

Supporting Information

Th@C₂(8)-C₈₄ and Th@C₅(15)-C₈₄: impact of actinide metal ions on the electronic structure of actinide endohedral metallofullerenes

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High-performance liquid chromatography (HPLC) isolation of two Th@C₈₄ isomers.

Th@C₈₄ was purified by multiple HPLC processes with UV detection at 310 nm using toluene as the mobile phase.

Th@C₂(8)-C₈₄ was purified by a four-stage HPLC process, as shown in Figure S1. The first stage was performed on a Buckyprep-M column (25 mm × 250 mm, Cosmosil Nacalai Tesque) with a 13 mL/min flow rate. After that, the fraction from 29.2 to 33.1 min was re-injected into a Buckyprep-D column (10 mm × 250 mm, Cosmosil Nacalai Tesque) for the second stage separation with a 4 mL/min flow rate. The fraction from 32.9 to 39.2 min containing Th@C₂(8)-C₈₄ was collected. The third separation stage was conducted on a Buckyprep column (10 mm × 250 mm, Cosmosil Nacalai Tesque) with a 4 mL/min flow rate. The fraction from 77.4 to 82.5 min containing Th@C₂(8)-C₈₄ was collected. The final stage was performed on a Buckyprep column (10 mm × 250 mm, Cosmosil Nacalai Tesque) with a 4 mL/min flow rate under the recycle mode. After five rounds of recycling isolation, the fraction from 371.2 to 382.8 min containing pure Th@C₂(8)-C₈₄ was collected and stored for further characterization.

Th@C₅(15)-C₈₄ was purified by a four-stage HPLC process, as shown in Figure S2. The first stage was performed on a Buckyprep-M column (25 mm × 250 mm, Cosmosil Nacalai Tesque) with a 13 mL/min flow rate. The fraction from 29.2 to 33.2 min was re-injected into a Buckyprep column (10 mm × 250 mm, Cosmosil Nacalai Tesque) for the second stage separation with a 4 mL/min flow rate. The fraction from 82.9 to 94.6 min containing Th@C₅(15)-C₈₄ was collected. The third separation stage was conducted on a 5PBB column (10 mm × 250 mm, Cosmosil Nacalai Tesque) with a 4 mL/min flow rate. The fraction from 106.4 to 116.3 min containing Th@C₅(15)-C₈₄ was collected. The final stage was performed on a Buckyprep column (10 mm × 250 mm, Cosmosil Nacalai Tesque) with a 4 mL/min flow rate under the recycle mode. After three rounds of recycling isolation, the fraction from 243.5 to 253.6 min containing pure Th@C₅(15)-C₈₄ was collected and stored for further characterization.

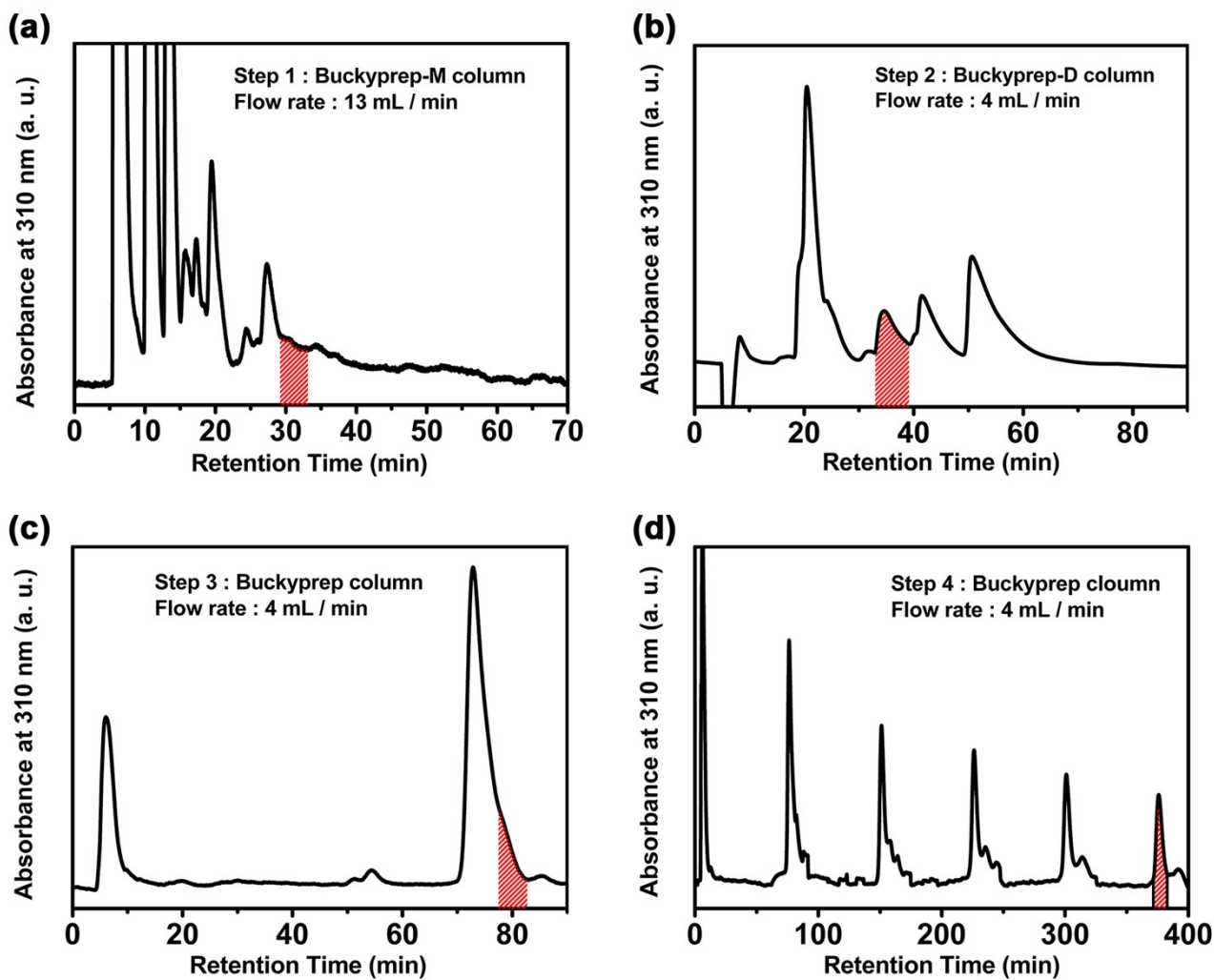


Fig. S1 HPLC isolation procedures of Th@C₂(8)-C₈₄.

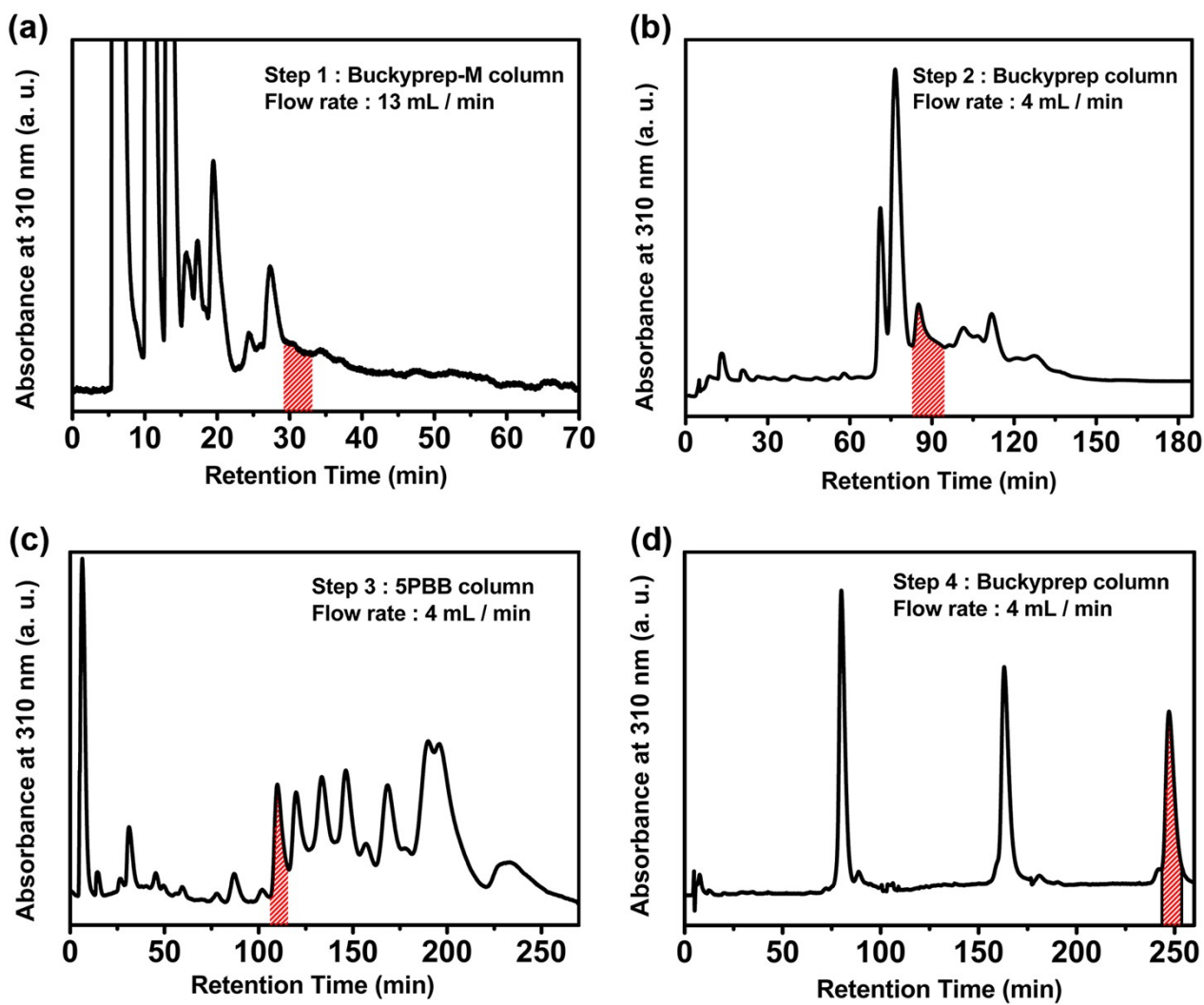


Fig. S2 HPLC isolation procedures of Th@C₅(15)-C₈₄.

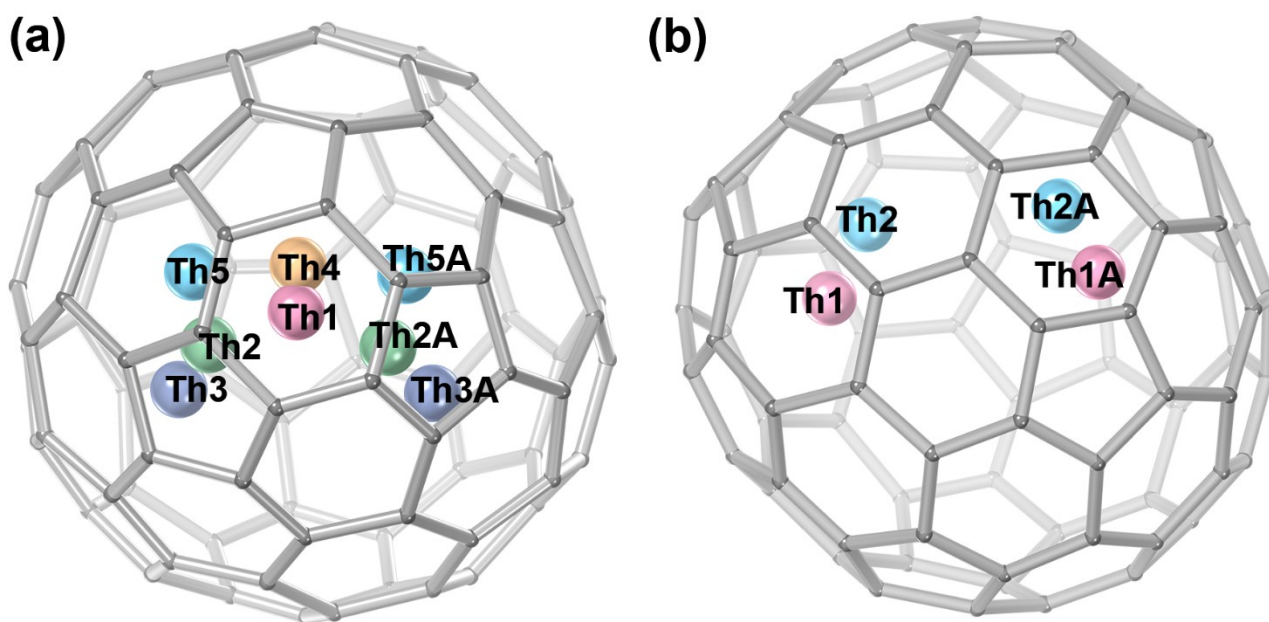


Fig. S3 Ball and stick representation of disordered Th sites inside (a) $\text{Th}@C_2(8)\text{-C}_{84}$ and (b) $\text{Th}@C_5(15)\text{-C}_{84}$, respectively. For clarity, only the major cage orientations are shown for all EMFs. For $\text{Th}@C_2(8)\text{-C}_{84}$, three positions (Th2, Th3, and Th5) and the mirror-related site (Th2A, Th3A, and Th5A) are observed. For $\text{Th}@C_5(15)\text{-C}_{84}$, two positions (Th1 and Th2) and the mirror-related site (Th1A and Th2A) are observed.

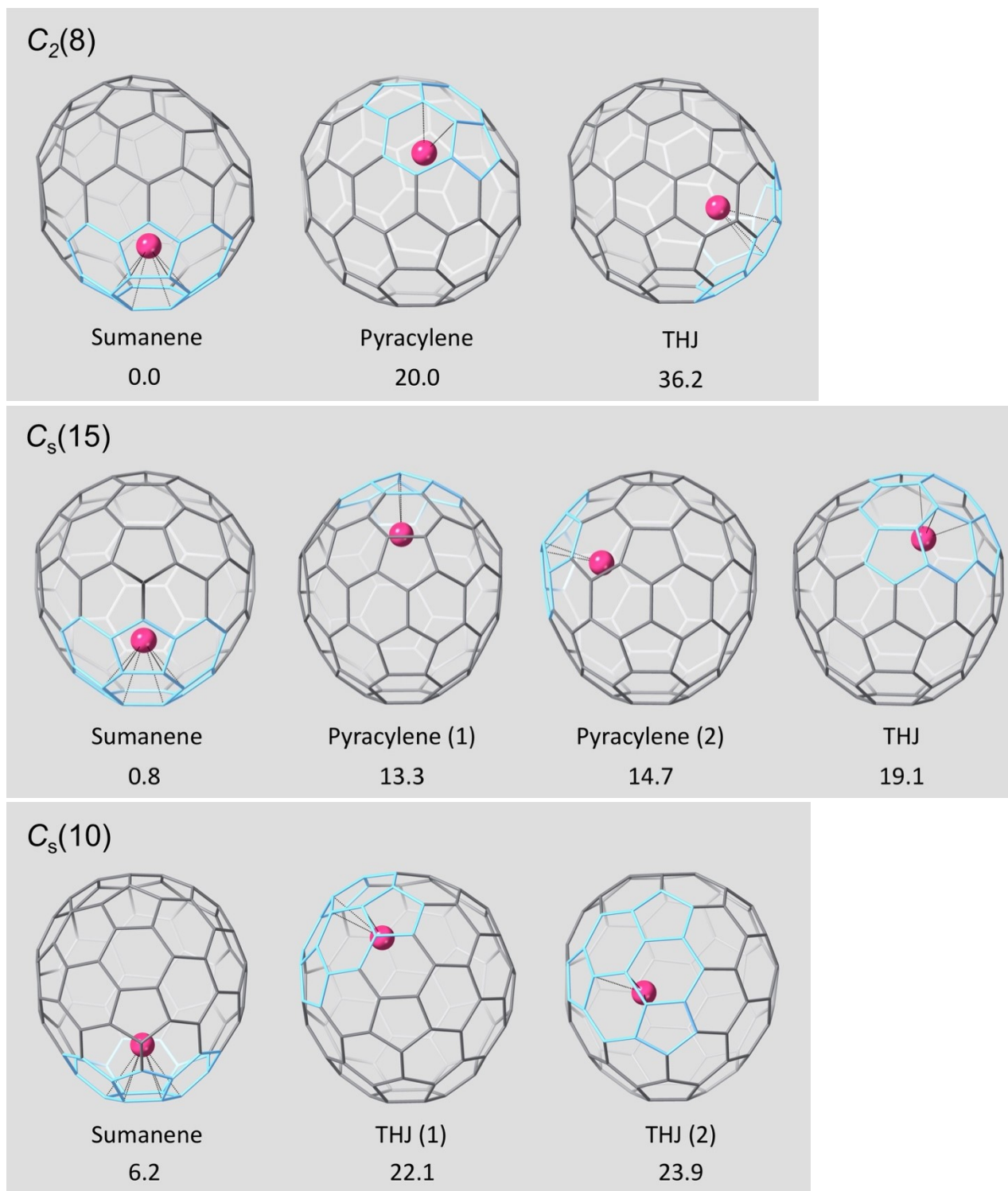


Figure S4. Optimized structures at PBE0/TZP level for different Th positions in Th@ $C_2(8)$ - C_{84} , Th@ $C_s(15)$ - C_{84} and Th@ $C_s(10)$ - C_{84} . Relative energies (in kcal·mol⁻¹) are indicated (see also Table S4).

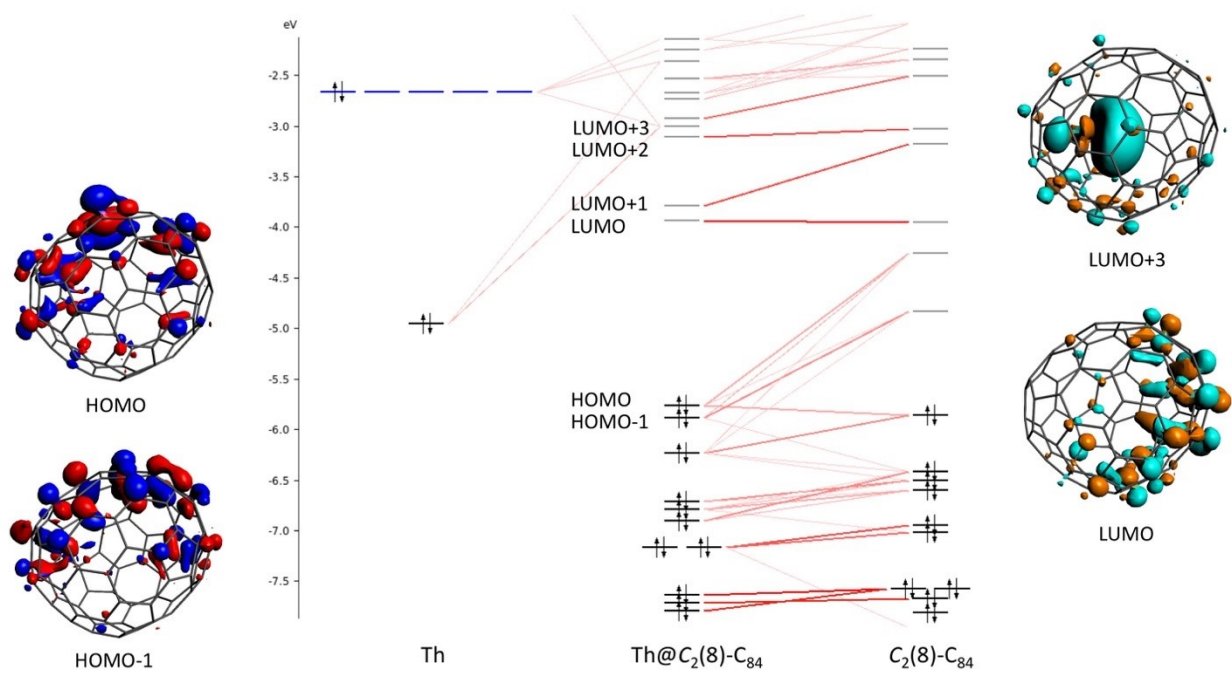


Fig. S5 Molecular orbitals (MO) diagram and MO isosurfaces for some frontier MO of Th@C₂(8)-C₈₄. The occupied MO shows a rather small contribution from Th orbitals, with 7s, 6d, and 5f Th orbitals essentially empty. Therefore, we can consider Th(IV) formally.

Table S1. Occupancies of disordered thorium sites in Th@C₂(8)-C₈₄ and Th@C₅(15)-C₈₄.

Compounds	Fractional occupancy of atom position				
	Th1	Th2/Th2A	Th3/Th3A	Th4	Th5/Th5A
Th@C ₂ (8)-C ₈₄	0.730(3)	0.0616(10)	0.0454(11)	0.037(3)	0.0090(7)
Th@C ₅ (15)-C ₈₄	Th1/Th1A		Th2/Th2A		
	0.3159(10)		0.1841(10)		

Table S2. Closest Th-Cage distances (Å) in Th@C₂(8)-C₈₄ and Th@C₅(15)-C₈₄ from X-ray structures and from optimized structures (PBE0/TZP).

Th@C ₂ (8)-C ₈₄			Th@C ₅ (15)-C ₈₄		
Label	X-ray structures	DFT structures	Label	X-ray structures	DFT structures
Th1-C1	2.465(17) Å	2.460	Th1-C1	2.313(15) Å	2.462
Th1-C2	2.374(16) Å	2.472	Th1-C2	2.275(17) Å	2.462
Th1-C3	2.357(16) Å	2.475	Th1-C3	2.270(18) Å	2.474
Th1-C4	2.393(14) Å	2.480	Th1-C4	2.417(15) Å	2.474
Th1-C5	2.530(15) Å	2.517	Th1-C5	2.424(15) Å	2.534
Th1-C6	2.502(15) Å	2.525	Th1-C6	2.312(15) Å	2.534

Table S3. Relative energies at PBE0/TZP level for different Th positions in Th@C₂(8)-C₈₄, Th@C_s(15)-C₈₄ and Th@C_s(10)-C₈₄.^a See also Figure S4.

IPR isomer	Th position	Relative energy
C ₂ (8)	Sumanene	0.0
	Pyrcylene	20.0
	THJ	36.2
C _s (15)	Sumanene	0.8
	Pyrcylene (1)	13.3
	Pyrcylene (2)	14.7
	THJ	19.1
C _s (10)	Sumanene	6.2
	THJ (1)	22.1
	THJ (2)	23.9

^a Relative energies in kcal·mol⁻¹. THJ stands for Triple Hexagon Junction

Table S4. Crystallographic information of Th@C₂(8)-C₈₄ and Th@C₅(15)-C₈₄.

	Th@C ₂ (8)-C ₈₄	Th@C ₅ (15)-C ₈₄
Formula	C ₁₂₈ H ₅₁ N ₄ Ni Th	C ₁₂₆ H ₅₀ N ₄ Ni Th
Formula weight	1935.47	1910.45
Crystal size, mm ³	0.1×0.08×0.06	0.14×0.1×0.06
Crystal system	Monoclinic	Monoclinic
Space group	C2/m (No. 12)	C2/m (No. 12)
a, Å	27.462(2)	25.3891(17)
b, Å	16.9912(14)	15.1408(11)
c, Å	17.7357(14)	19.9283(14)
α, deg	90	90
β, deg	107.907(4)	94.647(4)
γ, deg	90	90
Volume, Å ³	7874.7(11)	7635.5(9)
Z	4	4
ρ, g cm ⁻³	1.633	1.662
F(000)	3860	3808
θ, deg	2.699 to 54.097	1.935 to 53.946
T, K	122(2)	120(2)
Radiation (λ, mm ⁻¹)	1.34139	1.34139
R ₁ / wR ₂ (all data)	0.1069 / 0.2168	0.1237 / 0.2660
R ₁ / wR ₂ (I > 2.0σ(I))	0.0719 / 0.1922	0.0921 / 0.2444
obs reflects	4838	5073
total reflects	7520	7270
R _{int}	0.0841	0.0799
Goodness-of-fit indicator	1.029	1.057
Parameters	1031	999
density, e Å ⁻³	-0.772 / 0.793	-1.804 / 1.198

Optimized xyz coordinates for the structures in Figure S4:

Th@C ₂ (8)-C ₈₄ Sumanene							
C				C	-0.859133	0.958075	3.736907
C				C	-1.199044	2.167877	2.981073
C	-4.438473	-1.388787	-0.121009	C	-0.148574	3.061210	2.655731
C	-4.385909	-0.632199	-1.352041	C	-0.149181	3.817278	1.446683
C	-3.460520	-1.303216	-2.241925	C	-1.232803	3.764352	0.547209
C	-3.046868	-2.518217	-1.607444	C	-0.929759	3.944060	-0.844302
C	-3.567001	-2.530621	-0.273697	C	0.416461	3.931731	-1.322135
C	-4.406067	-0.694004	1.171967	C	0.457605	3.172726	-2.547913
C	-4.307832	0.753965	1.213631	C	1.595707	2.401932	-2.897646
C	-4.301429	1.517392	-0.015732	C	1.374251	1.129162	-3.585091
C	-4.326410	0.822351	-1.315856	C	2.414295	0.167236	-3.505420
C	-3.341984	1.469578	-2.162610	C	2.119254	-1.236497	-3.475835
C	-2.413348	0.802788	-3.073617	C	2.917250	-1.870769	-2.441694
C	-2.536686	-0.637140	-3.152554	C	2.337531	-2.814707	-1.557525
C	-1.432102	-1.376783	-3.600958	C	2.736474	-2.774567	-0.145032
C	-1.087025	-2.668838	-3.021647	C	1.833457	-3.276113	0.892310
C	-1.848698	-3.211317	-1.967754	C	1.837549	-2.686737	2.231547
C	-1.175318	-3.929574	-0.955727	C	0.660732	-2.786871	3.015836
C	-1.668925	-3.904730	0.409033	C	0.240092	-1.694700	3.871252
C	-2.797227	-3.150724	0.785021	C	1.043839	-0.598150	4.059888
C	-2.787804	-2.466342	2.080624	C	0.492099	0.733594	4.086392
C	-3.505106	-1.212373	2.166175	C	1.541700	1.603393	3.639458
C	-2.909087	-0.103525	2.857191	C	1.229822	2.759072	2.960637
C	-3.318686	1.100846	2.215629	C	2.071802	3.238354	1.898081
C	-2.384732	2.216223	2.143984	C	1.223929	3.912097	0.973989
C	-2.408789	3.002300	0.945283	C	1.511354	3.913192	-0.416560
C	-3.337333	2.583323	-0.105853	C	2.706029	3.280605	-0.840333
C	-2.885573	2.627715	-1.464277	C	2.766239	2.589200	-2.113677
C	-1.711337	3.272900	-1.823674	C	3.737209	1.550173	-1.981547
C	-0.865887	2.728630	-2.836144	C	3.574324	0.360077	-2.667569
C	-1.145026	1.442483	-3.388317	C	3.862096	-0.894358	-2.003681
C	0.000784	0.653665	-3.819176	C	4.282288	-0.898075	-0.677810
C	-0.208577	-0.734635	-3.981317	C	3.712474	-1.834559	0.242532
C	0.850230	-1.675188	-3.740997	C	3.670610	-1.191596	1.546471
C	0.326808	-2.813415	-3.042220	C	2.736191	-1.575647	2.524790
C	1.034481	-3.361132	-1.925931	C	2.345044	-0.556964	3.443092
C	0.252865	-3.965681	-0.919168	C	2.681883	0.813537	3.226902
C	0.668739	-3.950168	0.468186	C	3.502337	1.221858	2.141335
C	-0.519890	-3.987817	1.266033	C	3.208475	2.488648	1.463869
C	-0.530738	-3.383831	2.512330	C	3.570302	2.621211	0.096724
C	-1.677616	-2.609084	2.924630	C	4.222462	1.548371	-0.610882
C	-1.175689	-1.516151	3.739047	C	4.491317	0.347091	0.020875
C	-1.708552	-0.217219	3.618476	C	4.098378	0.165405	1.397896

Th	-2.345222	0.008294	-0.106839	C	-1.921722	2.153689	3.007903
				C	-2.929989	1.167344	2.854339
				C	-0.490004	3.773505	1.779786
Th@C ₂ (8)-C ₈₄ Pyracylene				C	-0.757783	1.579830	3.612775
C	-1.641210	-3.265086	1.892972	C	0.551246	1.990244	3.216584
C	-2.464300	-3.210601	0.748178	C	0.717944	3.147153	2.340053
C	-3.592276	-2.332992	0.813523	C	2.968730	2.337282	1.751932
C	-4.150085	-1.757812	-0.379794	C	1.936751	3.265668	1.544371
C	-3.613713	-2.094728	-1.607684	C	1.827106	3.819876	0.189468
C	-0.420146	-3.830984	-0.613768	C	-2.418095	-0.034320	3.447100
C	-1.857902	-3.534364	-0.538948	C	-2.772259	-1.307344	2.914017
C	-2.504284	-3.018809	-1.696515	C	-3.705584	-1.351216	1.848218
C	0.242525	-3.611904	-1.839009	C	-1.798157	-2.332744	2.970266
C	-0.417476	-2.961400	-2.933015	C	-1.083526	0.221843	3.914373
C	-1.752169	-2.645440	-2.854141	C	-0.088911	-0.789805	3.916628
C	0.414568	-3.835990	0.585574	C	-0.501884	-2.094150	3.555031
C	1.852754	-3.540912	0.512931	C	1.748308	-2.668918	2.834610
C	-0.247791	-3.624976	1.812400	C	0.413154	-2.983502	2.911158
C	2.499877	-3.034823	1.674258	C	2.847501	1.272777	2.718441
C	-4.356394	0.596253	-1.067753	C	1.622289	1.003766	3.367349
C	-3.754906	0.248405	-2.333038	C	1.305247	-0.387350	3.716985
C	-4.548035	-0.394263	-0.098022	C	2.220820	-1.391633	3.326987
C	-3.422803	-1.068345	-2.612498	C	4.357238	0.582037	1.072110
C	-2.222818	-1.363883	-3.337084	C	3.755230	0.225779	2.334802
C	-2.845684	1.296901	-2.709007	C	3.421215	-1.092513	2.604561
C	-1.620854	1.030891	-3.359877	C	4.547470	-0.401584	0.095096
C	-1.305814	-0.358088	-3.719742	C	2.570410	3.164995	-0.856455
C	1.083854	0.249063	-3.912645	C	3.583545	2.160849	-0.651803
C	0.087756	-0.761109	-3.922365	C	3.867428	1.867010	0.695692
C	0.498845	-2.068657	-3.570335	C	2.931665	1.184027	-2.845657
C	-2.565820	3.162265	0.879741	C	1.924834	2.172951	-2.991966
C	-3.580431	2.161191	0.667711	C	1.760743	3.168120	-2.024323
C	-3.864722	1.877729	-0.681919	C	4.251803	-0.128194	-1.276489
C	-2.965437	2.354480	-1.734734	C	3.773782	1.144144	-1.680921
C	-1.932019	3.279686	-1.520290	C	1.794780	-2.313454	-2.987359
C	-1.821488	3.823567	-0.161347	C	3.703626	-1.342953	-1.858128
C	0.597385	4.332247	-0.396090	C	2.770369	-1.289908	-2.923573
C	-0.591065	4.329899	0.427931	C	2.418035	-0.012477	-3.447248
C	0.760075	1.605241	-3.601049	C	3.610644	-2.111732	1.592209
C	-0.548376	2.014683	-3.201875	C	4.147540	-1.766586	0.366830
C	-0.713376	3.165341	-2.316858	C	3.588889	-2.332151	-0.830688
C	0.495478	3.785879	-1.752004	C	2.459627	-3.208564	-0.771776
C	-3.772140	1.137216	1.689322	C	1.636470	-3.253444	-1.916937
C	-4.252013	-0.131408	1.275556	Th	0.002083	2.031604	0.007367
C	-1.756181	3.155682	2.047596				

				C	-1.228868	2.163236	2.982727
Th@C ₂ (8)-C ₈₄ THJ				C	-0.172145	3.043487	2.644410
C	-4.364019	-1.345831	-0.081676	C	-0.169221	3.811795	1.439503
C	-4.297950	-0.584281	-1.313202	C	-1.259800	3.773741	0.545843
C	-3.493533	-1.304088	-2.242560	C	-0.950966	3.955955	-0.839422
C	-3.093988	-2.573139	-1.624451	C	0.398740	3.933658	-1.314392
C	-3.621880	-2.559424	-0.263153	C	0.440496	3.176208	-2.541164
C	-4.323649	-0.678151	1.140174	C	1.576122	2.407611	-2.886619
C	-4.215602	0.766814	1.177943	C	1.351237	1.127228	-3.544516
C	-4.200636	1.496838	-0.001859	C	2.407393	0.157205	-3.488695
C	-4.229244	0.804597	-1.278513	C	2.123597	-1.239908	-3.444670
C	-3.343995	1.505975	-2.166945	C	2.963902	-1.891860	-2.465571
C	-2.439885	0.816237	-3.021746	C	2.341439	-2.844944	-1.586680
C	-2.568006	-0.632938	-3.074933	C	2.753564	-2.767749	-0.157653
C	-1.437591	-1.407356	-3.520769	C	1.829341	-3.231516	0.873076
C	-1.138737	-2.783419	-3.102174	C	1.827970	-2.673607	2.209957
C	-1.969815	-3.324874	-2.035483	C	0.644388	-2.777318	3.007546
C	-1.218278	-3.996536	-0.986137	C	0.218895	-1.691791	3.865610
C	-1.673233	-3.830546	0.372286	C	1.015955	-0.594410	4.037333
C	-2.850063	-3.099174	0.783934	C	0.467770	0.735679	4.084859
C	-2.827935	-2.428762	2.082971	C	1.510145	1.592533	3.638466
C	-3.538716	-1.203915	2.218469	C	1.207110	2.745465	2.954414
C	-2.971473	-0.088357	2.932233	C	2.054025	3.229495	1.899386
C	-3.340294	1.129255	2.250635	C	1.197669	3.900227	0.973948
C	-2.429124	2.214320	2.148637	C	1.496311	3.910459	-0.417680
C	-2.447748	3.020747	0.932942	C	2.696599	3.289766	-0.841096
C	-3.344312	2.636253	-0.111579	C	2.758006	2.593168	-2.104419
C	-2.932943	2.708175	-1.489559	C	3.729665	1.556867	-1.976980
C	-1.749974	3.317800	-1.834156	C	3.568837	0.353701	-2.667025
C	-0.892948	2.749259	-2.839997	C	3.881049	-0.898710	-2.017427
C	-1.155647	1.461717	-3.352965	C	4.318414	-0.891265	-0.685345
C	-0.010105	0.664062	-3.730187	C	3.730527	-1.832399	0.228354
C	-0.221671	-0.752237	-3.841461	C	3.670513	-1.195030	1.534820
C	0.833432	-1.698479	-3.666154	C	2.732258	-1.575421	2.509841
C	0.322781	-2.935953	-3.122001	C	2.336231	-0.560245	3.430294
C	1.104628	-3.508155	-2.001608	C	2.664620	0.798934	3.213967
C	0.250842	-4.059445	-0.962504	C	3.486075	1.210837	2.131026
C	0.644658	-3.895246	0.422113	C	3.187650	2.485353	1.456727
C	-0.535425	-3.886505	1.220007	C	3.563730	2.623204	0.095333
C	-0.544767	-3.341787	2.500563	C	4.220681	1.558626	-0.617339
C	-1.695617	-2.581134	2.930756	C	4.498902	0.343551	0.007740
C	-1.208305	-1.515010	3.741035	C	4.090281	0.163104	1.386555
C	-1.762760	-0.200423	3.652138	Th	-0.284674	-1.638866	-1.124082
C	-0.900053	0.966291	3.745090				

Th@C _s (15)-C ₈₄ Sumanene				C	-1.230093	1.627639	3.475438
C	-4.279714	-1.461403	-0.204436	C	-0.128183	2.477297	3.255103
C	-4.356967	-0.502760	-1.284705	C	-0.113139	3.409146	2.182012
C	-3.463920	-0.952075	-2.320051	C	-1.164952	3.483873	1.233611
C	-2.870996	-2.190457	-1.901436	C	-0.818516	3.864330	-0.138861
C	-3.290912	-2.461503	-0.566580	C	0.538566	4.111570	-0.454831
C	-4.282308	-0.996335	1.168606	C	1.082775	3.714375	-1.724792
C	-4.285418	0.447773	1.459557	C	0.267981	3.255696	-2.730564
C	-4.286187	1.408308	0.373568	C	0.676731	2.146988	-3.569106
C	-4.360335	0.942532	-0.993489	C	1.857703	1.413653	-3.294903
C	-3.469948	1.761567	-1.773292	C	1.860760	-0.018916	-3.583333
C	-2.762032	1.336543	-2.957277	C	2.762826	-0.906791	-2.844219
C	-2.758797	-0.098762	-3.246512	C	2.389567	-2.263081	-2.602480
C	-1.655482	-0.660785	-3.902882	C	2.729788	-2.933235	-1.390694
C	-1.135523	-1.971016	-3.552890	C	3.511260	-2.315213	-0.381403
C	-1.662457	-2.697905	-2.467145	C	3.213993	-2.596228	1.022821
C	-0.802088	-3.512271	-1.625389	C	2.109026	-3.449769	1.325513
C	-1.149072	-3.694830	-0.213060	C	1.253325	-3.205245	2.430133
C	-2.350107	-3.099050	0.347591	C	1.507886	-2.145915	3.343727
C	-2.389604	-2.680928	1.720121	C	0.385417	-1.532270	3.972716
C	-3.333261	-1.612999	2.065648	C	0.382332	-0.124482	4.256295
C	-2.903721	-0.608706	2.987865	C	1.501675	0.689853	3.915296
C	-3.338177	0.672693	2.526181	C	1.241778	2.019237	3.482923
C	-2.399380	1.795136	2.622174	C	2.095467	2.676138	2.559744
C	-2.363058	2.712371	1.518680	C	1.269918	3.582965	1.798988
C	-3.301955	2.474873	0.428041	C	1.586270	3.899095	0.504211
C	-2.881999	2.743832	-0.907265	C	2.716196	3.255027	-0.143835
C	-1.675938	3.435657	-1.231052	C	2.377703	3.104875	-1.520761
C	-1.146916	3.188259	-2.513216	C	2.756382	1.949537	-2.268511
C	-1.661710	2.113728	-3.343756	C	3.654677	1.078101	-1.617789
C	-0.528385	1.511781	-4.004520	C	3.657966	-0.351542	-1.905948
C	-0.525360	0.154972	-4.277841	C	4.057380	-1.046083	-0.729979
C	0.682753	-0.594019	-4.121054	C	4.326189	-0.046394	0.278439
C	0.279617	-1.942511	-3.777703	C	4.052154	-0.312688	1.596577
C	1.097241	-2.751466	-3.027573	C	3.512410	-1.599959	1.990418
C	0.555801	-3.612056	-2.011164	C	2.672007	-1.366551	3.114168
C	1.603331	-3.783023	-1.043740	C	2.668899	0.065153	3.402717
C	1.286799	-3.994597	0.272125	C	3.507268	0.719210	2.457666
C	-0.096727	-3.988765	0.691167	C	3.203856	2.011290	1.951185
C	-0.114924	-3.545229	2.041405	C	3.501099	2.297491	0.547984
C	-1.220239	-2.852028	2.572633	C	4.052205	1.264697	-0.264292
C	-0.950495	-1.921637	3.631117	Th	-2.288686	-0.024727	0.099418
C	-1.762545	-0.764205	3.771917				
C	-0.955559	0.360969	4.091183				

Th@C _s (15)-C ₈₄ Pyracylene (1)							
C	-3.518676	0.289265	-2.366555	C	0.994639	-3.151172	2.264583
C	-4.213205	-0.189767	-1.175849	C	0.782085	-1.022132	3.637165
C	-1.186824	1.027662	-3.892405	C	-0.607227	-1.312503	3.754916
C	-1.584098	-0.295094	-3.836805	C	-1.924343	2.025620	-3.152146
C	-2.759442	-0.670294	-3.100573	C	-3.057020	1.679320	-2.380843
C	0.199162	1.350016	-3.921086	C	-3.273818	2.465314	-1.175550
C	-0.605951	-1.336877	-3.746852	C	-2.202448	3.319752	-0.716970
C	0.782647	-1.046021	-3.630802	C	-1.010310	3.620907	-1.464110
C	1.199397	0.344125	-3.739107	C	-0.946767	3.017992	-2.735093
C	3.284370	-0.213626	-2.550840	C	1.476428	3.009176	-2.633749
C	2.451845	0.766543	-3.128354	C	0.320995	2.639406	-3.290446
C	2.593588	2.086820	-2.602640	C	1.436546	3.758916	1.391405
C	-2.540514	-2.023134	-2.654135	C	0.199381	3.980904	0.715393
C	-3.102882	-2.470659	-1.437445	C	0.199801	3.975654	-0.741120
C	-3.912320	-1.525649	-0.707805	C	1.436824	3.749922	-1.415256
C	-2.406477	-3.457248	-0.709373	C	-2.203887	3.325686	0.695811
C	-1.219554	-2.428975	-3.051762	C	-0.947352	3.035861	2.714638
C	-0.456701	-3.324171	-2.262900	C	-1.010740	3.631623	1.440406
C	-1.120390	-3.926532	-1.155196	C	3.341844	2.359687	1.408627
C	0.995272	-4.222390	0.014030	C	2.632361	3.389292	0.675806
C	-0.383118	-4.287167	0.014074	C	2.632408	3.385022	-0.697219
C	2.900483	-1.610839	-2.518618	C	4.105979	0.080116	1.409960
C	1.612203	-2.023716	-2.934067	C	4.036345	1.318024	0.728475
C	0.995245	-3.165795	-2.244045	C	0.320042	2.660758	3.273111
C	1.695018	-3.754306	-1.155569	C	3.283754	-0.197392	2.552033
C	-2.407581	-3.453101	0.731167	C	2.451019	0.786670	3.123117
C	-3.103836	-2.461684	1.451881	C	2.593092	2.103567	2.589066
C	-3.914554	-1.521171	0.717208	C	1.476004	3.026589	2.614399
C	-2.540594	-2.004599	2.664756	C	2.965614	-3.245316	0.730356
C	-1.220322	-2.408400	3.066753	C	3.564182	-2.201014	1.419338
C	-0.457179	-3.309436	2.284000	C	2.900013	-1.594322	2.529132
C	-1.120618	-3.918902	1.180531	C	1.611487	-2.004358	2.947119
C	-2.759870	-0.648751	3.100902	C	1.198610	0.368207	3.736452
C	-3.524402	0.306489	2.364393	C	0.198030	1.375962	3.912158
C	-4.220649	-0.182470	1.177539	C	4.270066	-1.169853	-0.687463
C	-4.503852	0.632089	-0.002811	C	3.564884	-2.210318	-1.405358
C	-4.009307	2.005031	-0.006982	C	2.965862	-3.250287	-0.709432
C	-1.584682	-0.269741	3.835882	C	4.269539	-1.165082	0.694569
C	-1.187515	1.053154	3.883610	C	3.341639	2.350288	-1.423341
C	-1.925702	2.045945	3.136601	C	4.036387	1.313287	-0.736643
C	-3.062158	1.697256	2.370399	C	4.106077	0.071026	-1.410582
C	-3.278712	2.477463	1.160415	Th	-2.100148	0.514817	0.015624
C	1.694588	-3.746956	1.180091				

Th@C _s (15)-C ₈₄ Pyracylene (2)							
C	-4.167481	-1.432444	-0.174011	C	-1.249551	1.593805	3.451871
C	-4.255928	-0.487285	-1.257537	C	-0.111628	2.420639	3.174851
C	-3.475167	-0.992838	-2.362906	C	-0.084989	3.444343	2.175851
C	-2.907160	-2.239364	-1.952861	C	-1.190904	3.483769	1.210703
C	-3.277498	-2.480865	-0.566445	C	-0.853036	3.852567	-0.140771
C	-4.169989	-0.990423	1.146411	C	0.557191	4.116791	-0.440536
C	-4.164882	0.425332	1.422198	C	1.066886	3.644623	-1.696874
C	-4.161828	1.334020	0.382448	C	0.255694	3.230965	-2.751260
C	-4.245903	0.874692	-0.988116	C	0.665871	2.140710	-3.574957
C	-3.491096	1.778219	-1.813064	C	1.854557	1.395786	-3.307917
C	-2.789407	1.322097	-2.952734	C	1.865994	-0.024757	-3.613684
C	-2.783375	-0.116966	-3.241765	C	2.764652	-0.908428	-2.876032
C	-1.659891	-0.676539	-3.905775	C	2.384681	-2.253901	-2.628832
C	-1.152721	-1.960041	-3.567575	C	2.710792	-2.924708	-1.404832
C	-1.694906	-2.716022	-2.486044	C	3.483972	-2.304998	-0.393135
C	-0.821150	-3.506334	-1.629547	C	3.179716	-2.588565	1.018705
C	-1.157522	-3.675970	-0.220405	C	2.087992	-3.445110	1.313567
C	-2.373602	-3.078914	0.336265	C	1.219723	-3.198610	2.437564
C	-2.417289	-2.660132	1.744107	C	1.486988	-2.150897	3.355677
C	-3.326719	-1.631753	2.105544	C	0.366712	-1.537202	3.977338
C	-2.951880	-0.622369	3.080798	C	0.375702	-0.124429	4.265843
C	-3.333660	0.665594	2.577235	C	1.487646	0.659546	3.913152
C	-2.432518	1.758927	2.630322	C	1.223273	1.981657	3.421560
C	-2.382560	2.692446	1.491526	C	2.117309	2.730593	2.570739
C	-3.283779	2.472587	0.420207	C	1.316490	3.729431	1.881455
C	-2.918152	2.774029	-0.936188	C	1.660569	4.053099	0.515420
C	-1.705647	3.428081	-1.243398	C	2.750921	3.320237	-0.119319
C	-1.158338	3.153963	-2.539857	C	2.349320	3.062582	-1.494660
C	-1.674336	2.107305	-3.365941	C	2.740236	1.906079	-2.266644
C	-0.544202	1.504507	-4.023289	C	3.669118	1.055659	-1.650550
C	-0.524613	0.149438	-4.291890	C	3.669570	-0.346908	-1.932329
C	0.682557	-0.598167	-4.164791	C	4.049912	-1.043522	-0.739013
C	0.276528	-1.931655	-3.797086	C	4.308282	-0.054191	0.270042
C	1.087424	-2.735310	-3.045323	C	4.039259	-0.334092	1.606252
C	0.543986	-3.596210	-2.014951	C	3.510661	-1.601261	1.998270
C	1.582975	-3.767240	-1.061992	C	2.662571	-1.366166	3.136993
C	1.267869	-3.980089	0.268239	C	2.664785	0.033185	3.430060
C	-0.106696	-3.958596	0.681200	C	3.492354	0.701301	2.449840
C	-0.127631	-3.525033	2.054685	C	3.256913	2.019175	1.963077
C	-1.238946	-2.846924	2.591591	C	3.563023	2.311203	0.567324
C	-0.972155	-1.929729	3.653508	C	4.046437	1.247520	-0.255839
C	-1.799151	-0.774542	3.816569	Th	0.934915	1.755752	0.547054
C	-0.971141	0.364242	4.083617				

Th@C _s (15)-C ₈₄ THJ				C	-1.272620	1.620370	3.502145
C	-4.170147	-1.397782	-0.158511	C	-0.162944	2.454526	3.270366
C	-4.256949	-0.444439	-1.248311	C	-0.136616	3.393010	2.169477
C	-3.496113	-0.959461	-2.360107	C	-1.180825	3.462480	1.222359
C	-2.922165	-2.207925	-1.937230	C	-0.836822	3.842868	-0.148376
C	-3.295133	-2.456394	-0.564173	C	0.525364	4.077318	-0.466345
C	-4.181672	-0.961395	1.154920	C	1.079324	3.692675	-1.751179
C	-4.184953	0.453832	1.443679	C	0.264676	3.230697	-2.755319
C	-4.180877	1.369841	0.394833	C	0.674750	2.146137	-3.600282
C	-4.263466	0.911252	-0.972116	C	1.858813	1.411499	-3.324019
C	-3.487171	1.807642	-1.800992	C	1.867034	-0.019509	-3.618850
C	-2.797134	1.341373	-2.950060	C	2.751397	-0.899460	-2.876751
C	-2.798691	-0.097772	-3.240027	C	2.385478	-2.246926	-2.625553
C	-1.679227	-0.658875	-3.914932	C	2.732061	-2.924750	-1.392120
C	-1.157610	-1.933124	-3.556253	C	3.521709	-2.336484	-0.352529
C	-1.706641	-2.685924	-2.474638	C	3.357782	-2.713519	1.076280
C	-0.830278	-3.463667	-1.614110	C	2.161703	-3.525150	1.387236
C	-1.168357	-3.610341	-0.223042	C	1.261344	-3.245094	2.508687
C	-2.381190	-3.050452	0.337615	C	1.498813	-2.195251	3.474320
C	-2.428696	-2.639808	1.750434	C	0.358219	-1.542212	3.990983
C	-3.341589	-1.615018	2.122879	C	0.326399	-0.115595	4.281646
C	-2.976800	-0.625989	3.098950	C	1.434107	0.690183	3.940333
C	-3.350200	0.679628	2.581027	C	1.180735	2.009584	3.509218
C	-2.446377	1.772105	2.641694	C	2.046464	2.669631	2.553284
C	-2.397176	2.698098	1.504075	C	1.234849	3.577941	1.801221
C	-3.293872	2.487157	0.433717	C	1.563122	3.880825	0.487478
C	-2.920817	2.796957	-0.939050	C	2.691481	3.249691	-0.149157
C	-1.708535	3.441455	-1.245301	C	2.369187	3.099497	-1.555904
C	-1.160898	3.158856	-2.531807	C	2.746743	1.947601	-2.289757
C	-1.672758	2.110639	-3.347117	C	3.643554	1.055137	-1.630510
C	-0.540247	1.502875	-4.023183	C	3.645283	-0.337785	-1.913986
C	-0.543521	0.158083	-4.294716	C	4.027146	-1.036891	-0.714302
C	0.673824	-0.600096	-4.154133	C	4.297052	-0.049948	0.284485
C	0.272268	-1.917327	-3.796275	C	4.017110	-0.353363	1.638505
C	1.093794	-2.724810	-3.029247	C	3.624765	-1.667060	2.095958
C	0.550900	-3.572845	-2.004066	C	2.700721	-1.415084	3.236459
C	1.589047	-3.725265	-1.049158	C	2.587814	0.015372	3.402715
C	1.285506	-3.912723	0.300803	C	3.399300	0.663980	2.427551
C	-0.083099	-3.838517	0.691621	C	3.113309	1.989775	1.934329
C	-0.105180	-3.438775	2.047012	C	3.446347	2.284335	0.540955
C	-1.260492	-2.807845	2.600494	C	4.017583	1.237101	-0.252221
C	-1.008672	-1.929430	3.675916	Th	1.500791	-1.165132	1.044660
C	-1.831822	-0.778276	3.848682				
C	-1.004600	0.361694	4.132666				

Th@C _s (10)-C ₈₄ Sumanene							
				C	-0.200462	3.153173	2.690992
C	-4.421840	-1.389062	0.006833	C	-0.197033	3.879652	1.460375
C	-4.418624	-0.654234	-1.237719	C	-1.290805	3.811543	0.563944
C	-3.508274	-1.324494	-2.137096	C	-0.991620	3.943903	-0.821044
C	-3.058667	-2.522089	-1.497542	C	0.354679	3.927192	-1.307390
C	-3.513823	-2.502679	-0.141946	C	0.380327	3.148887	-2.517621
C	-4.389630	-0.678051	1.281576	C	1.502445	2.372264	-2.871010
C	-4.354180	0.790522	1.288558	C	1.271542	1.103928	-3.560803
C	-4.350815	1.520649	0.051887	C	2.304883	0.137515	-3.484513
C	-4.382754	0.805521	-1.230497	C	2.027200	-1.261518	-3.513894
C	-3.413719	1.449028	-2.093715	C	2.857013	-1.943432	-2.532617
C	-2.499449	0.781809	-3.007404	C	2.335028	-3.035383	-1.785742
C	-2.617904	-0.666009	-3.081213	C	2.851240	-3.163474	-0.466658
C	-1.527998	-1.401793	-3.555830	C	2.015852	-3.691523	0.600904
C	-1.174050	-2.709966	-3.011041	C	2.290285	-2.990814	1.812882
C	-1.889971	-3.231180	-1.913063	C	1.254200	-2.587915	2.691377
C	-1.179873	-3.942866	-0.923688	C	1.484827	-1.371996	3.469754
C	-1.539234	-3.787240	0.483398	C	0.362285	-0.684772	3.974470
C	-2.628887	-3.013620	0.894098	C	0.339542	0.751053	4.071722
C	-2.513772	-2.250180	2.126798	C	1.444140	1.530496	3.628166
C	-3.425784	-1.125541	2.265777	C	1.157066	2.766235	2.977432
C	-2.977606	0.031176	2.975736	C	1.996989	3.261679	1.931419
C	-3.414723	1.212821	2.301850	C	1.162783	3.940684	0.988982
C	-2.494875	2.346135	2.203891	C	1.455631	3.912738	-0.406299
C	-2.491656	3.069172	0.979551	C	2.632631	3.254941	-0.832893
C	-3.408452	2.610012	-0.063874	C	2.670486	2.543635	-2.069816
C	-2.965790	2.628645	-1.422240	C	3.607271	1.466406	-1.898855
C	-1.790160	3.262531	-1.797778	C	3.433221	0.298831	-2.591855
C	-0.959735	2.708877	-2.801944	C	3.729724	-0.974938	-1.960791
C	-1.240673	1.421865	-3.345630	C	4.133532	-1.031275	-0.597212
C	-0.098173	0.631729	-3.790742	C	3.724214	-2.197415	0.108787
C	-0.307966	-0.756324	-3.954063	C	3.422004	-2.133993	1.527783
C	0.753180	-1.707184	-3.769369	C	3.595605	-0.963337	2.215646
C	0.233819	-2.879894	-3.106308	C	2.655576	-0.590456	3.237522
C	0.982769	-3.525765	-2.079264	C	2.620959	0.836346	3.263023
C	0.228121	-4.111477	-1.020863	C	3.488677	1.340257	2.205357
C	0.741774	-4.127188	0.328552	C	3.148666	2.528211	1.501530
C	-0.322501	-3.827165	1.245879	C	3.494725	2.570090	0.122859
C	-0.115240	-3.013989	2.383051	C	4.082778	1.451735	-0.529533
C	-1.257819	-2.240015	2.855393	C	4.317791	0.219980	0.141893
C	-0.977800	-1.142977	3.720801	C	4.076999	0.227546	1.543740
C	-1.805375	0.005657	3.717242	Th	-2.368788	0.003127	-0.004931
C	-1.004654	1.188179	3.845727				
C	-1.297656	2.337744	3.059659				

Th@C _s (10)-C ₈₄ THJ (1)							
				C	-0.239723	3.136423	2.688065
C	-4.308753	-1.342409	0.041227	C	-0.236186	3.867762	1.447274
C	-4.305398	-0.601843	-1.213161	C	-1.341215	3.811262	0.548534
C	-3.527861	-1.331705	-2.161272	C	-1.029467	3.951185	-0.829387
C	-3.114018	-2.553175	-1.516331	C	0.327685	3.927290	-1.304838
C	-3.533477	-2.526926	-0.136993	C	0.358614	3.140490	-2.522836
C	-4.279706	-0.664355	1.245412	C	1.459857	2.334736	-2.836202
C	-4.261264	0.781112	1.256849	C	1.249657	1.083894	-3.539237
C	-4.257752	1.487939	0.059534	C	2.304902	0.117132	-3.467933
C	-4.272538	0.779959	-1.200629	C	2.030849	-1.277125	-3.507316
C	-3.403166	1.479356	-2.122705	C	2.855270	-1.962198	-2.551331
C	-2.527423	0.792347	-3.004836	C	2.322800	-3.031702	-1.783686
C	-2.645471	-0.663986	-3.061380	C	2.849493	-3.188802	-0.474208
C	-1.545331	-1.407294	-3.545604	C	2.019360	-3.692983	0.583834
C	-1.210685	-2.695153	-3.009972	C	2.290080	-2.985722	1.786766
C	-1.937158	-3.229248	-1.912267	C	1.232108	-2.578398	2.663144
C	-1.216596	-3.934335	-0.911559	C	1.441892	-1.359134	3.419494
C	-1.556565	-3.780507	0.473400	C	0.340263	-0.693124	3.969680
C	-2.656380	-2.994702	0.885933	C	0.312405	0.753547	4.071273
C	-2.541958	-2.242371	2.134511	C	1.392241	1.541166	3.638388
C	-3.415882	-1.136140	2.306717	C	1.097451	2.764202	2.982869
C	-3.015855	0.023001	3.048096	C	1.969767	3.242576	1.920762
C	-3.418581	1.217599	2.334803	C	1.103110	3.941802	0.984395
C	-2.543720	2.325484	2.219516	C	1.403870	3.924909	-0.401895
C	-2.540216	3.072510	0.954177	C	2.604912	3.232197	-0.774190
C	-3.411596	2.640422	-0.075364	C	2.616084	2.477794	-1.980320
C	-3.002946	2.687401	-1.464134	C	3.586943	1.448128	-1.836268
C	-1.828633	3.301354	-1.824932	C	3.430625	0.278244	-2.581903
C	-0.977272	2.709655	-2.816288	C	3.727267	-0.969995	-1.962184
C	-1.249262	1.428521	-3.354768	C	4.129311	-1.009988	-0.584708
C	-0.110718	0.626770	-3.783544	C	3.721920	-2.196280	0.113695
C	-0.320040	-0.770793	-3.951169	C	3.419172	-2.134972	1.504732
C	0.734097	-1.715310	-3.764628	C	3.574426	-0.916741	2.168580
C	0.214095	-2.875940	-3.108223	C	2.600503	-0.543035	3.135394
C	0.952641	-3.515742	-2.073531	C	2.592968	0.877395	3.214678
C	0.208255	-4.110953	-1.016704	C	3.567505	1.428241	2.280405
C	0.722564	-4.126637	0.318935	C	3.233590	2.658380	1.578791
C	-0.334703	-3.831334	1.231637	C	3.573830	2.677814	0.163927
C	-0.128026	-3.009776	2.375073	C	4.178501	1.497873	-0.521587
C	-1.266726	-2.244456	2.865518	C	4.429837	0.238515	0.152913
C	-0.995781	-1.154940	3.728531	C	4.171689	0.256809	1.580242
C	-1.844521	0.000774	3.764731	Th	1.985530	0.815930	0.485730
C	-1.042894	1.184511	3.856767				
C	-1.348329	2.324365	3.067611				

Th@C _s (10)-C ₈₄ THJ (2)							
C	-4.290470	-1.340874	0.035092	C	-0.239122	3.199604	2.764433
C	-4.306368	-0.609249	-1.215733	C	-0.225005	3.781234	1.450886
C	-3.520806	-1.328136	-2.152524	C	-1.333107	3.771783	0.535958
C	-3.098914	-2.562976	-1.511668	C	-1.012967	3.929675	-0.828896
C	-3.508602	-2.534068	-0.143885	C	0.351767	3.897404	-1.316164
C	-4.254083	-0.661291	1.238496	C	0.379082	3.141252	-2.528929
C	-4.261013	0.792128	1.254704	C	1.503266	2.357425	-2.877968
C	-4.284543	1.494048	0.042520	C	1.268832	1.099412	-3.565567
C	-4.282313	0.788378	-1.198193	C	2.310988	0.124258	-3.490540
C	-3.404907	1.483393	-2.119533	C	2.025674	-1.268582	-3.518512
C	-2.523216	0.799186	-2.995684	C	2.859267	-1.962987	-2.544408
C	-2.637147	-0.658381	-3.051974	C	2.342362	-3.047323	-1.799696
C	-1.534490	-1.390959	-3.539176	C	2.869568	-3.190705	-0.479550
C	-1.184232	-2.685290	-2.996661	C	2.042273	-3.714264	0.581956
C	-1.915606	-3.229848	-1.906436	C	2.324128	-3.010300	1.794077
C	-1.182604	-3.937162	-0.917608	C	1.271158	-2.586766	2.662816
C	-1.522509	-3.783846	0.476316	C	1.505533	-1.377250	3.429146
C	-2.628038	-3.003137	0.880564	C	0.378239	-0.653828	3.948124
C	-2.501452	-2.236638	2.112992	C	0.343559	0.798414	4.211393
C	-3.393635	-1.128373	2.299367	C	1.495224	1.574886	3.775571
C	-2.993581	0.033473	3.009040	C	1.148135	2.808850	3.071259
C	-3.448872	1.234364	2.334671	C	1.949199	3.175704	1.922825
C	-2.531379	2.333536	2.232009	C	1.116786	3.815512	0.968412
C	-2.542207	3.066508	0.943622	C	1.441025	3.861763	-0.425384
C	-3.417493	2.642756	-0.084666	C	2.635598	3.234702	-0.841160
C	-3.002147	2.694713	-1.465589	C	2.680037	2.525286	-2.076580
C	-1.819348	3.298035	-1.825950	C	3.620951	1.454108	-1.907375
C	-0.969002	2.714157	-2.819787	C	3.431071	0.279081	-2.597820
C	-1.244090	1.438018	-3.352245	C	3.739530	-0.992111	-1.971792
C	-0.100445	0.640423	-3.787916	C	4.139269	-1.050619	-0.609297
C	-0.319466	-0.751151	-3.938734	C	3.742544	-2.219321	0.100286
C	0.744675	-1.705815	-3.759591	C	3.449895	-2.163910	1.519425
C	0.227412	-2.876339	-3.106909	C	3.616874	-0.981648	2.217223
C	0.978641	-3.525506	-2.085679	C	2.684232	-0.616808	3.229625
C	0.233445	-4.116845	-1.027926	C	2.596410	0.840814	3.254404
C	0.755365	-4.132050	0.310775	C	3.483281	1.320715	2.195176
C	-0.308927	-3.851061	1.235534	C	3.144810	2.494770	1.483309
C	-0.096908	-3.012631	2.352851	C	3.494064	2.559719	0.115861
C	-1.229121	-2.226254	2.803075	C	4.087937	1.431916	-0.542308
C	-0.932700	-1.091123	3.625567	C	4.318281	0.205398	0.132932
C	-1.793295	0.044125	3.705004	C	4.081651	0.207924	1.542544
C	-1.035604	1.241354	3.968633	Th	0.124029	0.921008	1.792898
C	-1.397893	2.419605	3.158698				