Supporting Information

Theoretical Insights into Monometallofullerene Th@C_{76}: Strong Covalent Interaction between Thorium and the Carbon Cage

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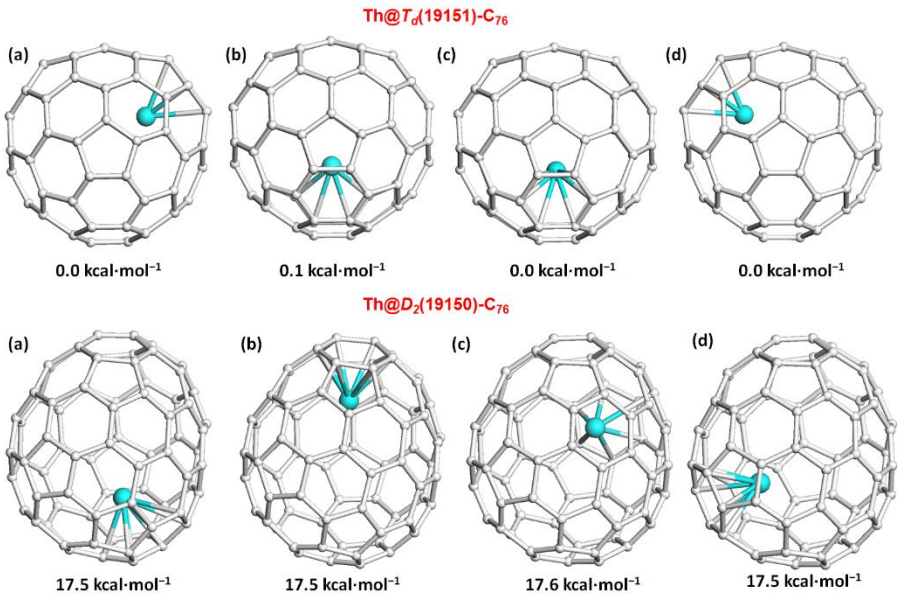
Contents

I. Table S1. Relative energies (in kcal·mol^{-1}) and HOMO–LUMO gaps (in eV) of C_{76}^{4-} at the level of B3LYP/6-31G*.

PA	Spiral No.	Sym.	ΔE	Gap
0	19151	T_d	0.0	1.72
1	19138	C_{2v}	16.5	0.88
1	17459	C_1	26.2	0.93
1	19142	C_s	31.6	1.03
1	17418	C_1	33.3	1.04
1	17894	C_1	33.8	0.83
1	17750	C_1	35.3	1.01
0	19150	D_2	37.6	0.85
1	18542	C_1	40.6	0.99
1	18632	C_1	42.7	0.89
1	17646	C_2	45.3	0.66
1	17410	C_s	47.4	0.88
2	16030	C_1	63.2	0.89
1	18439	C_1	63.5	0.92
1	18720	C_1	65.2	0.94
2	15021	C_s	65.7	1.06
2	13453	C_1	66.2	1.07
2	12118	C_1	76.2	1.01
2	11708	C_s	106.2	0.65

II. Table S2. Relative energies (in kcal·mol^{-1}) and HOMO–LUMO gaps (in eV) of Th@C_{76} isomers at the level of B3LYP/3-21G∼SDD.

PA	Spiral No.	Sym.	ΔE	Gap
0	19151	T_d	0.0	1.41
1	17418	C_1	2.0	1.90
1	17750	C_1	10.5	1.61
1	19138	C_{2v}	12.0	1.14
1	17894	C_1	13.3	1.23
1	17459	C_1	13.9	1.07
1	18542	C_1	16.8	1.43
0	19150	D_2	17.5	1.19
2	12118	C_1	21.6	1.80
1	17646	C_2	22.2	1.18
1	17410	C_s	22.7	1.32
2	15021	C_s	27.3	1.14
1	18632	C_1	27.9	1.03
2	13453	C_1	29.0	1.84
1	18720	C_1	30.5	1.76
1	18439	C_1	31.9	1.36
1	19142	C_s	36.2	1.30
2	16030	C_1	39.8	1.13
2	11708	C_s	54.6	1.29



III. Figure S1. Different positions of Th atom in Th@T_d(19151)-C_{76} and

Th@D_2(19150)-C_{76} at the B3LYP/3-21G~SDD.

For two IPR isomers, different positions of Th atom in starting structures were considered to determine the most stable one. As shown in Figure S1, these structures always possess rather similar relative energies in Th@T_d(19151)-C_{76} and Th@D_2(19150)-C_{76} due to the high symmetry of carbon cages. They also exhibit similar interaction between Th atom and carbon cages, in which the Th atom coordinates with a sumanene-type hexagon. As for non-IPR isomers, the initial position of Th atom was located near the joint pentagons or the triple sequentially fused pentagons.

IV. Table S3. Relative energies (in kcal·mol^{-1}), HOMO–LUMO gaps (in eV) and HOMA-based aromaticity of Th@C_{76} isomers at the B3LYP/6-31G*~SDD level of theory.

PA	Spiral No.	Sym.	ΔE	Gap	HOMA
0	19151	T_d	0.0	1.39	11.2
1	17418	C_1	8.3	1.85	10.3
1	19138	C_{2v}	13.2	1.10	10.9
1	17750	C_1	15.8	1.57	9.6
1	17894	C_1	16.8	1.23	9.7
1	17459	C_1	17.3	1.04	9.8
0	19150	D_2	21.5	1.18	9.6
1	18542	C_1	22.4	1.40	9.0
1	17646	C_2	28.2	1.15	9.5
1	17410	C_s	28.7	1.30	9.9
1	18632	C_1	32.8	1.01	9.3
2	12118	C_1	33.7	1.75	8.5
2	13453	C_1	37.1	1.79	7.9
2	15021	C_s	38.0	1.08	7.6

V. Table S4. Relative energies (in kcal·mol^{-1}) and HOMO–LUMO gaps (in eV) of Th@C_{76} isomers at various levels of theory.

PA	Spiral No.	Sym.	M06-2X/6-31G*~SDD		PBE0/6-31G*~SDD		BP86/ def-SVP~Th-ECP	
			ΔE	Gap	ΔE	Gap	ΔE	Gap
0	19151	T_d	0.0	2.81	0.0	1.62	0.0	0.53
1	17418	C_1	4.4	3.29	6.2	2.09	5.1	0.94
1	19138	C_{2v}	14.2	2.36	13.4	1.28	10.3	0.34
1	17750	C_1	14.0	2.95	14.3	1.79	11.3	0.73
1	17894	C_1	16.3	2.54	15.7	1.43	12.0	0.46
1	17459	C_1	18.0	2.27	16.8	1.22	12.8	0.30
0	19150	D_2	22.0	2.55	21.5	1.38	17.1	0.39
1	18542	C_1	21.0	2.79	20.9	1.62	/	/
1	17646	C_2	26.9	2.49	27.2	1.35	/	/
1	17410	C_s	27.3	2.62	27.3	1.52	/	/

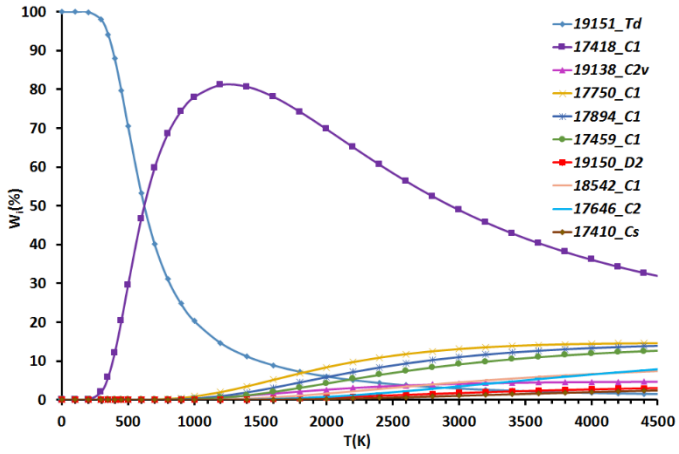
VI. Computational method of statistical thermodynamic analyses.

Rotational-vibrational partition functions were calculated from the computed structural and vibrational data at the B3LYP/6-31G*~SDD level of theory (though only of the rigid rotator and harmonic oscillator (RRHO) quality and with no frequency scaling). Relative concentrations (mole fractions) w_i of i isomers can be expressed through the partition functions q_i and the ground-state energies $\Delta H^{o}_{0,i}$ by a compact formula

$$w_i = \frac{q_i \exp[-\Delta H^{o}_{0,i}/(RT)]}{\sum_{j=1}^{m} q_j \exp[-\Delta H^{o}_{0,j}/(RT)]} \qquad (1)$$

where R is the gas constant and T is the absolute temperature. The conventional heats of formation at room temperature $\Delta H^{o}_{f,298}$ have to be converted to the heats of formation at the absolute zero temperature $\Delta H^{o}_{f,0}$. Chirality contributions, frequently ignored, must be also taken into account in eq. 1 as its partition function q_i is

doubled for an enantiomeric pair. In this way, the equilibrium concentrations can finally be evaluated, where the partial thermodynamic equilibrium is described by a set of equilibrium constants so that both enthalpy and entropy terms are considered accordingly. It is noticed that eq. 1 is an exact relationship derived from the principle of equilibrium statistical thermodynamics, that is, from the standard Gibbs energies of isomers, and it is strongly temperature-dependent. All entropy contributions are evaluated through the isomeric partition functions.



VII. Figure S2. Relative concentrations of Th@C_{76} isomers at the level of M06-2X/6-31G*～SDD.

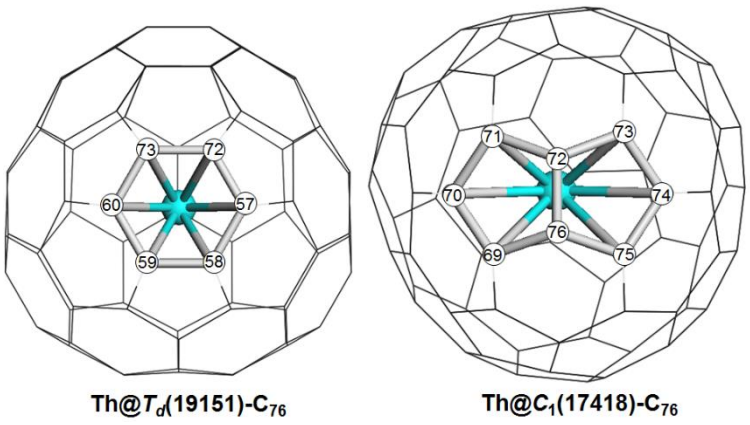
VIII. Table S5. Natural electron configuration populations of Th atoms in Th@T_d(19151)-C_{76} and Th@C_1(17418)-C_{76} at the level of B3LYP/6-311G**~SDD.

Isomer	Atom	Charge	Populations
Th@T_d(19151)-C_{76}	Th	1.711	$7s^{0.08}\ 5f^{0.39}\ 6d^{0.72}\ 7p^{0.32}$
Th@C_1(17418)-C_{76}	Th	1.548	$7s^{0.09}\ 5f^{0.41}\ 6d^{0.61}\ 7p^{0.24}$

IX. Table S6. Bond lengths (*d*), Wiberg bond orders (WBOs) and BCP parameters[a] of Th–C bonds at the B3LYP/6-31G*~SDD level of theory.

Bond	*d* (Å)	WBO	ρ_{BCP}	$\nabla^2\rho_{BCP}$	H_{BCP}	$\lvert V_{BCP}\rvert/G_{BCP}$	G_{BCP}/ρ_{BCP}
Th@T_d(19151)-C_{76}							
Th-C57	2.489	0.642	0.071	0.146	-0.018	1.331	0.774
Th-C58	2.489	0.642	0.071	0.146	-0.018	1.331	0.774
Th-C59	2.489	0.643	0.071	0.146	-0.018	1.332	0.774
Th-C60	2.488	0.644	0.071	0.146	-0.018	1.333	0.774
Th-C72	2.489	0.642	0.071	0.146	-0.018	1.331	0.774
Th-C73	2.488	0.643	0.071	0.146	-0.018	1.332	0.774
Th@C_1(17418)-C_{76}							
Th-C69	2.534	0.570	0.062	0.158	-0.013	1.247	0.842
Th-C70	2.508	0.636	0.069	0.133	-0.018	1.352	0.743
Th-C71	2.520	0.602	0.066	0.155	-0.015	1.280	0.817
Th-C72	2.497	0.621	0.069	0.153	-0.017	1.309	0.798
Th-C73	2.561	0.570	0.061	0.143	-0.013	1.259	0.793
Th-C74	2.624	0.511	0.054	0.135	-0.009	1.209	0.793
Th-C75	2.586	0.549	/	/	/	/	/
Th-C76	2.512	0.616	0.068	0.148	-0.016	1.305	0.786

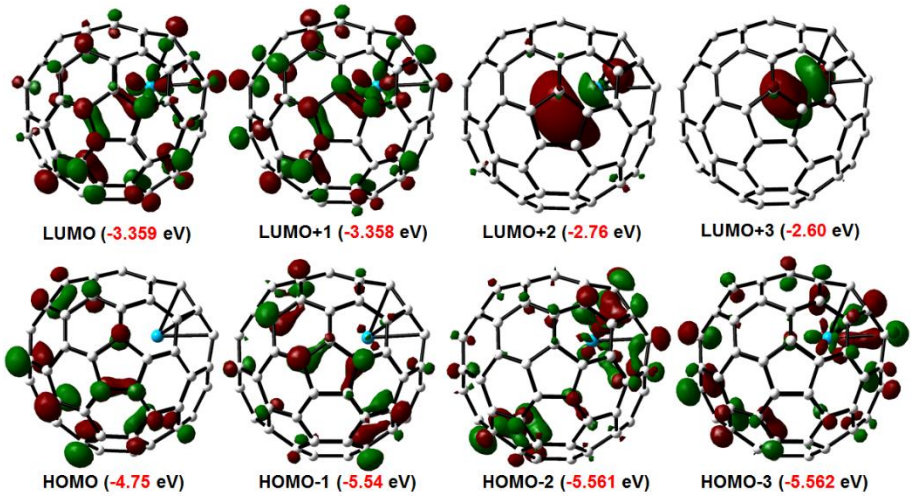
[a]The unit of all BCPs' parameters is a.u.



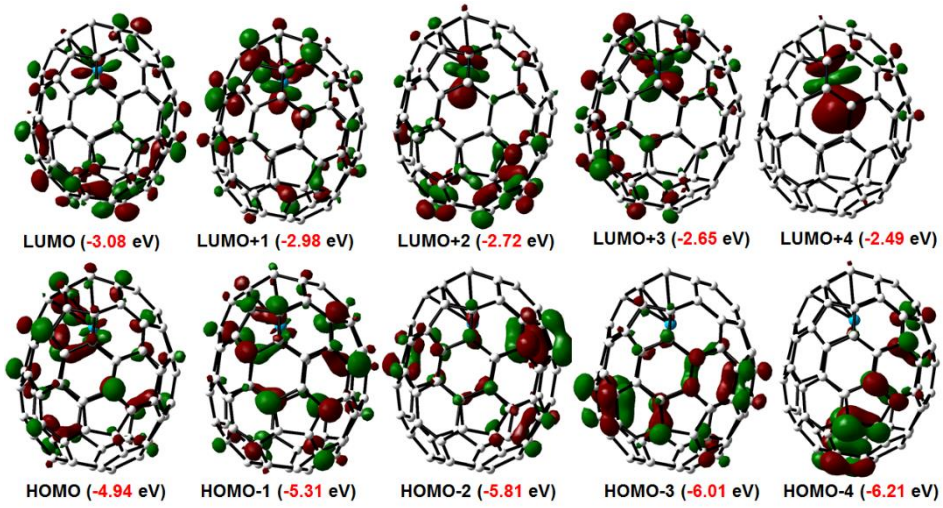
X. Figure S3. Carbon atoms adjacent to thorium atoms in Th@T_d(19151)-C_{76} and Th@C_1(17418)-C_{76} at the B3LYP/6-31G*~SDD level of theory.

XI. Table S7. Vertical/adiabatic electron affinity (VEA/AEA, in eV) and vertical/adiabatic ionization potential (VIP/AIP, in eV) of Th@T_d(19151)-C_{76} and Th@C_1(17418)-C_{76} at the B3LYP/6-31G*~SDD level of theory.

Isomer	VEA	AEA	VIP	AIP
Th@T_d(19151)-C_{76}	2.26	2.32	5.80	5.75
Th@C_1(17418)-C_{76}	1.99	2.06	5.99	5.94



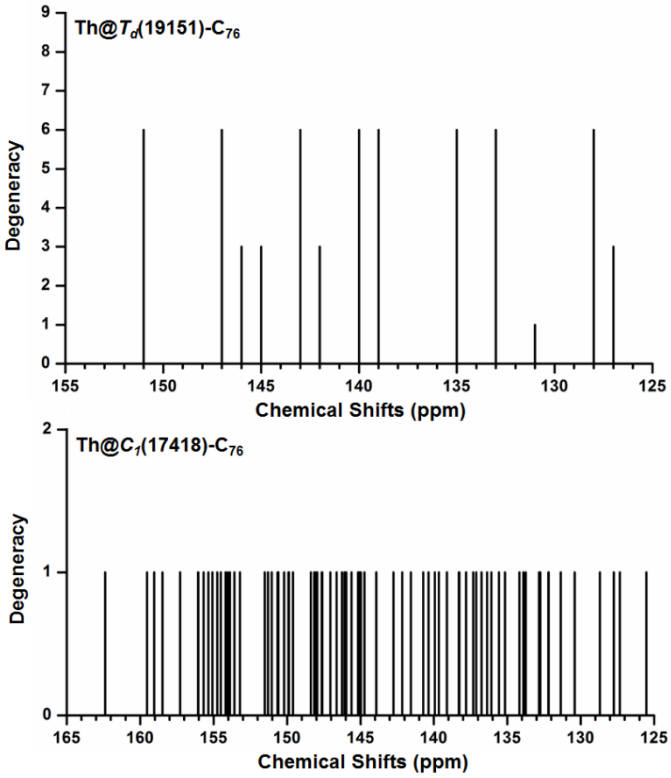
XII. Figure S4. Main molecular orbitals of Th@T_d(19151)-C_{76} at the B3LYP/6-31G*~SDD level of theory (isovalue=0.04).



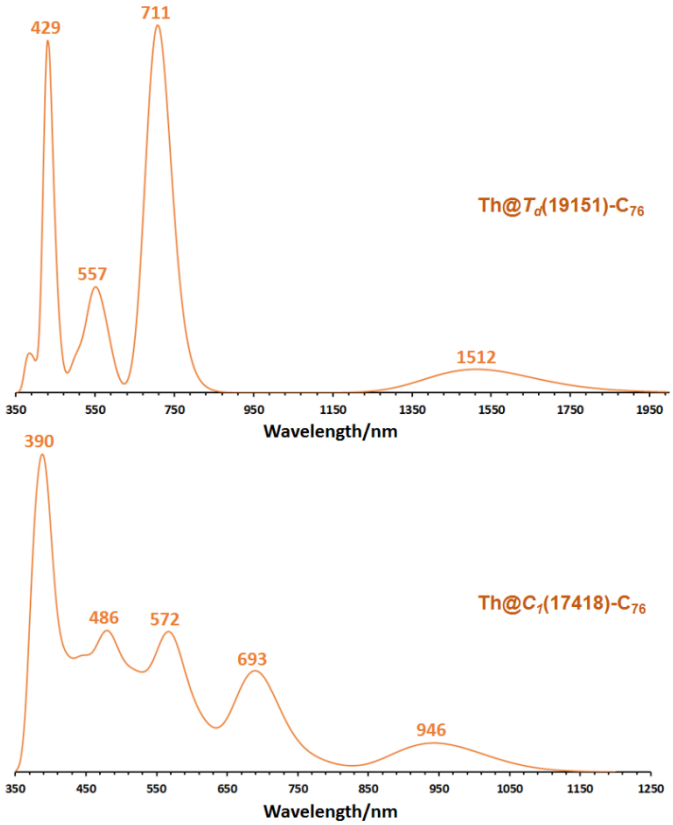
XIII. Figure S5. Main molecular orbitals of Th@C_1(17418)-C_{76} at the B3LYP/6-31G*~SDD level of theory (isovalue=0.04).

XIV. Table S8. Wiberg bond orders (WBOs) and distances (*d*) of M-C in different EMFs at the level of B3LYP/6-31G*~SDD.

Isomer	WBO (*d*, Å)
Th@C_s(10)-C_{84}	0.601 (2.480), 0.623 (2.491), 0.624 (2.491), 0.557 (2.501), 0.601 (2.480), 0.557 (2.501)
Th@C_{3v}(8)-C_{82}	0.641 (2.468), 0.641 (2.468), 0.639 (2.471), 0.709 (2.378)
La@T_d(19151)-C_{76}	0.496 (2.562), 0.495 (2.563), 0.495 (2.564), 0.495 (2.563), 0.496 (2.562), 0.496 (2.562)
Sc_2C_2@D_{3h}(14246)-C_{74}	0.501 (2.274), 0.537 (2.209), 0.517(2.257), 0.508 (2.269), 0.535(2.210), 0.511(2.261)



XV. Figure S6. Simulated ^{13}C NMR spectra of Th@T_d(19151)-C_{76} and Th@C_1(17418)-C_{76} at the B3LYP/6-311G**~SDD level of theory.



XVI. Figure S7. Simulated UV-vis-near-IR absorption spectra of Th@T_d(19151)-C_{76} and Th@C_1(17418)-C_{76} at the B3LYP/6-31G*~SDD level of theory.

XVII. The full references of ref. 13, 14, 15, 16, 17, 23, 25, 30, 31, 32, 36, 37, 38, 43, 47 and 51.

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XVIII. Cartesian coordinates of Th@T_d(19151)-C_{76} and Th@C_1(17418)-C_{76}.

Th@T_d(19151)-C_{76}

C	-0.02128700	-0.02087100	0.06982200
C	1.40748700	-0.01496600	0.03239700
C	2.10654600	1.28525800	0.03286900
C	3.38207600	1.36873300	-0.60136300
C	3.73443500	2.51708300	-1.40125400
C	4.53135000	2.09817600	-2.52920700
C	4.38966100	2.73479100	-3.79837200
C	4.41222400	1.89272500	-5.01048500
C	3.69342600	2.33669400	-6.16337300
C	2.96064800	1.41943400	-6.97688700
C	1.73600200	2.08245900	-7.42928500
C	0.51405000	1.38040400	-7.54114300
C	-0.72238300	2.04469200	-7.13207000
C	-1.79513400	1.19530800	-6.62267100
C	-2.56561800	1.62655100	-5.49218200
C	-2.92918800	0.47515200	-4.71871700
C	-3.02632000	0.58220700	-3.26562400
C	-2.50200200	-0.53411600	-2.48027300
C	-1.98156700	-0.27730400	-1.19136500
C	-0.77769100	-0.95327600	-0.70389600
C	-0.78776000	1.20870200	0.13978700
C	-1.99104300	1.04344600	-0.63009900
C	-2.49575600	2.11762200	-1.38582200

C	-2.99649400	1.88172700	-2.70976800
C	-2.66077200	3.05310700	-3.52125300
C	-2.40731300	2.92700300	-4.90573200
C	-1.47732000	3.80405900	-5.50768600
C	-0.65552500	3.36776300	-6.63832500
C	0.59012800	4.07652300	-6.56430300
C	1.78005300	3.43705500	-6.95824000
C	2.97587200	3.59735400	-6.17565200
C	2.95293600	4.37299100	-5.01833100
C	3.65694700	3.95861800	-3.83788000
C	2.86011300	4.37752900	-2.70989000
C	2.86650900	3.64022900	-1.49355800
C	1.67382400	3.62478400	-0.71870100
C	1.32152100	2.47590400	0.08078100
C	-0.11234300	2.42745900	0.12574000
C	-0.63396300	3.53729100	-0.65449400
C	-1.80855600	3.38103200	-1.38774700
C	-1.88602700	3.94737000	-2.72104800
C	-0.80732100	4.69822700	-3.28275600
C	-0.70240700	4.69899800	-4.70822100
C	0.56969300	4.88991000	-5.37858200
C	1.72381900	5.03357000	-4.61128200
C	1.66108000	5.03087400	-3.17719400
C	0.42378900	4.86573000	-2.48571900
C	0.47477000	4.27790400	-1.18642100
C	3.98280400	0.22660000	-1.23001200
C	4.69083200	0.67567300	-2.41742500
C	4.72745500	-0.13215800	-3.55218700
C	4.56488200	0.48004200	-4.85691900
C	3.83248300	-0.43665900	-5.67111500

C	2.97170700	0.03623200	-6.68702400
C	1.76220200	-0.69920200	-6.92462000
C	0.56399100	-0.07225200	-7.40179500
C	-0.55614900	-0.91702700	-7.04374700
C	-1.79248800	-0.25278500	-6.63547700
C	-2.50361700	-0.70365200	-5.44394200
C	-1.97890900	-1.82003400	-4.65865100
C	-1.92829900	-1.65439000	-3.22079700
C	-0.72893500	-2.27967600	-2.74433300
C	-0.12526100	-1.92901600	-1.49038000
C	1.27793400	-2.05866500	-1.38429300
C	2.03513400	-1.12652100	-0.61099000
C	3.34294400	-1.01127600	-1.22792000
C	3.36925600	-1.83757900	-2.40467600
C	4.05438700	-1.40306500	-3.55429700
C	3.46091800	-1.58896700	-4.84766600
C	2.21208200	-2.23347000	-4.99994900
C	1.39978100	-1.85166700	-6.15147700
C	-0.03306100	-2.03105200	-6.26085100
C	-0.74524400	-2.48277300	-5.06691900
C	0.04158500	-2.71350300	-3.87310500
C	1.50035600	-2.68609700	-3.80556700
C	2.08427200	-2.46277300	-2.53750400
Th	-0.20388200	-0.07810800	-4.72686500

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C	-0.37311600	-1.82408700	3.21390200
C	1.06999900	-1.83958100	3.23091800
C	1.80631300	-0.61103300	3.19165900
C	2.91492700	-0.78595500	2.31211600

C	3.36736000	0.29742800	1.49723700
C	3.86494900	-0.06549800	0.21261200
C	3.66255100	0.80905000	-0.89806100
C	3.23578000	0.05436400	-2.03993200
C	2.17689800	0.54409000	-2.86746300
C	1.33886300	-0.43986900	-3.45768100
C	-0.04757600	-0.17539900	-3.71134900
C	-0.77517200	-1.39020800	-3.50601600
C	-2.07570500	-1.35943300	-2.91660500
C	-2.38572400	-2.37387900	-1.95420400
C	-3.05215700	-2.01175800	-0.73115900
C	-2.53261400	-2.82171500	0.31831900
C	-2.24244800	-2.25509900	1.61304800
C	-1.08756600	-2.76080700	2.34351800
C	-0.96650200	-0.59707100	3.53247900
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C	-2.80082400	-0.92976600	1.89077700
C	-3.51820900	-0.17075400	0.84915900
C	-3.55997400	-0.69895000	-0.50804300
C	-3.52861100	0.18613300	-1.61708100
C	-2.69409300	-0.10536700	-2.76684000
C	-2.01460000	1.11524500	-3.13812700
C	-0.62714400	1.10548100	-3.46053400
C	0.23374800	2.18671500	-2.97258500
C	1.63456700	1.89130300	-2.63881100
C	2.26123600	2.68039900	-1.63427700
C	3.19171700	2.09317800	-0.69725400
C	2.86889800	2.54699800	0.62727600
C	2.80146200	1.63134600	1.71619700
C	1.73781000	1.82729200	2.71253300

C	1.18938200	0.65930500	3.39371300
C	-0.17985300	0.61805800	3.74867400
C	-1.02951600	1.73517800	3.50847500
C	-2.30385200	1.23622600	3.03706100
C	-3.02030800	1.94342000	2.08633300
C	-3.65671100	1.23984900	1.00183800
C	-3.63466900	2.12751200	-0.13871900
C	-3.51707600	1.60336800	-1.42036900
C	-2.58615700	2.18112300	-2.36812700
C	-1.81006300	3.27296500	-2.00461700
C	-0.40066600	3.29270700	-2.32933200
C	0.25588900	4.03440800	-1.28284700
C	1.55205100	3.70914600	-0.92369900
C	1.91965700	3.62189300	0.47914400
C	0.97352800	3.85600400	1.45900000
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C	-0.49908100	2.91679200	2.98621800
C	-1.28278200	3.69331700	2.04136300
C	-2.52835400	3.22559600	1.60646300
C	-2.90006600	3.33056900	0.21381800
C	-2.00598800	3.89422700	-0.70767500
C	-0.71951600	4.37409100	-0.25714900
C	-0.36696600	4.28421700	1.09077300
C	1.81253800	-2.82360800	2.50356700
C	2.93137100	-2.16110700	1.86805600
C	3.34887100	-2.50597600	0.52432600
C	3.74928900	-1.42051400	-0.29140800
C	3.34042300	-1.33498300	-1.68371800
C	2.47889500	-2.31476000	-2.24695800
C	1.47731400	-1.83833600	-3.14137700

C	0.15911300	-2.43242300	-3.16963700
C	-0.17950300	-3.51347400	-2.30501100
C	-1.49400100	-3.46092500	-1.68511900
C	-1.65757700	-3.79570000	-0.28269600
C	-0.63631200	-4.42950500	0.46203000
C	-0.31222000	-3.89618300	1.78507000
C	1.14658100	-3.93201000	1.89945800
C	1.69376100	-4.39947700	0.64085300
C	2.69239100	-3.64301700	-0.10690600
C	2.19597400	-3.51401500	-1.47377900
C	0.88480000	-4.15205400	-1.56100400
C	0.59911200	-4.70926800	-0.24088300
Th	0.57267700	-2.22632500	0.13599400