ₆	this work	1134	1.3473	3.7139	14.7986	89.3	59.8% ±1/2>
	Ref	1103	2.01	6.98	12.46	88.3	67% ±1/2>
KD ₇	this work	1330	0.0489	0.0988	19.6975	74.2	28% ±3/2> +25.6% ±5/2> +21.3% ±1/2>
	Ref	1281	0.09	0.18	19.57	74.4	29% ±3/2> +26% ±5/2> +21% ±1/2>

Ref—*Chem. Commun.*, 2021,57, 9208-9211

Table S3 *ab initio* results of JEYRAK

JEYRAK		E (K)	g _x	g _y	g _z	θ (°)	wave functions
KD ₀	this work	0	0.0017	0.0023	19.9646	0	99.6% ±15/2>
	Ref	0	0.002	0.002	19.817		99.6% ±15/2>
KD ₁	this work	347	0.0547	0.0754	17.1035	9.4	93.6% ±13/2>

	Ref	338	0.043	0.058	17.021		93.4% ±13/2>
KD ₂	this work	533	1.7251	3.1800	14.3892	57.2	36.4% ±11/2> +16.9% ±7/2>
	Ref	521	1.459	2.620	14.296		38.9% ±11/2> +16.1% ±7/2>
KD ₃	this work	610	1.0976	4.6792	9.1213	58.1	43.8% ±11/2> +18.4% ±1/2>
	Ref	598	1.370	4.229	9.634		
KD ₄	this work	734	4.3266	5.0258	9.2448	84.9	46.6% ±9/2> +17% ±3/2>
	Ref	716	4.527	5.165	8.900		
KD ₅	this work	881	0.7098	0.9973	14.1518	86.6	36.7% ±7/2> +24.2% ±9/2> +18.3% ±1/2>
	Ref	852	0.810	1.163	13.987		
KD ₆	this work	1079	0.0377	0.0629	17.4555	88.2	34.9% ±5/2> +25.5% ±3/2> +23.5% ±7/2>
	Ref	1043	0.034	0.059	17.296		
KD ₇	this work	1467	0.0010	0.0012	19.9473	87.1	41.5% ±1/2> +31.3% ±3/2> +17.5% ±5/2>
	Ref	1424	0.001	0.001	19.838		

Ref—*Inorg. Chem. Front.*, **2023**,10, 485-492

Table S4 *ab initio* results of ABILEG

ABILEG		E (K)	g_x	g_y	g_z	θ (°)	wave functions
KD ₀	this work	0	0.0050	0.0077	19.8518	0	97.8% ±15/2>
	Ref	0	0.01	0.01	19.74	0	97% ±15/2>
KD ₁	this work	267	0.3641	0.7089	16.4251	2.2	89.2% ±13/2>
	Ref	257	0.38	0.75	16.32	1.4	30% ±13/2>
KD ₂	this work	406	3.2029	4.6900	13.3386	80.6	26.7% ±11/2> +21.1% ±3/2>
	Ref	394	3.19	4.70	13.06	77.4	27% ±11/2> +20% ±3/2>
KD ₃	this work	501	0.7831	5.0024	7.6665	81.3	48.6% ±11/2>
	Ref	490	0.86	4.92	7.63	81.9	46% ±11/2>
KD ₄	this work	638	2.4552	2.8252	11.2593	82.3	43.3% ±9/2>
	Ref	628	2.41	2.70	11.23	82.7	34% ±9/2>
KD ₅	this work	777	0.0604	0.1695	14.7117	85.8	36.6% ±7/2> +25.8% ±9/2>
	Ref	770	0.02	0.17	14.59	86.4	32% ±7/2>
KD ₆	this work	913	0.1681	0.1903	17.6305	82.2	32.9% ±5/2> +25.1% ±7/2> +22.6% ±3/2>
	Ref	912	0.14	0.16	17.34	83.0	25% ±5/2>
KD ₇	this work	1042	0.0194	0.0381	19.6720	88.3	45.5% ±1/2> +33.3% ±3/2>

Ref	1041	0.02	0.03	19.56	87.0	23% ±1/2>
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Ref—*Chem. Commun.*, **2021**,57, 9208-9211

Table S5 *ab initio* results of ZOTSAE01

ZOTSAE01		E (K)	g_x	g_y	g_z	θ (°)	wave functions
KD ₀	this work	0	0.1938	0.7053	17.5942	0	64.1% ±15/2> +28.7% ±11/2>
	Ref	0					69.8% ±15/2> +30.1% ±7/2>
KD ₁	this work	107	0.0698	0.5404	14.9352	2.0	64.6% ±13/2> +28.6% ±9/2>
	Ref	35					69.6% ±7/2> +30.1% ±15/2>
KD ₂	this work	391	2.2315	2.5447	13.2084	1.7	31.4% ±15/2> +30.2% ±11/2> +26.2% ±7/2>
	Ref	50					95.7% ±5/2> +4.0% ±3/2>
KD ₃	this work	578	3.3415	6.0572	8.2534	8.7	27.9% ±5/2> +26.4% ±13/2> +22.9% ±9/2>

	Ref	105					100% ±9/2>
KD ₄	this work	770	3.1099	3.6711	10.5989	88.7	27.8% ±3/2> +24.5% ±11/2>
	Ref	140					95.4% ±3/2>
KD ₅	this work	987	0.7563	0.8859	14.3308	87.2	25.6% ±7/2> +23.9% ±1/2> +22.9% ±9/2>
	Ref	201					99.6% ±1/2>
KD ₆	this work	1303	0.0675	0.0967	17.2856	88.2	33.7% ±5/2> +27.7% ±3/2> +22% ±7/2>
	Ref	281					99.4% ±11/2>
KD ₇	this work	1920	0.0014	0.0022	19.9090	89.6	45.7% ±1/2> +31.7% ±3/2>
	Ref	387					99.7% ±13/2>

Ref—*Inorg. Chem. Front.*, **2016**, 3, 1028-1034

Table S6 *ab initio* results of ANOVUW

ANOVUW		E (K)	g _x	g _y	g _z	θ (°)	wave functions
KD ₀	this work	0	0.0104	0.0198	19.7995	0	97.6% ±15/2>
	Ref	0					92.0% ±15/2>
KD ₁	this work	173	0.2827	0.3824	16.6781	18.6	79.2% ±13/2>

	Ref	86					97.1% ±13/2>
KD ₂	this work	281	2.5426	3.9501	13.6424	74.8	26.4% ±1/2> +26.9% ±3/2>
	Ref	230					80.3% ±11/2>
KD ₃	this work	371	0.3301	5.3080	7.8416	25.4	38.5% ±11/2>
	Ref	314					47.4% ±9/2> +47.3% ±3/2>
KD ₄	this work	471	3.3375	3.6119	13.9040	57.6	37.3% ±7/2>
	Ref	332					47.9% ±1/2> +36.7% ±7/2>
KD ₅	this work	573	0.3228	0.5972	13.6596	73.7	27.8% ±9/2> +24% ±5/2>
	Ref	399					69.5% ±5/2>
KD ₆	this work	815	0.2941	0.3341	16.3397	74.1	26.7% ±7/2> +20.9% ±9/2>
	Ref	520					52.5% ±3/2> +44.8% ±9/2>
KD ₇	this work	1037	0.0533	0.1306	19.2225	81.0	28% ±3/2> +31% ±1/2> +21.8% ±5/2>
	Ref	592					41.2% ±7/2> +30.3% ±1/2> +27.2% ±5/2>

Ref—*Inorg. Chem. Front.*, **2016**, 3, 1028-1034

Table S7 *ab initio* results of LAJKAL

LAJKAL		E (K)	g_x	g_y	g_z	θ (°)	wave functions
KD ₀	this work	0	0.0127	0.0172	17.8478	0	98.4% ±15/2>
	Ref	0	0.004	0.005	17.858		
KD ₁	this work	72	0.2044	0.2189	15.5239	3.1	99.1% ±13/2>
	Ref	72					
KD ₂	this work	141	0.0620	0.3320	12.9213	1.9	96.2% ±11/2>
	Ref	144					
KD ₃	this work	221	0.7540	0.9595	10.1895	1.7	90% ±9/2>
	Ref	229					
KD ₄	this work	298	5.3823	5.9678	6.9359	84.0	77.9% ±7/2>
	Ref	314					
KD ₅	this work	441	3.5998	5.6360	6.6467	84.5	77.5% ±5/2>
	Ref	447					
KD ₆	this work	516	2.5123	4.4345	5.5500	62.3	86.1% ±3/2>
	Ref	524					
KD ₇	this work	574	0.8142	4.3631	13.9312	88.6	79.2% ±1/2>
	Ref	584					

Table S8 *ab initio* results of FOXWUM

FOXWUM		E (K)	g_x	g_y	g_z	θ ($^\circ$)	wave functions
KD ₀	this work	0	0.0223	0.0286	17.8104	0	98% $\pm 15/2$ >
	Ref						
KD ₁	this work	51	0.2607	0.2938	15.5137	5.9	97.2% $\pm 13/2$ >
	Ref						
KD ₂	this work	106	0.1945	0.3328	12.8584	5.6	90.7% $\pm 11/2$ >
	Ref						
KD ₃	this work	176	0.9088	1.0302	10.1236	5.4	80% $\pm 9/2$ >
	Ref						
KD ₄	this work	243	5.3938	5.8273	7.3924	89.1	65.7% $\pm 7/2$ >
	Ref						

		Ref					
KD ₅	this work	382	3.3741	6.3794	6.5394	85.7	64.5% ±5/2>
		Ref					
KD ₆	this work	450	2.4069	3.7692	5.1360	58.4	71% ±3/2>
		Ref					
KD ₇	this work	501	0.8857	5.1305	13.3313	86.9	69% ±1/2>
		Ref					

Ref—*Angew. Chem. Int. Ed.* **2015**, *54*, 5864 -5868

Table S9 *ab initio* results of LAJJUE

LAJJUE		E (K)	g _x	g _y	g _z	θ (°)	wave functions
KD ₀	this	0	0.7026	2.7052	17.2934	0	71% ±15/2>

	work						
	Ref	0					
KD ₁	this work	90	3.2350	5.5243	8.7894	3.2	36.3% ±13/2> +24.8% ±9/2>
	Ref	98					
KD ₂	this work	213	0.6303	4.0542	6.5376	89.4	26.7% ±13/2>
	Ref	219					
KD ₃	this work	403	1.4654	1.6861	9.4520	90.0	27.4% ±11/2>
	Ref	406					
KD ₄	this work	651	0.1516	0.1767	12.2213	89.8	26.5% ±11/2> +23.5% ±9/2>
	Ref	650					
KD ₅	this work	944	0.0097	0.0275	14.7284	89.6	28.5% ±9/2> +25.2% ±7/2>
	Ref	935					
KD ₆	this work	1219	0.0101	0.0109	17.2744	89.2	31.5% ±5/2> +27.2% ±7/2>
	Ref	1201					
KD ₇	this work	1402	0.0007	0.0009	19.8781	89.0	39.1% ±1/2> +31% ±3/2>
	Ref	1371					

Ref—*Inorg. Chem.* **2016**, *55*, 1905-1911

Table S10 The experimental values and theoretical predictions of τ_{QTM} (in s) and U_{eff} (in K) of the systems studied here.

	$\tau_{QTM}^{exp\ a}$	$\tau_{QTM}^{Zee\ b}$ 20 mT	$\tau_{QTM}^{Zee\ c}$ Ref	$\tau_{QTM}^{Zee\ d}$ aniso	$U_{eff}^{exp\ e}$	$U_{eff}^{Zee\ f}$	$U_{eff}^{Zee\ g}$ Ref
DUXGUB	3.70×10^{-1}	2.95	7.10		1278	1522/348	1500/468
ABIKUV	1.75×10^{-1}	1.67×10^{-1}	1.41×10^{-1}		916±126	986/649	1031/593
JEYRAK		1.74×10^{-2}	1.77×10^{-2}		593	650/536	650/531
ABILEG	4.90×10^{-2}	1.68×10^{-3}	1.14×10^{-3}			470/411	457/397
LAJKAL	1.08×10^{-2}		3.11×10^{-3}		71	378/11	
FOXWUM	6.74×10^{-3}	1.01×10^{-4}			66	325/30	
ANOVUV	1.81×10^{-2}	2.83×10^{-4}		1.03×10^{-3}	36	360/~0	
ZOTSAE01	2.89×10^{-2}	2.35×10^{-7}		1.89×10^{-6}	25	545/~0	
LAJJUE	5.53×10^{-2}	1.58×10^{-8}	2.67×10^{-8}	8.40×10^{-8}	17	120/~0	

^a τ_{QTM} fitted from experimental data. ^b τ_{QTM} calculated from eqn 1b using results calculated here and 20 mT B_{ave} . ^c τ_{QTM} calculated from eqn 1b using results reported in references. ^d τ_{QTM} calculated from eqn 1c. ^e U_{eff} fitted from experimental data. ^f U_{eff} calculated from eqn 3a using results calculated here. ^g U_{eff} calculated from eqn 3a using results reported in references. ^h result using 300 K in eqn 3a is at the left side of “/”, result using T_{AC} in eqn 3a is at the right side of “/”.

Table S11 Various $U_{\text{eff}}^{\text{KD}}$ values according to transition magnetic moment $|\mu|$, angle of easy axis of excited KD with respect to that of ground KD (θ) and crystal field wave function composition.

	$U_{\text{eff}}^{\text{Zee}}$ (K)		$U_{\text{eff}}^{\text{KD}}$ by $ \mu $ for QTM and TA-QTM			$U_{\text{eff}}^{\text{KD}}$ by $ \mu $ for spin-phonon transition		
	300 K	T_{AC}	KD	$ \mu $	$U_{\text{eff}}^{\text{KD}}$ (K)	KD	$ \mu $	$U_{\text{eff}}^{\text{KD}}$ (K)
DUXGUB	1500	468	KD ₃	4.40E-01	1337	KD ₄	0.47	1479
ABIKUV	986	649	KD ₂	1.80E-02	541	KD ₄	0.58	927
JEYRAK	650	536	KD ₁	2.40E-02	347	KD ₂	0.38	533
ABILEG	470	411	KD ₁	1.80E-01	267	KD ₂	1.80	406
ZOTSAE01	545	0	KD ₀	1.50E-01	0	KD ₁	0.18	107
ANOVUW	360	0	KD ₁	1.30E-01	173	KD ₂	0.67	281
LAJKAL	378	11	KD ₁	7.20E-02	72	KD ₃	0.11	221
LAJJUE	120	0	KD ₀	5.70E-01	0	KD ₁	0.84	90
FOXWUM	325	30	KD ₁	9.70E-02	51	KD ₂	0.11	106

	$U_{\text{eff}}^{\text{KD}}$ by θ			$U_{\text{eff}}^{\text{KD}}$ by crystal field wave function composition		
	KD	θ (°)	E (K)	KD	composition	E (K)
DUXGUB	KD ₄	88.7	1479	KD ₄	51.6% $ \pm 1/2\rangle + 33.5\% \pm 3/2\rangle$	1479
ABIKUV	KD ₃	13.0	754	KD ₄	44.6% $ \pm 7/2\rangle + 23.7\% \pm 5/2\rangle$	927
JEYRAK	KD ₂	57.2	533	KD ₂	36.4% $ \pm 11/2\rangle + 16.9\% \pm 7/2\rangle$	533
ABILEG	KD ₂	80.6	406	KD ₂	26.7% $ \pm 11/2\rangle + 21.1\% \pm 3/2\rangle$	406
ZOTSAE01	KD ₄	88.7	770	KD ₂	31.4% $ \pm 15/2\rangle + 30.2\% \pm 11/2\rangle$	391
ANOVUW	KD ₁	18.6	173	KD ₂	26.4% $ \pm 1/2\rangle + 26.9\% \pm 3/2\rangle$	281
LAJKAL	KD ₄	84.0	298	KD ₄	77.9% $ \pm 7/2\rangle$	298

LAJJUE	KD ₂	89.4	213	KD ₁	36.3% ±13/2>+24.8% ±9/2>	90
FOXWUM	KD ₄	89.1	243	KD ₃	80% ±9/2>	176

Table S12 The contributions of various KDs to U^{Zee}_{eff} angles between *ab initio* magnetic easy axis of ground KD and excited KDs and crystal field wave function compositions of DUXCUB and JEYRAK.

DUXCUB	E (K)	contribution ^a		θ (°)	composition
KD ₀	0	0.0%	0.3%		> 99.9% ±15/2>
KD ₁	487	0.0%	14.3%	0.2	99.9% ±13/2>
KD ₂	969	0.0%	0.8%	0.8	99.0% ±11/2>
KD ₃	1337	12.6%	39.1%	3.7	94.0% ±9/2>
KD ₄	1479	25.3%	18.7%	88.7	51.6% ±1/2>+33.5% ±3/2>
KD ₅	1534	21.3%	12.0%	80.7	72.0% ±7/2>+13.4% ±5/2>
KD ₆	1624	40.7%	14.7%	89.2	44.6% ±5/2>+27.4% ±3/2>+14.8% ±7/2>
KD ₇	1733	0.1%	0.0%	88.2	30.8% ±3/2>+30.7% ±1/2>+27.4% ±5/2>
JEYRAK	E (K)	contribution ^a		θ (°)	composition
KD ₀	0	0.0%	0.0%		99.6% ±15/2>
KD ₁	347	0.0%	0.3%	9.4	93.6% ±13/2>
KD ₂	533	19.1%	44.3%	57.2	36.4% ±11/2>+16.9% ±7/2>+12.2% ±3/2>
KD ₃	610	37.4%	41.1%	58.1	43.8% ±11/2>+18.4% ±1/2>+15.3% ±5/2>
KD ₄	734	42.8%	14.2%	84.9	46.6% ±9/2>+17% ±3/2>+13.2% ±7/2>
KD ₅	881	0.7%	0.1%	86.6	36.7% ±7/2>+24.2% ±9/2>+18.3% ±1/2>
KD ₆	1079	0.0%	0.0%	88.2	34.9% ±5/2>+25.5% ±3/2>+23.5% ±7/2>
KD ₇	1467	0.0%	0.0%	87.1	41.5% ±1/2>+31.3% ±3/2>+17.5% ±5/2>

^a contribution to saturated U^{Zee}_{eff} is at the left side, contribution to U^{Zee}_{eff} reproducing $U^{\text{exp}}_{\text{eff}}$ is at the right side.

Table S13 The distance R to Ln³⁺ (in Å), atomic charge Q (in |e|) and angle θ with respect to the *ab initio* magnetic easy axis (in °) of the atoms in the first sphere.

DUXCUB	N ₂ -a ^a	N ₃ -a	I ₄ -e ^b	I ₅ -e
R	2.402	2.438	2.977	2.936
Q ^c	0.734	0.728	0.745	0.760
θ	10.2	9.4	87.5	89.5
ABIKUV	O ₂ -a	O ₃ -a	Cl ₄ -e	Cl ₅ -e
R	2.103	2.082	2.549	2.549
Q	0.949	0.949	0.841	0.833
θ	25.7	32.8	74.0	79.6
JEYRAK	N ₃ -a	N ₄ -a	O ₂ -e	C ₅ -e
R	2.132	2.145	2.339	2.464
Q	1.117	1.102	0.562	0.823
θ	31.4	25.7	89.5	82.6
ABILEG	O ₂ -a	O ₃ -a	O ₄ -e	Cl ₅ -e
R	2.117	2.133	2.091	2.553
Q	0.951	0.954	0.953	0.834
θ	31.4	25.4	86.7	82.3
ZOTSAE01	N ₂ -a	N ₄ -a	N ₃ -e	N ₅ -e
R	2.295	2.295	2.282	2.282

Q	0.733	0.733	0.729	0.729
θ	44.7	44.7	49.4	49.4
ANOVUW	N ₂ -a	O ₃ -a	O ₄ -e	O ₅ -e
R	2.273	2.195	2.068	2.152
Q	0.748	1.008	1.024	1.011
θ	14.1	38.6	78.1	67.2
LAJKAL	Cl ₅ -a	N ₂ -e	N ₃ -e	N ₄ -e
R	2.571	2.249	2.247	2.242
Q	0.779	1.261	1.262	1.264
θ	0.6	78.8	79.0	78.9
FOXWUM	Cl ₅ -a	N ₂ -e	N ₃ -e	N ₄ -e
R	2.528	2.231	2.251	2.246
Q	0.814	1.265	1.262	1.265
θ	7.4	82.9	79.4	72.8
LAJJUE	N ₃ -a	N ₂ -e	N ₄ -e	Cl ₅ -e
R	2.274	2.269	2.265	2.601
Q	1.265	1.261	1.263	0.780
θ	10.4	63.0	56.3	89.7

^a “-a” indicates the atom occupying the axial position. ^b “-e” indicates the atom occupying the equatorial position.

^cThe atomic charges are absolute values obtained from the LoProp analysis.

Table S14 Theoretical prediction of τ_{QTM} and U_{eff} in different Dy-O.

Dy-O _{ave} (Å)	$\tau_{\text{QTM-20}}^{\text{Zee}}$ (s)	$U_{\text{eff}}^{\text{Zee}}$ (K)	θ (°) ^a
		300 K	

2.09	1.671E-01	986	0.0
1.79	8.798E-02	1364	4.4
1.89	1.756E-01	1377	2.4
1.99	2.072E-01	1236	1.3
2.19	1.382E-01	885	2.0
2.29	9.632E-02	720	3.8
2.39	3.894E-02	562	6.9
2.49	8.259E-03	429	12.4
2.59	3.347E-03	349	25.2

^a The angle between the different magnetic easy axis.

Table S15 Theoretical prediction of τ_{QTM} and U_{eff} with different $\angle\text{O-Dy-O}$.

$\angle\text{O-Dy-O}$ (°)	$\tau_{\text{QTM-20}}^{\text{Zee}}$ (s)	$U_{\text{eff}}^{\text{Zee}}$ (K)	θ (°) ^a
		300 K	
122.4	1.671E-01	986	0.0
115	3.300E-03	757	5.7
120	4.432E-02	955	2.0
130	3.975E+00	1279	0.8
140	3.615E+01	1632	2.1
150	1.506E+02	1916	2.9
160	4.357E+02	2181	3.6
170	7.961E+02	2335	4.1
180	1.002E+03	2423	4.4

^a The angle between the different magnetic easy axis.

Table S16 Theoretical prediction of τ_{QTM} and U_{eff} of structures having different Dy-Cl lengths.

Dy-Cl _{ave} (Å)	$\tau_{\text{QTM-20}}^{\text{Zee}}$ (s)	$U_{\text{eff}}^{\text{Zee}}$ (K)	θ (°) ^a
		300 K	
2.55	1.671E-01	986	0.0
2.35	8.576E-02	974	1.5
2.45	1.076E-01	1004	1.4
2.65	2.366E-01	1106	0.6
2.75	4.657E-01	1169	0.5
2.85	1.006E+00	1231	0.9
2.95	2.266E+00	1290	1.5
3.05	5.174E+00	1344	1.9

^a The angle between the different magnetic easy axis.

Table S17 Theoretical prediction of τ_{QTM} and U_{eff} with different equatorial atom.

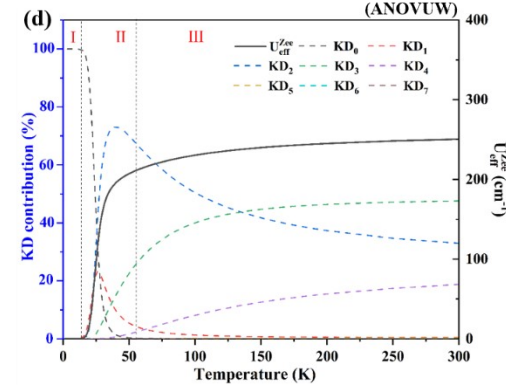
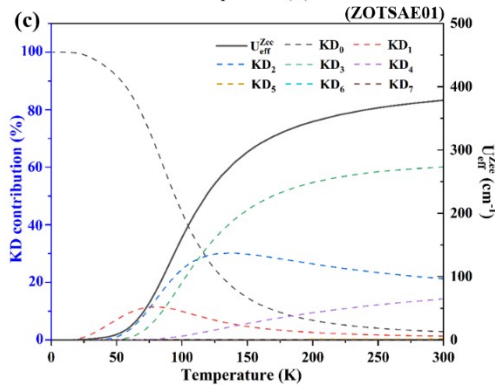
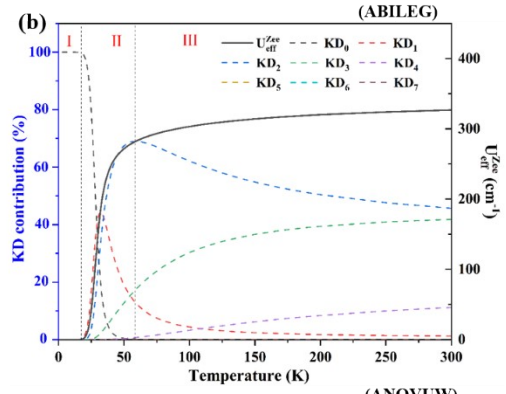
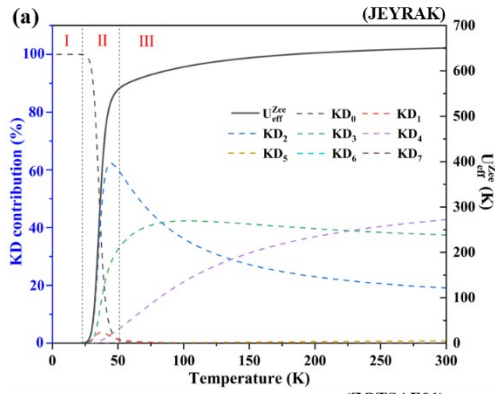
equatorial atom	$\tau_{\text{QTM-20}}^{\text{Zee}}$ (s)	$U_{\text{eff}}^{\text{Zee}}$ (K)	θ (°) ^a
		300 K	
Cl	1.671E-01	986	0.0
Br	6.282E-01	1144	0.5
I	3.361E+00	1254	1.5
None	1.471E+04	2183	6.0

^a The angle between the different magnetic easy axis.

Table S18 Prediction of T_{B} from calculated U_{eff} .

$\angle\text{O-Dy-O}$ (°)	$U_{\text{eff}}^{\text{Zee}}$ (K)	T_{B}^{100} (K)

115	757	
120	955	
122.4	986	
130	1279	
140	1632	
150	1916	49
160	2181	57
170	2335	62
180	2423	64



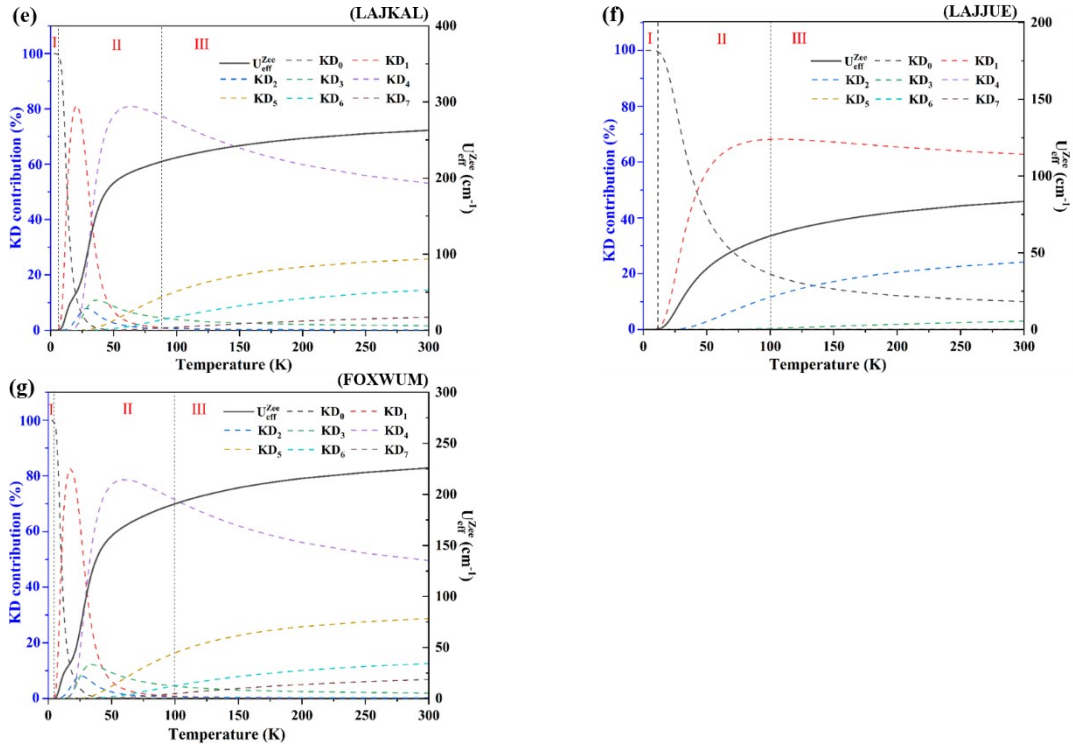
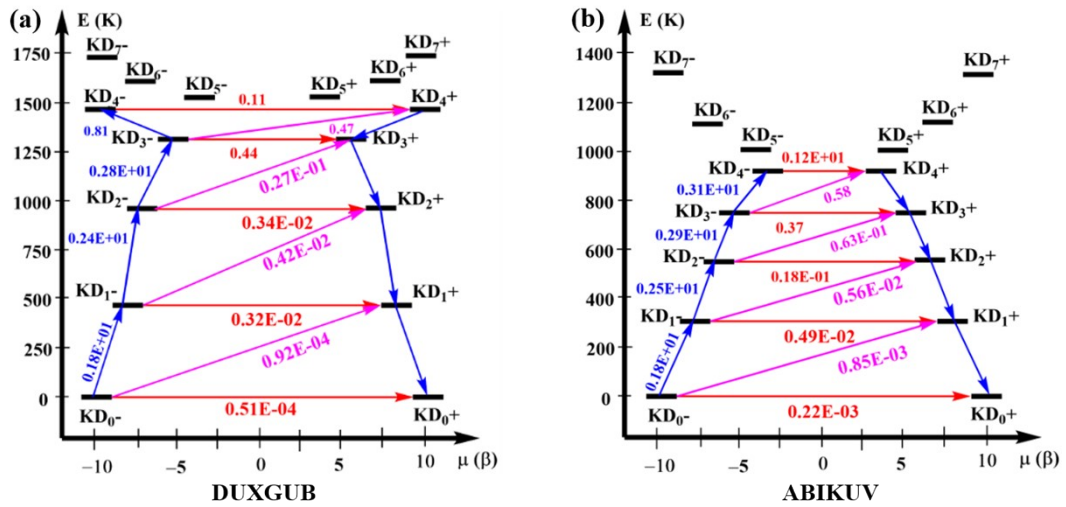
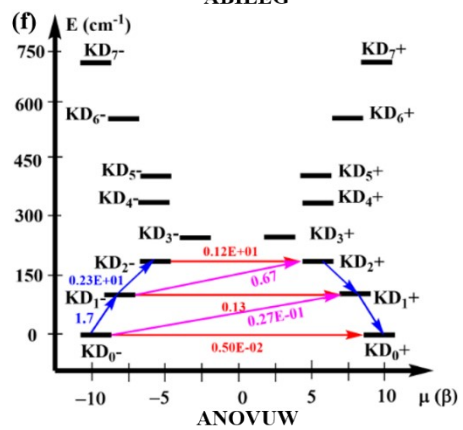
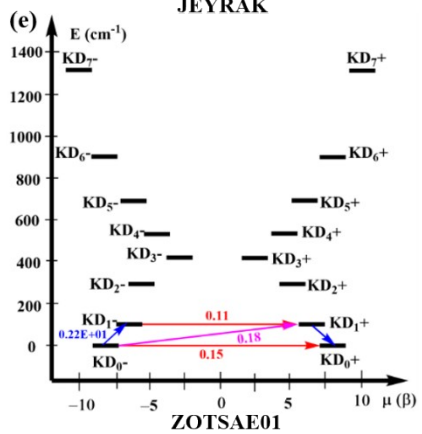
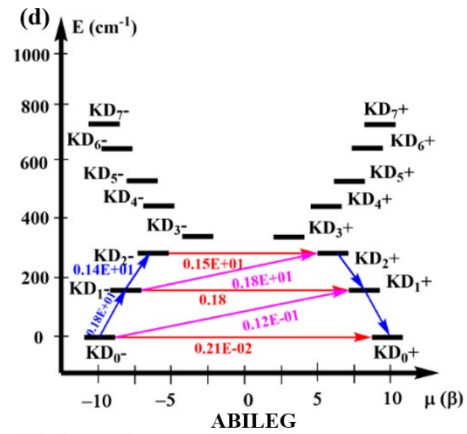
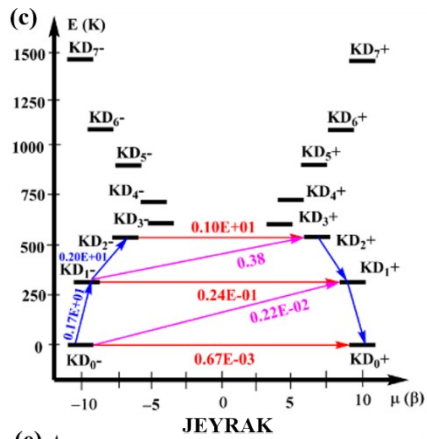


Figure S1 $U_{\text{eff}}^{\text{Zee}}$ and the contributions from various KDs of other SIMs.





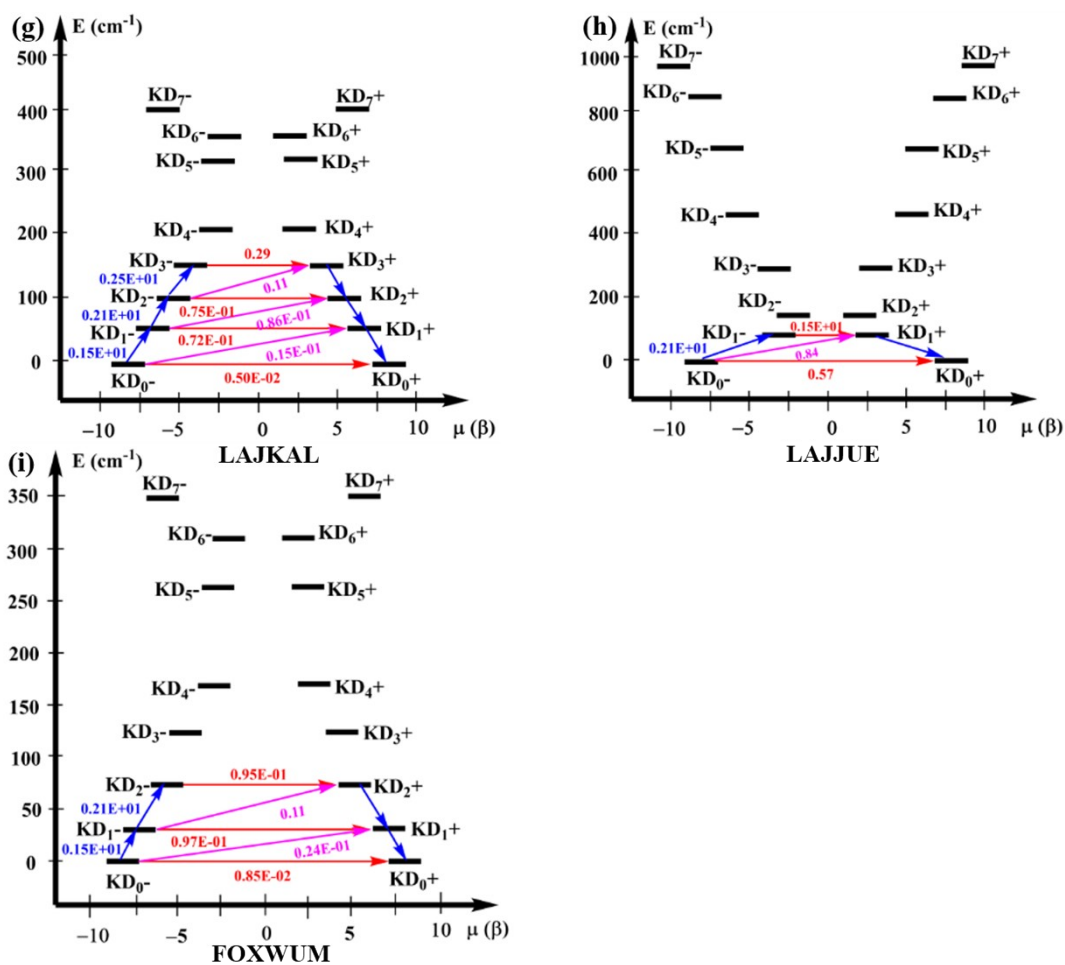


Figure S2 Possible relaxation mechanism based on transition magnetic moment for the Ln-SIMs studied here.

Cartesian coordinates used in our calculations

1Dy (DUXGUB)

Dy	2.008338000	5.995324000	12.677982000
N	-0.108367000	7.092785000	12.387598000
N	3.711990000	4.251897000	12.661612000
I	3.255756000	8.033121000	14.454095000
I	0.583493000	4.214839000	14.526514000
C	1.537311000	6.360277000	9.884100000
C	2.629210000	5.504386000	9.949935000

C	3.981193000	7.278037000	10.857386000
C	3.849792000	5.961328000	10.471274000
C	4.954004000	5.010575000	10.709703000
C	1.634712000	7.680452000	10.353840000
C	2.864550000	8.147006000	10.795110000
C	-1.253995000	6.673948000	13.154483000
C	3.632192000	3.151437000	13.586857000
C	-1.546607000	7.275116000	14.398225000
C	-0.437312000	8.147363000	11.547761000
C	4.828993000	4.149379000	11.828893000
C	0.416283000	8.503769000	10.480171000
C	4.060541000	3.289180000	14.916006000
C	3.113418000	1.908898000	13.145586000
C	-2.113660000	5.690398000	12.615350000
C	0.119447000	9.546990000	9.613644000
C	6.059723000	4.971605000	9.866307000
C	-0.632703000	8.298036000	15.029882000
C	-3.273897000	5.349264000	13.302166000
C	-1.772735000	4.989731000	11.312891000
C	5.894969000	3.237511000	12.022838000
C	2.586825000	1.715313000	11.727472000
C	-1.047813000	10.276154000	9.754210000
C	-2.717203000	6.881284000	15.054792000
C	6.997166000	3.215014000	11.175884000
C	-2.103125000	3.503740000	11.320008000
C	-0.125077000	7.808251000	16.399955000
C	7.097036000	4.064670000	10.086942000

C	3.979720000	2.189797000	15.768298000
C	3.064208000	0.840671000	14.022789000
C	-1.906420000	9.965907000	10.800448000
C	4.547587000	4.640603000	15.432007000
C	-3.577091000	5.949949000	14.508542000
C	-1.621978000	8.927297000	11.668754000
C	3.502977000	0.972127000	15.334145000
C	1.153681000	1.210799000	11.743485000
C	-2.418471000	5.677347000	10.111853000
C	3.489310000	0.774866000	10.930338000
C	4.122420000	4.919142000	16.862577000
C	-1.304444000	9.670261000	15.181124000
C	6.040870000	4.829710000	15.266531000
H	0.716689000	6.049107000	9.519234000
H	2.549268000	4.609407000	9.642629000
H	4.820422000	7.601480000	11.165226000
H	2.957750000	9.054484000	11.058876000
H	0.726049000	9.762468000	8.914248000
H	6.109723000	5.571019000	9.131805000
H	0.161199000	8.409535000	14.432922000
H	-3.862921000	4.698824000	12.938278000
H	-0.782332000	5.066289000	11.192752000
H	5.856782000	2.625882000	12.748621000
H	2.593102000	2.605671000	11.272287000
H	-1.257454000	10.975374000	9.146716000
H	-2.926174000	7.264160000	15.899772000
H	7.701370000	2.600130000	11.348246000

H	-1.704706000	3.084998000	12.111573000
H	-1.740875000	3.084978000	10.511647000
H	-3.075286000	3.386048000	11.342178000
H	-0.887987000	7.656065000	16.995741000
H	0.465120000	8.485607000	16.790746000
H	0.370784000	6.970591000	16.283908000
H	7.848245000	4.032053000	9.506512000
H	4.259137000	2.281196000	16.672137000
H	2.726553000	0.004234000	13.724683000
H	-2.699427000	10.473639000	10.920409000
H	4.108534000	5.337304000	14.863641000
H	-4.380468000	5.722207000	14.961663000
H	-2.234820000	8.729703000	12.366851000
H	3.474391000	0.229691000	15.924949000
H	1.133672000	0.297016000	12.099989000
H	0.795545000	1.213131000	10.832120000
H	0.608363000	1.793791000	12.311603000
H	-3.394101000	5.636868000	10.197972000
H	-2.144157000	5.223502000	9.288101000
H	-2.132794000	6.614647000	10.079095000
H	4.388792000	1.158271000	10.869557000
H	3.123003000	0.655368000	10.029364000
H	3.534878000	-0.094534000	11.381786000
H	3.165308000	4.729891000	16.962166000
H	4.292024000	5.860501000	17.077554000
H	4.632934000	4.347754000	17.473150000
H	-1.593955000	9.989636000	14.301021000

H	-0.664866000	10.305841000	15.565100000
H	-2.081306000	9.590374000	15.772124000
H	6.515697000	4.174603000	15.819845000
H	6.288783000	5.735124000	15.547183000
H	6.284354000	4.700578000	14.326216000

2Dy (ABIKUV)

Dy	4.707736000	28.425086000	11.121782000
O	4.172541000	28.749041000	13.129320000
O	5.496315000	29.932346000	9.920675000
Cl	3.009356000	27.373521000	9.537666000
Cl	6.374928000	26.534331000	11.503099000
C	3.696091000	29.372573000	14.216962000
C	2.390744000	29.051431000	14.694665000
C	1.833031000	29.871868000	15.676621000
C	2.509778000	30.950156000	16.249189000
C	3.837528000	31.137684000	15.858402000
C	4.468693000	30.355222000	14.885409000
C	1.617895000	27.811399000	14.192443000
C	0.325147000	27.567612000	15.010880000
C	2.503924000	26.553553000	14.348013000
C	1.167546000	27.948764000	12.714521000
C	-0.408095000	26.294763000	14.528949000
C	0.504931000	25.088018000	14.689593000
C	1.769705000	25.296175000	13.847482000
C	1.397831000	25.469638000	12.388161000
C	0.465905000	26.673102000	12.220753000
C	-0.800675000	26.452756000	13.056100000

C	1.809255000	31.867170000	17.268684000
C	1.151990000	31.055172000	18.353958000
C	0.742502000	32.666978000	16.553059000
C	2.739044000	32.869040000	17.905847000
C	5.987386000	30.519309000	14.648502000
C	6.627753000	31.495395000	15.659035000
C	6.674071000	29.151759000	14.835186000
C	6.321670000	31.071112000	13.244307000
C	8.152434000	31.599004000	15.450536000
C	8.787333000	30.216920000	15.628090000
C	8.193158000	29.257243000	14.608932000
C	8.459618000	29.765914000	13.196790000
C	7.845055000	31.162063000	13.021773000
C	8.445998000	32.116114000	14.041945000
C	5.535722000	30.908900000	9.008388000
C	4.558358000	31.933274000	8.968988000
C	4.668483000	32.908890000	7.966403000
C	5.663278000	32.933738000	7.008628000
C	6.608724000	31.921553000	7.080664000
C	6.602720000	30.917807000	8.044864000
C	3.361330000	32.141430000	9.934034000
C	3.131859000	31.068299000	11.013390000
C	3.545346000	33.493041000	10.674854000
C	2.044817000	32.207534000	9.106972000
C	1.924979000	31.402099000	11.907583000
C	2.154776000	32.743865000	12.596829000
C	2.333904000	33.830592000	11.552814000

C	1.081691000	33.902791000	10.670120000
C	0.839953000	32.555399000	9.988652000
C	0.662988000	31.472423000	11.050591000
C	5.725188000	33.986710000	5.897143000
C	4.836187000	35.200018000	6.190699000
C	5.267599000	33.351457000	4.587644000
C	7.153821000	34.517415000	5.725677000
C	7.747093000	29.874681000	8.075471000
C	7.202152000	28.438213000	7.866465000
C	8.518297000	29.944066000	9.398329000
C	8.764584000	30.135814000	6.940143000
C	8.354944000	27.413839000	7.907049000
C	9.093206000	27.516042000	9.244619000
C	9.662788000	28.918755000	9.427245000
C	10.641246000	29.210361000	8.295976000
C	9.906950000	29.108627000	6.966861000
C	9.340358000	27.712009000	6.774089000
H	0.967111000	29.690950000	15.963649000
H	4.325962000	31.816443000	16.265084000
H	0.550297000	27.473379000	15.949969000
H	-0.264051000	28.333010000	14.919550000
H	3.323212000	26.671461000	13.842612000
H	2.740042000	26.438645000	15.281336000
H	0.562003000	28.701409000	12.631849000
H	1.942627000	28.125322000	12.157866000
H	-1.217093000	26.163259000	15.066902000
H	0.043691000	24.285631000	14.399200000

H	0.744965000	24.979486000	15.623304000
H	2.356936000	24.516994000	13.942819000
H	0.954886000	24.668048000	12.066992000
H	2.200359000	25.602784000	11.859931000
H	0.224728000	26.774508000	11.275695000
H	-1.398751000	27.209058000	12.953221000
H	-1.261935000	25.655901000	12.750539000
H	0.549473000	30.420154000	17.959654000
H	0.662546000	31.638854000	18.939259000
H	1.823770000	30.588882000	18.857027000
H	1.157976000	33.270539000	15.932687000
H	0.233733000	33.167726000	17.194754000
H	0.160033000	32.070263000	16.077723000
H	2.245091000	33.420561000	18.517122000
H	3.132119000	33.419249000	17.224532000
H	3.431701000	32.405048000	18.381775000
H	6.229162000	32.373356000	15.555394000
H	6.447380000	31.188786000	16.561378000
H	6.503848000	28.825506000	15.732711000
H	6.298408000	28.514162000	14.208067000
H	5.932331000	30.492118000	12.570500000
H	5.929313000	31.952777000	13.144099000
H	8.530397000	32.218176000	16.109902000
H	9.746996000	30.276929000	15.503362000
H	8.617070000	29.889870000	16.525546000
H	8.601185000	28.372672000	14.718745000
H	8.073438000	29.154478000	12.550597000

H	9.416369000	29.807827000	13.039444000
H	8.026184000	31.490378000	12.116437000
H	8.063171000	33.000685000	13.929494000
H	9.404119000	32.180389000	13.907173000
H	4.029305000	33.584133000	7.945739000
H	7.289131000	31.913396000	6.446257000
H	2.984805000	30.210356000	10.585063000
H	3.927175000	30.993991000	11.564211000
H	4.340068000	33.448222000	11.229092000
H	3.674850000	34.199882000	10.023436000
H	2.136299000	32.876588000	8.410844000
H	1.891530000	31.350201000	8.679271000
H	1.819427000	30.702478000	12.585414000
H	1.396664000	32.955491000	13.163089000
H	2.946189000	32.693420000	13.156173000
H	2.477152000	34.693457000	11.995785000
H	0.312950000	34.136310000	11.212571000
H	1.197311000	34.592051000	9.996786000
H	0.032583000	32.607673000	9.435345000
H	0.506312000	30.615230000	10.624260000
H	-0.102791000	31.679548000	11.608346000
H	5.094593000	35.591062000	7.028430000
H	3.918582000	34.920789000	6.237606000
H	4.937598000	35.848304000	5.489988000
H	4.358447000	33.056897000	4.674290000
H	5.829514000	32.600453000	4.382392000
H	5.328216000	33.998196000	3.879848000

H	7.436404000	34.944230000	6.537638000
H	7.174780000	35.153042000	5.006112000
H	7.744456000	33.787836000	5.524974000
H	6.558494000	28.230666000	8.561799000
H	6.749743000	28.383642000	7.010455000
H	7.910871000	29.770040000	10.134635000
H	8.880903000	30.836279000	9.513266000
H	8.310932000	30.090057000	6.084133000
H	9.132627000	31.028262000	7.036851000
H	7.994027000	26.509249000	7.799891000
H	8.480822000	27.316840000	9.970846000
H	9.812555000	26.866022000	9.270237000
H	10.130611000	28.973325000	10.286604000
H	11.011537000	30.101027000	8.401426000
H	11.372312000	28.572765000	8.319125000
H	10.532823000	29.304876000	6.237776000
H	10.058219000	27.060254000	6.780751000
H	8.885635000	27.655516000	5.918568000

3Dy (JEYRAK)

Dy	0.234462000	7.615890000	6.218107000
O	1.634834000	9.378595000	6.852734000
N	1.075383000	6.106734000	7.466919000
N	0.436096000	7.621615000	4.082930000
N	2.539058000	4.882245000	8.950013000
N	-0.014004000	7.006870000	1.781229000
N	0.460344000	4.182843000	8.798419000
N	0.945385000	8.962261000	2.114735000

C	5.565949000	6.335462000	7.386758000
C	0.216111000	4.612552000	1.439223000
C	1.641677000	4.824987000	0.965607000
C	3.740047000	5.639658000	8.776369000
C	6.006495000	7.181629000	8.390494000
C	4.441986000	5.528996000	7.559024000
C	-0.551363000	5.684925000	1.908935000
C	-2.476885000	10.085343000	7.644008000
C	-1.908130000	8.797002000	7.809384000
C	3.416181000	6.627754000	11.121251000
C	-0.952430000	3.400228000	6.987791000
C	-1.969339000	4.416223000	8.979872000
C	1.324050000	5.184467000	8.299308000
C	3.976787000	4.554568000	6.493043000
C	4.296206000	3.107864000	6.895226000
C	-2.221435000	3.333662000	6.405991000
C	0.143626000	7.630175000	0.545049000
C	-2.678963000	6.699194000	2.875691000
C	4.170692000	6.476656000	9.813180000
C	-0.365559000	3.342786000	1.451627000
C	0.460041000	7.822559000	2.834117000
C	-1.834010000	4.968329000	10.386480000
C	1.142826000	3.319030000	9.646197000
C	5.334346000	7.238307000	9.587167000
C	4.553062000	4.830603000	5.110553000
C	-3.221469000	4.295661000	8.356041000
C	2.404908000	3.753037000	9.758514000

C	0.241569000	2.792918000	6.273232000
C	-1.860989000	5.516892000	2.411492000
C	4.329945000	6.536678000	12.343420000
C	-3.334601000	3.793964000	7.083570000
C	-0.846834000	3.976114000	8.254059000
C	-0.716918000	9.720236000	9.741058000
C	1.203386000	10.234828000	2.720881000
C	-2.140456000	7.716935000	6.867664000
C	-3.802287000	6.333786000	3.849567000
C	0.704629000	8.825575000	0.748552000
C	-1.012649000	8.654251000	8.898104000
C	-2.178690000	11.131783000	8.489259000
C	-1.654146000	3.153518000	1.911002000
C	2.084139000	3.834204000	-0.107953000
C	2.637398000	7.949339000	11.139856000
C	2.525916000	10.620030000	2.985941000
C	-2.885267000	6.034397000	10.714934000
C	1.669277000	12.751666000	3.757692000
C	0.110258000	11.082366000	2.962972000
C	3.683036000	9.683877000	2.701128000
C	0.381476000	12.356341000	3.482066000
C	2.905717000	9.212440000	7.533758000
C	2.601322000	4.764593000	2.159065000
C	-1.909181000	3.824829000	11.413185000
C	0.546385000	3.486884000	4.956662000
C	0.033438000	1.297435000	6.072944000
C	-1.307337000	10.954275000	9.545823000

C	4.944199000	10.401478000	2.246346000
C	2.726041000	11.893681000	3.528004000
C	-2.375482000	4.207225000	2.400237000
C	1.265021000	10.778171000	6.830914000
C	-1.326816000	10.655002000	2.685050000
C	-3.270974000	7.442867000	1.669830000
C	3.961227000	8.808844000	3.886317000
C	-2.151332000	10.661846000	3.964411000
C	2.411521000	11.501070000	7.304071000
C	3.454926000	10.589965000	7.660087000
C	-1.967909000	11.500061000	1.605517000
H	6.030643000	6.303400000	6.581703000
H	1.698017000	5.724585000	0.582075000
H	6.758123000	7.713016000	8.253531000
H	-3.070033000	10.228594000	6.942496000
H	2.766575000	5.895874000	11.178099000
H	3.001648000	4.633886000	6.426732000
H	5.247361000	2.985020000	6.919734000
H	3.911022000	2.505053000	6.255316000
H	3.927964000	2.928923000	7.764503000
H	-2.317533000	2.974990000	5.553253000
H	-0.099354000	7.275220000	-0.279599000
H	-2.074125000	7.316004000	3.338167000
H	0.122406000	2.613028000	1.144626000
H	-0.950575000	5.384145000	10.463678000
H	0.784778000	2.568693000	10.063287000
H	5.653518000	7.791897000	10.263299000

H	4.209729000	5.663375000	4.780905000
H	4.304148000	4.121645000	4.513089000
H	5.510591000	4.878791000	5.167952000
H	-3.987411000	4.560013000	8.813027000
H	3.071704000	3.370396000	10.281674000
H	1.022068000	2.907415000	6.854158000
H	4.849195000	5.731064000	12.296173000
H	3.796478000	6.527629000	13.141677000
H	4.917672000	7.295922000	12.360463000
H	-4.168163000	3.763667000	6.672429000
H	-0.117005000	9.601429000	10.442203000
H	-2.725766000	7.969003000	6.135213000
H	-2.455955000	6.902845000	7.289371000
H	-4.459266000	5.802080000	3.395061000
H	-4.212403000	7.136398000	4.180087000
H	-3.438455000	5.834423000	4.584407000
H	0.900116000	9.456560000	0.093483000
H	-0.613986000	7.828589000	9.052844000
H	-2.568463000	11.964886000	8.346807000
H	-2.033757000	2.304660000	1.887390000
H	2.024002000	2.939848000	0.237911000
H	2.991983000	4.018753000	-0.359232000
H	1.515275000	3.918726000	-0.875914000
H	3.246556000	8.680970000	11.017685000
H	2.188726000	8.043819000	11.983407000
H	1.990284000	7.949221000	10.431223000
H	-3.756255000	5.631672000	10.728807000

H	-2.860839000	6.723851000	10.048403000
H	-2.695554000	6.415236000	11.576470000
H	1.828871000	13.600244000	4.103050000
H	3.404306000	9.096299000	1.967528000
H	-0.321684000	12.944616000	3.640712000
H	2.777858000	8.810827000	8.408111000
H	2.311175000	5.380832000	2.834462000
H	3.486422000	5.000630000	1.869153000
H	2.609821000	3.874689000	2.518320000
H	-1.821532000	4.184480000	12.299113000
H	-1.197736000	3.201582000	11.249165000
H	-2.753456000	3.376407000	11.331576000
H	1.336564000	3.105528000	4.568214000
H	0.686554000	4.424034000	5.112849000
H	-0.193551000	3.371400000	4.354581000
H	-0.710460000	1.153514000	5.483175000
H	-0.143237000	0.881898000	6.919160000
H	0.825278000	0.913487000	5.686862000
H	-1.118531000	11.661082000	10.120088000
H	5.299479000	10.916930000	2.973675000
H	4.733465000	10.985744000	1.513367000
H	5.595523000	9.755902000	1.962751000
H	3.589233000	12.169643000	3.736377000
H	-3.229308000	4.053467000	2.735604000
H	0.503379000	10.935933000	7.410761000
H	-1.301373000	9.731807000	2.358434000
H	-2.558841000	7.785207000	1.125562000

H	-3.815912000	8.169758000	1.979656000
H	-3.807269000	6.837439000	1.153538000
H	4.683290000	8.210725000	3.681550000
H	3.175436000	8.299944000	4.101075000
H	4.202385000	9.355402000	4.638659000
H	-2.125594000	11.537444000	4.358095000
H	-1.787961000	10.023185000	4.583144000
H	-3.060307000	10.428964000	3.762102000
H	2.160856000	12.043816000	8.063533000
H	2.721726000	12.099693000	6.596839000
H	3.740431000	10.754125000	8.573325000
H	4.218297000	10.701919000	7.073923000
H	-2.882435000	11.231211000	1.487688000
H	-1.491645000	11.380506000	0.779859000
H	-1.937250000	12.425007000	1.860632000
H	3.635842000	9.108302000	6.903955000
H	1.380015000	11.153507000	5.944204000

4Dy (ABILEG)

Dy	9.646741000	8.971268000	8.178028000
O	10.929617000	9.427767000	6.557348000
O	7.681931000	8.181703000	7.925511000
O	10.710859000	7.680142000	9.432804000
Cl	9.595745000	11.253172000	9.321731000
C	11.945424000	9.402297000	5.678021000
C	13.190484000	10.007696000	5.964381000
C	14.248768000	9.760834000	5.087947000
C	14.126238000	9.022208000	3.936723000

C	12.846677000	8.595098000	3.601190000
C	11.749368000	8.785142000	4.422666000
C	13.378106000	10.983387000	7.147422000
C	12.314364000	12.088387000	7.037506000
C	13.311867000	10.283946000	8.504015000
C	14.737026000	11.708299000	7.075109000
C	15.295532000	8.702855000	2.999545000
C	16.610573000	9.341561000	3.488382000
C	15.021206000	9.251437000	1.596672000
C	15.481604000	7.172704000	2.912770000
C	10.334227000	8.428564000	3.910690000
C	9.475236000	9.700098000	3.939615000
C	9.690604000	7.329442000	4.746629000
C	10.352069000	7.919167000	2.452859000
C	6.370687000	7.864309000	7.812702000
C	5.434219000	8.890940000	7.540805000
C	4.078725000	8.563751000	7.474277000
C	3.603117000	7.274584000	7.630473000
C	4.555342000	6.281259000	7.858983000
C	5.908321000	6.530080000	7.951543000
C	5.829603000	10.356437000	7.378824000
C	4.681605000	11.208698000	6.806105000
C	6.173427000	10.908937000	8.778805000
C	6.991103000	10.546481000	6.395367000
C	2.108199000	6.908210000	7.537913000
C	1.224482000	8.166029000	7.508988000
C	1.697158000	6.057908000	8.746987000

C	1.869026000	6.106889000	6.253633000
C	6.863374000	5.334956000	8.145342000
C	7.825044000	5.548511000	9.337062000
C	7.670763000	5.168422000	6.835030000
C	6.122630000	4.022279000	8.394099000
C	11.150214000	6.749513000	10.326304000
C	10.841205000	6.867066000	11.680005000
C	11.237224000	5.838476000	12.550654000
C	11.932699000	4.717802000	12.113883000
C	12.306905000	4.680577000	10.789108000
C	11.951238000	5.648431000	9.849038000
C	10.168058000	8.120967000	12.241154000
C	9.962670000	8.034761000	13.782868000
C	11.019929000	9.351357000	11.972149000
C	8.753736000	8.297297000	11.662649000
C	12.400980000	3.614761000	13.079985000
C	11.784864000	3.757784000	14.465503000
C	13.914720000	3.622598000	13.175438000
C	11.957846000	2.229592000	12.510158000
C	12.412144000	5.513245000	8.394099000
C	13.346991000	4.302447000	8.185838000
C	11.212098000	5.346711000	7.471385000
C	13.221289000	6.763227000	7.997824000
H	15.100242000	10.125014000	5.300402000
H	12.719567000	8.154548000	2.768722000
H	12.399082000	12.698567000	7.799484000
H	11.422482000	11.683436000	7.039965000

H	12.445788000	12.586049000	6.203766000
H	13.417540000	10.945163000	9.219336000
H	14.030256000	9.619535000	8.564845000
H	12.444963000	9.835735000	8.599353000
H	15.460423000	11.059190000	7.203103000
H	14.782008000	12.388442000	7.780914000
H	14.833943000	12.138348000	6.201105000
H	16.486416000	10.309161000	3.585715000
H	17.320965000	9.167347000	2.836812000
H	16.858877000	8.955791000	4.354316000
H	15.773406000	9.034355000	1.006395000
H	14.910633000	10.223739000	1.640494000
H	14.201641000	8.845761000	1.241008000
H	14.683214000	6.769144000	2.513949000
H	15.618470000	6.809269000	3.811939000
H	16.262957000	6.970435000	2.355988000
H	8.560458000	9.484055000	3.661065000
H	9.854086000	10.365645000	3.328801000
H	9.460865000	10.063573000	4.850384000
H	9.635313000	7.621111000	5.681290000
H	10.233529000	6.515876000	4.690485000
H	8.789644000	7.145785000	4.408493000
H	10.796747000	8.579052000	1.880139000
H	9.432995000	7.783276000	2.140785000
H	10.839860000	7.069238000	2.408921000
H	3.453395000	9.259058000	7.310358000
H	4.255518000	5.385739000	7.954812000

H	3.954135000	11.258854000	7.461550000
H	4.351212000	10.799417000	5.980897000
H	5.010657000	12.112368000	6.615198000
H	6.551972000	11.808728000	8.688876000
H	6.827920000	10.320857000	9.209617000
H	5.360208000	10.948729000	9.322252000
H	7.037432000	9.776273000	5.791205000
H	7.831898000	10.624458000	6.891434000
H	6.844294000	11.362869000	5.871415000
H	1.302799000	8.638612000	8.363728000
H	0.291115000	7.906589000	7.362886000
H	1.517746000	8.754637000	6.782126000
H	0.739228000	5.857872000	8.695616000
H	1.885346000	6.550691000	9.571674000
H	2.205762000	5.219107000	8.743863000
H	0.920994000	5.866688000	6.189737000
H	2.411419000	5.289816000	6.273071000
H	2.122422000	6.648123000	5.477714000
H	7.305375000	5.715201000	10.150468000
H	8.403337000	6.319151000	9.155064000
H	8.376436000	4.748111000	9.458634000
H	8.294689000	4.418198000	6.929847000
H	8.174341000	5.990217000	6.655433000
H	7.056767000	4.992014000	6.093590000
H	5.501542000	4.134914000	9.145201000
H	6.769064000	3.317861000	8.609592000
H	5.621488000	3.772537000	7.591048000

H	11.021938000	5.912181000	13.471662000
H	12.841658000	3.951923000	10.496269000
H	10.835856000	7.982430000	14.226523000
H	9.439067000	7.235243000	13.999113000
H	9.486176000	8.832066000	14.094075000
H	11.805976000	9.338348000	12.556815000
H	10.492770000	10.157772000	12.150531000
H	11.309126000	9.350534000	11.035608000
H	8.170273000	7.586825000	12.001248000
H	8.791114000	8.250902000	10.684167000
H	8.396608000	9.169620000	11.933737000
H	12.054654000	4.614041000	14.855589000
H	12.093923000	3.024487000	15.036805000
H	10.807583000	3.724771000	14.391802000
H	14.299776000	3.559981000	12.276876000
H	14.212442000	2.860030000	13.713390000
H	14.210217000	4.456305000	13.599627000
H	12.304240000	1.514516000	13.081721000
H	12.311194000	2.122384000	11.601328000
H	10.978885000	2.184765000	12.485688000
H	13.626491000	4.262636000	7.247909000
H	12.872178000	3.477890000	8.421058000
H	14.137891000	4.397273000	8.758355000
H	10.659605000	6.155634000	7.504649000
H	10.680532000	4.576131000	7.761129000
H	11.523606000	5.201886000	6.553356000
H	14.012168000	6.835895000	8.571382000

H	12.663333000	7.560610000	8.106091000
H	13.502501000	6.685133000	7.061861000
5Dy (ZOTSAE01)			
Dy	0.000000000	13.193372000	5.017800000
N	1.806078000	14.608770000	5.049914000
N	0.884111000	11.782215000	6.578737000
N	-1.806078000	14.608770000	4.985686000
N	-0.884111000	11.782215000	3.456863000
C	2.831633000	15.010868000	4.205519000
C	3.866997000	15.899566000	4.573022000
C	4.835251000	16.294543000	3.661990000
C	4.822174000	15.832787000	2.352345000
C	3.802297000	14.971307000	1.975408000
C	2.823546000	14.577596000	2.869981000
C	1.895040000	14.946462000	6.424992000
C	0.803581000	15.572634000	7.041378000
C	0.819584000	15.849403000	8.407224000
C	1.914484000	15.526268000	9.178760000
C	3.005427000	14.892501000	8.585054000
C	2.994931000	14.606554000	7.233460000
C	-1.380025000	11.216651000	7.201747000
C	-0.129399000	11.750725000	7.547975000
C	-0.020649000	12.349362000	8.823701000
C	-1.089910000	12.368984000	9.694390000
C	-2.324362000	11.814814000	9.330699000
C	-2.461332000	11.258586000	8.073038000
C	2.171561000	11.352108000	6.912321000

C	3.231875000	11.581720000	6.014134000
C	4.521218000	11.134206000	6.275060000
C	4.806687000	10.430812000	7.439792000
C	3.778723000	10.186799000	8.325333000
C	2.482669000	10.640485000	8.082472000
C	-2.831633000	15.010868000	5.830081000
C	-3.866997000	15.899566000	5.462578000
C	-4.835251000	16.294543000	6.373610000
C	-4.822174000	15.832787000	7.683255000
C	-3.802297000	14.971307000	8.060192000
C	-2.823546000	14.577596000	7.165619000
C	-1.895040000	14.946462000	3.610608000
C	-0.803581000	15.572634000	2.994222000
C	-0.819584000	15.849403000	1.628376000
C	-1.914484000	15.526268000	0.856840000
C	-3.005427000	14.892501000	1.450546000
C	-2.994931000	14.606554000	2.802140000
C	1.380025000	11.216651000	2.833853000
C	0.129399000	11.750725000	2.487625000
C	0.020649000	12.349362000	1.211899000
C	1.089910000	12.368984000	0.341210000
C	2.324362000	11.814814000	0.704901000
C	2.461332000	11.258586000	1.962562000
C	-2.171561000	11.352108000	3.123279000
C	-3.231875000	11.581720000	4.021466000
C	-4.521218000	11.134206000	3.760540000
C	-4.806687000	10.430812000	2.595808000

C	-3.778723000	10.186799000	1.710267000
C	-2.482669000	10.640485000	1.953128000
H	3.900895000	16.232670000	5.461374000
H	5.520102000	16.892547000	3.937969000
H	5.490849000	16.098162000	1.732145000
H	3.775282000	14.645482000	1.083845000
H	2.130264000	13.999847000	2.573128000
H	0.044739000	15.811740000	6.523140000
H	0.067108000	16.265901000	8.811257000
H	1.925497000	15.732618000	10.105849000
H	3.759795000	14.656559000	9.112325000
H	3.744308000	14.172333000	6.842272000
H	-1.490152000	10.814395000	6.348521000
H	0.801860000	12.744972000	9.086232000
H	-0.987699000	12.763961000	10.553437000
H	-3.054296000	11.820827000	9.937251000
H	-3.300360000	10.903012000	7.803683000
H	3.061179000	12.055028000	5.208476000
H	5.215533000	11.311281000	5.650043000
H	5.688733000	10.126034000	7.621035000
H	3.957679000	9.697192000	9.120353000
H	1.799884000	10.464676000	8.718929000
H	-3.900895000	16.232670000	4.574226000
H	-5.520102000	16.892547000	6.097631000
H	-5.490849000	16.098162000	8.303455000
H	-3.775282000	14.645482000	8.951755000
H	-2.130264000	13.999847000	7.462472000

H	-0.044739000	15.811740000	3.512460000
H	-0.067108000	16.265901000	1.224343000
H	-1.925497000	15.732618000	-0.070249000
H	-3.759795000	14.656559000	0.923275000
H	-3.744308000	14.172333000	3.193328000
H	1.490152000	10.814395000	3.687079000
H	-0.801860000	12.744972000	0.949368000
H	0.987699000	12.763961000	-0.517837000
H	3.054296000	11.820827000	0.098349000
H	3.300360000	10.903012000	2.231917000
H	-3.061179000	12.055028000	4.827124000
H	-5.215533000	11.311281000	4.385557000
H	-5.688733000	10.126034000	2.414565000
H	-3.957679000	9.697192000	0.915247000
H	-1.799884000	10.464676000	1.316671000

6Dy (ANOVUW)

Dy	-0.864269000	13.041542000	4.400018000
N	-2.020499000	12.531279000	2.510962000
O	-0.889826000	14.938751000	5.502935000
O	-0.764937000	11.460730000	5.729191000
O	1.136480000	13.768153000	4.083394000
Li	0.940918000	15.319619000	5.175971000
O	2.149054000	16.417619000	6.134912000
C	-1.929915000	15.771099000	5.984716000
C	-1.691316000	17.212224000	5.501395000
C	-1.087522000	17.445187000	4.288277000
C	-0.967768000	18.740032000	3.789550000

C	-1.445620000	19.807331000	4.511644000
C	-2.034140000	19.590620000	5.707432000
C	-2.162992000	18.306611000	6.211935000
C	-1.915472000	15.702474000	7.527110000
C	-0.774304000	16.144925000	8.195287000
C	-0.707407000	16.143119000	9.572080000
C	-1.768270000	15.702474000	10.303802000
C	-2.888980000	15.272665000	9.676062000
C	-2.969274000	15.274471000	8.295418000
C	-3.260452000	15.236547000	5.399339000
C	-3.546160000	13.869466000	5.484065000
C	-4.649526000	13.324078000	4.854398000
C	-5.509765000	14.134936000	4.155411000
C	-5.270414000	15.483958000	4.089941000
C	-4.150227000	16.025734000	4.704203000
C	2.293404000	13.623860000	3.285047000
C	2.628138000	15.028866000	2.743958000
C	1.686087000	15.630238000	1.921733000
C	1.860133000	16.926888000	1.469221000
C	2.977768000	17.636615000	1.821603000
C	3.915179000	17.064138000	2.638051000
C	3.738733000	15.763876000	3.098265000
C	3.444111000	13.020683000	4.116900000
C	3.239122000	12.612545000	5.422446000
C	4.271452000	12.049098000	6.156094000
C	5.509817000	11.882954000	5.611153000
C	5.729749000	12.258585000	4.311384000

C	4.705141000	12.823838000	3.568108000
C	2.017312000	12.607128000	2.156655000
C	2.482474000	12.760631000	0.860736000
C	2.235673000	11.772792000	-0.094354000
C	1.515978000	10.647704000	0.236847000
C	1.058356000	10.481560000	1.505807000
C	1.317348000	11.445921000	2.458971000
C	-0.800465000	10.658540000	6.882039000
C	0.285413000	11.158780000	7.864087000
C	0.421551000	12.518637000	8.091306000
C	1.357972000	13.011654000	8.977075000
C	2.188153000	12.139394000	9.666434000
C	2.061477000	10.797596000	9.468099000
C	1.119040000	10.300968000	8.572702000
C	-2.221170000	10.774119000	7.488598000
C	-2.482851000	11.238240000	8.755633000
C	-3.792361000	11.333954000	9.211996000
C	-4.834334000	10.961934000	8.432134000
C	-4.595319000	10.485172000	7.168951000
C	-3.301788000	10.391264000	6.699108000
C	-0.550302000	9.186715000	6.500773000
C	0.157948000	8.845396000	5.368529000
C	0.367611000	7.510821000	5.037329000
C	-0.083233000	6.512148000	5.842223000
C	-0.765724000	6.824572000	6.974467000
C	-1.002352000	8.141087000	7.299891000
C	-1.841959000	13.495640000	1.503881000

C	-2.075356000	14.835633000	1.773463000
C	-1.770376000	15.823471000	0.851108000
C	-1.256222000	15.492988000	-0.358159000
C	-1.028852000	14.169248000	-0.656624000
C	-1.318900000	13.175992000	0.252252000
C	-3.697628000	11.263523000	1.243928000
C	-2.692813000	11.355625000	2.210571000
C	-2.424502000	10.198030000	2.942293000
C	-3.113764000	9.025988000	2.736256000
C	-4.086803000	8.971811000	1.779240000
C	-4.380873000	10.077034000	1.047518000
C	2.227290000	17.844296000	6.007824000
C	3.261766000	15.957109000	6.891667000
C	4.195702000	17.091227000	7.030309000
C	3.415733000	18.248822000	6.762653000
H	-0.749332000	16.713790000	3.785699000
H	-0.553179000	18.886311000	2.948070000
H	-1.363899000	20.690425000	4.170816000
H	-2.363744000	20.327436000	6.210010000
H	-2.581016000	18.172973000	7.053416000
H	-0.027401000	16.450125000	7.692710000
H	0.077983000	16.448319000	10.011114000
H	-1.721880000	15.697057000	11.253116000
H	-3.628321000	14.967465000	10.190193000
H	-3.764615000	14.974689000	7.871789000
H	-2.968869000	13.304213000	5.984716000
H	-4.813840000	12.388611000	4.906389000

H	-6.266132000	13.762916000	3.718304000
H	-5.874647000	16.051017000	3.622024000
H	-3.993816000	16.961201000	4.644510000
H	0.908528000	15.146251000	1.665631000
H	1.203645000	17.325996000	0.912727000
H	3.100714000	18.521516000	1.500030000
H	4.687927000	17.557154000	2.890302000
H	4.394198000	15.375603000	3.666313000
H	2.382941000	12.717289000	5.821042000
H	4.114659000	11.776404000	7.053416000
H	6.212821000	11.507322000	6.127210000
H	6.587136000	12.133976000	3.918564000
H	4.867257000	13.080279000	2.668860000
H	2.969015000	13.540788000	0.621964000
H	2.568152000	11.877536000	-0.978197000
H	1.339238000	9.986738000	-0.423629000
H	0.562194000	9.705014000	1.736877000
H	1.006853000	11.312283000	3.346666000
H	-0.143526000	13.125427000	7.627240000
H	1.435155000	13.948926000	9.113791000
H	2.838488000	12.475295000	10.272993000
H	2.622095000	10.196224000	9.943718000
H	1.044609000	9.361889000	8.443688000
H	-1.763676000	11.496487000	9.321754000
H	-3.959128000	11.668049000	10.086211000
H	-5.725417000	11.028753000	8.759484000
H	-5.321011000	10.219701000	6.618234000

H	-3.146871000	10.060780000	5.822967000
H	0.506409000	9.529840000	4.808184000
H	0.831852000	7.294111000	4.236286000
H	0.077719000	5.603770000	5.615004000
H	-1.078975000	6.131098000	7.544440000
H	-1.489782000	8.341544000	8.091306000
H	-2.453370000	15.081238000	2.609167000
H	-1.923605000	16.737267000	1.068699000
H	-1.053944000	16.170208000	-0.993602000
H	-0.666987000	13.936285000	-1.503881000
H	-1.161382000	12.267615000	0.025033000
H	-3.913447000	12.023815000	0.714392000
H	-1.742882000	10.219701000	3.602769000
H	-2.912547000	8.256666000	3.256163000
H	-4.557425000	8.160952000	1.625193000
H	-5.066440000	10.035497000	0.392819000
H	1.416259000	18.272299000	6.381387000
H	2.313300000	18.104348000	5.056585000
H	3.704903000	15.204040000	6.425675000
H	2.966385000	15.646491000	7.783212000
H	4.571447000	17.125539000	7.944961000
H	4.940117000	17.011766000	6.381387000
H	3.944872000	18.898953000	6.236968000
H	3.146430000	18.680436000	7.611835000
7Dy (LAJJUE)			
Dy	-8.134438000	7.566128000	14.849607000
N	-8.444458000	5.356593000	14.437406000
N	-7.897398000	8.955329000	13.065295000

N	-9.208587000	8.364587000	16.677009000
Cl	-5.676667000	7.531641000	15.699333000
Li	-3.440445000	7.582253000	16.512583000
Si	-7.646832000	4.230990000	15.467057000
Si	-9.370050000	4.874420000	13.104039000
Si	-6.441215000	8.870710000	12.177581000
Si	-9.068654000	10.141603000	12.699966000
Si	-8.403686000	9.592373000	17.544123000
Si	-10.689492000	7.717964000	17.251179000
O	-2.254624000	7.183103000	15.146141000
O	-3.006237000	9.341707000	17.223208000
O	-3.195376000	6.373627000	17.911153000
C	-5.879569000	3.838226000	14.932576000
C	-7.632053000	4.860050000	17.238327000
C	-8.436453000	2.544980000	15.577052000
C	-8.401303000	3.954778000	11.816032000
C	-10.094995000	6.381610000	12.263952000
C	-10.872993000	3.803101000	13.494316000
C	-5.064359000	9.852619000	12.921658000
C	-5.841495000	7.200666000	12.073066000
C	-6.594440000	9.405571000	10.400451000
C	-10.496034000	10.088915000	13.925227000
C	-8.401970000	11.888284000	12.808261000
C	-9.839147000	9.940432000	10.990119000
C	-7.386231000	10.652515000	16.401075000
C	-9.519946000	10.764277000	18.425223000
C	-7.239010000	8.936170000	18.882593000

C	-12.082041000	8.982472000	17.274237000
C	-10.605309000	6.980335000	18.961971000
C	-11.281670000	6.311360000	16.176170000
C	-1.199286000	7.845692000	14.564034000
C	-0.698315000	7.162348000	13.333670000
C	-1.582022000	6.209177000	13.019936000
C	-2.457518000	6.130944000	14.337238000
C	-3.354125000	10.559912000	16.826316000
C	-2.897608000	11.594509000	17.446223000
C	-2.461680000	11.029313000	18.621778000
C	-2.916554000	9.657833000	18.421443000
C	-3.847079000	6.258672000	19.018670000
C	-3.569542000	4.963829000	19.691496000
C	-2.472114000	4.443338000	19.186877000
C	-2.563663000	5.184160000	17.899814000
H	-5.894086000	3.372019000	14.093434000
H	-5.460412000	3.288996000	15.597842000
H	-5.386203000	4.655686000	14.834298000
H	-6.944472000	5.522639000	17.334715000
H	-7.458216000	4.130404000	17.835555000
H	-8.483060000	5.251217000	17.446223000
H	-9.262508000	2.608844000	16.058992000
H	-7.843881000	1.943062000	16.034423000
H	-8.606565000	2.212888000	14.690661000
H	-7.907429000	4.579049000	11.279283000
H	-9.002470000	3.458236000	11.256603000
H	-7.790529000	3.349667000	12.245052000

H	-10.695765000	6.827062000	12.864959000
H	-10.571293000	6.110188000	11.475839000
H	-9.385685000	6.981932000	12.018257000
H	-10.733500000	2.918585000	13.150343000
H	-11.654381000	4.186285000	13.084195000
H	-11.000700000	3.761590000	14.444966000
H	-5.330957000	10.770664000	13.001037000
H	-4.286169000	9.791948000	12.360340000
H	-4.858084000	9.504560000	13.792930000
H	-5.718337000	6.849414000	12.957568000
H	-5.004967000	7.189490000	11.604356000
H	-6.476520000	6.661015000	11.600576000
H	-7.231298000	8.846761000	9.950641000
H	-5.738041000	9.327337000	9.967650000
H	-6.887593000	10.318826000	10.364542000
H	-10.926625000	9.231541000	13.879868000
H	-11.126418000	10.777050000	13.707882000
H	-10.159172000	10.231013000	14.813508000
H	-8.074626000	12.051137000	13.694652000
H	-9.103921000	12.510958000	12.607925000
H	-7.687695000	11.998449000	12.177014000
H	-9.169553000	10.088915000	10.317293000
H	-10.548432000	10.579072000	10.880501000
H	-10.191198000	9.052722000	10.899401000
H	-6.655568000	10.136813000	16.053322000
H	-7.042252000	11.407707000	16.884905000
H	-7.934021000	10.960659000	15.675330000

H	-10.210399000	11.059648000	17.827995000
H	-9.011554000	11.522662000	18.727616000
H	-9.918771000	10.323616000	19.179317000
H	-7.516533000	8.054847000	19.143407000
H	-7.268295000	9.518929000	19.646137000
H	-6.345023000	8.902642000	18.540510000
H	-11.832772000	9.721697000	17.833665000
H	-12.880408000	8.573742000	17.618209000
H	-12.243272000	9.297002000	16.382175000
H	-9.933612000	6.293797000	18.980871000
H	-11.458467000	6.600344000	19.188766000
H	-10.381653000	7.665277000	19.595108000
H	-11.321273000	6.600344000	15.261429000
H	-12.157971000	6.036745000	16.461554000
H	-10.674297000	5.570537000	16.253658000
H	-0.475064000	7.911153000	15.206620000
H	-1.474983000	8.746175000	14.335349000
H	-0.617498000	7.799391000	12.604145000
H	0.174689000	6.772777000	13.498096000
H	-1.138870000	5.364576000	12.836610000
H	-2.118338000	6.461440000	12.252612000
H	-3.397105000	6.091029000	14.093434000
H	-2.239427000	5.315081000	14.815398000
H	-3.097544000	10.644532000	15.894566000
H	-4.321171000	10.611004000	16.856556000
H	-3.590066000	12.253905000	17.603090000
H	-2.167493000	12.008029000	16.958613000

H	-2.881376000	11.438042000	19.394772000
H	-1.497710000	11.078807000	18.710607000
H	-2.293912000	9.052722000	18.858023000
H	-3.781394000	9.549265000	18.842904000
H	-4.796228000	6.328922000	18.839124000
H	-3.602432000	6.986722000	19.612118000
H	-3.459371000	5.104330000	20.644036000
H	-4.312717000	4.357121000	19.557309000
H	-2.528619000	3.482185000	19.071589000
H	-1.678706000	4.673248000	19.695276000
H	-1.660915000	5.329451000	17.572850000
H	-3.012572000	4.612577000	17.259117000

1Er (LAJKAL)

Er	0.523209000	15.687681000	5.381978000
N	0.692039000	17.073229000	3.618739000
N	0.199382000	13.504221000	4.963806000
N	-0.559476000	16.464161000	7.184950000
Cl	2.956769000	15.676563000	6.211887000
Li	5.142062000	15.779363000	7.055508000
Si	-0.484974000	18.254949000	3.248235000
Si	2.166706000	17.008938000	2.711709000
Si	-0.736085000	13.019707000	3.624742000
Si	1.004586000	12.374868000	5.987896000
Si	-2.026466000	15.809977000	7.785634000
Si	0.235452000	17.721451000	8.046019000
O	6.389429000	15.318534000	5.680425000
O	5.578998000	17.514722000	7.749616000

O	5.416872000	14.504833000	8.475615000
C	-1.928485000	18.147959000	4.451668000
C	0.140112000	20.010611000	3.371111000
C	-1.259372000	18.128624000	1.553300000
C	3.510806000	18.033558000	3.427390000
C	2.027552000	17.550171000	0.937983000
C	2.807378000	15.278252000	2.613221000
C	-1.505724000	14.524168000	2.806445000
C	0.252669000	12.123346000	2.326198000
C	-2.214262000	11.904211000	4.003312000
C	1.060708000	13.011167000	7.770252000
C	2.741719000	11.975107000	5.445930000
C	0.131533000	10.703799000	6.102518000
C	-2.640234000	14.393654000	6.730966000
C	-1.884638000	15.112289000	9.520528000
C	-3.467823000	17.008777000	7.757120000
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C	6.134410000	19.254915000	9.220373000
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C	5.839886000	13.170684000	8.333041000
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