Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary data to:

Theoretical insights into the effect of conjugated core on hole transport properties of hole-transporting materials for perovskite solar cells

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Table S5 Electron density difference plots of the electronic transition $S_0 \rightarrow S_1$ for all the molecules performed in dichloromethane solvent using the BMK functional together with the 6-31G** basis set.

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Table S1 Calculated molecular orbital energy levels (HOMO and LUMO, eV) and band gap for molecule FDT with different functional in dichloromethane.

Scheme	HOMO	LUMO	Band gap
Exp.[a]	-5.16	-2.28	2.88
BMK/6-31G**	-5.15	-0.57	4.58
PBE0/6-31G**	-4.70	-1.06	3.64
M06/6-31G**	-4.80	-1.04	3.76
HSE06/6-31G**	-4.34	-1.42	2.92
B3LYP/6-31G**	-4.48	-1.17	3.31

[a] Experimental value from Ref [18].

Table S2 Calculated molecular orbital energy levels (HOMO, eV) for molecule FDT, DT1 and DT2 with different functional (BMK, M06 and PBE0) in dichloromethane.

Scheme	FDT	DT1	DT2
BMK/6-31G**	-5.15	-5.22	-5.23
M06/6-31G**	-4.83	-4.91	-4.92
PBE0/6-31G**	-4.73	-4.78	-4.81

Table S3 Calculated wavelength of maximum absorption λ_{max} (nm) and corresponding energy $E_{\lambda max}$ (eV) of molecule FDT in chlorobenzene with B3LYP/6-31+G** method.

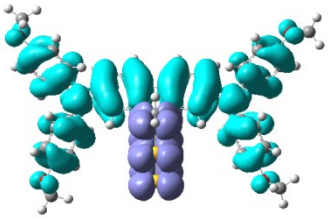
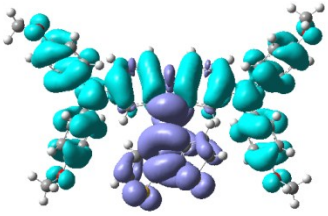
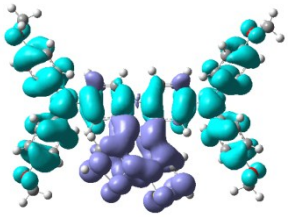
Scheme	λ_{max}(nm)	$E_{\lambda max}$(eV)
Exp.[a]	420.0	2.88
B3LYP/6-31+G**	418.2	2.96
B3LYP/6-31G**	402.6	3.08
B3LYP/6-311G**	410.7	3.02
CAM-B3LYP/6-31G**	343.5	3.61
M06-2X/6-31G**	347.6	3.57
M06/6-31G**	390.8	3.17
BMK/6-31G**	357.6	3.47
PBE0/6-31G**	389.5	3.18

[a] Experimental value from Ref [18].

Table S4 The absorption wavelengths λ_{abs} (nm) and emission wavelengths λ_{em} (nm) of molecules FDT-DT2 based on the S_0 and S_1 states, respectively, along with the Stokes shift at the B3LYP/6-31+G** level in chlorobenzene. (H=HOMO, L=LUMO.)

Compounds	Absorption			Emission	
	λ_{abs}	f	Composition	λ_{em}	Shift
FDT	418($S_0 \rightarrow S_1$)	0.922	H → L+1 (96%)	486	68
	403($S_0 \rightarrow S_2$)	0.322	H → L+1 (94%) H-1 → L+3 (3%)		
DT1	458($S_0 \rightarrow S_1$)	0.630	H-3 → L (98%)	538	124
	414($S_0 \rightarrow S_2$)	0.750	H-4 → L (15%) H→ L+1 (81%)		
DT2	458($S_0 \rightarrow S_1$)	0.117	H → L (39%) H → L+1 (58%)	526	111
	416($S_0 \rightarrow S_2$)	0.747	H → L (39%) H → L+1 (58%)		
	394($S_0 \rightarrow S_3$)	0.100	H-1 → L (32%) H-1 → L+1 (53%) H → L+2 (9%)		

Table S5 Electron density difference plots of the electronic transition $S_0 \rightarrow S_1$ for all the molecules performed in dichloromethane solvent using the BMK functional together with the 6-31G** basis set.

Molecules	Picture	*L* (Ang)	Δ*e*	Ω
FDT		3.56	1.47	0.21
DT1		3.36	1.20	0.28
DT2		3.71	1.10	0.23

L is the electron transfer distance (Å), Δ*e* is the fraction of electron exchange ($|e^-|$), *Ω* is overlap between the regions of density depletion and increment (isovalue: 4×10^{-4} e au^{-3})

Table S6 The calculated first singlet exciton energies (E_1, eV) and the exciton binding energies (E_b, eV) of molecules FDT, DT1 and DT2 at BMK/6-31G** level.

Molecules	E_1	$E_{H\text{-}L}$	E_b
FDT	2.55	2.96	0.41
DT1	2.30	2.99	0.69
DT2	2.36	2.98	0.63

Figure Captions

Fig. S1 The optimized geometries of the investigated molecules at the BMK/6-31G** level.

Fig. S2 The crystal structures of FDT, DT1 and DT2 and centroid-to-centroid distances of the correlated dimers.

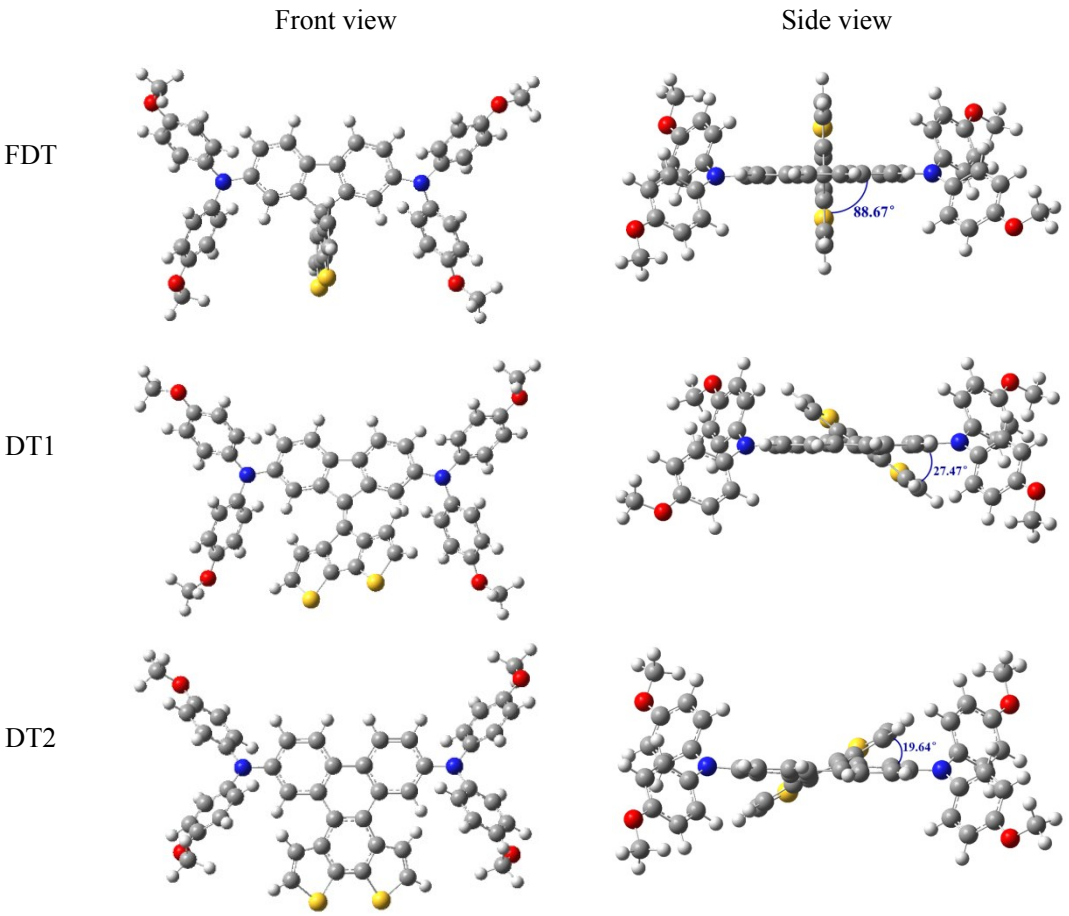


Fig. S1 The optimized geometries of the investigated molecules at the BMK/6-31G** level.

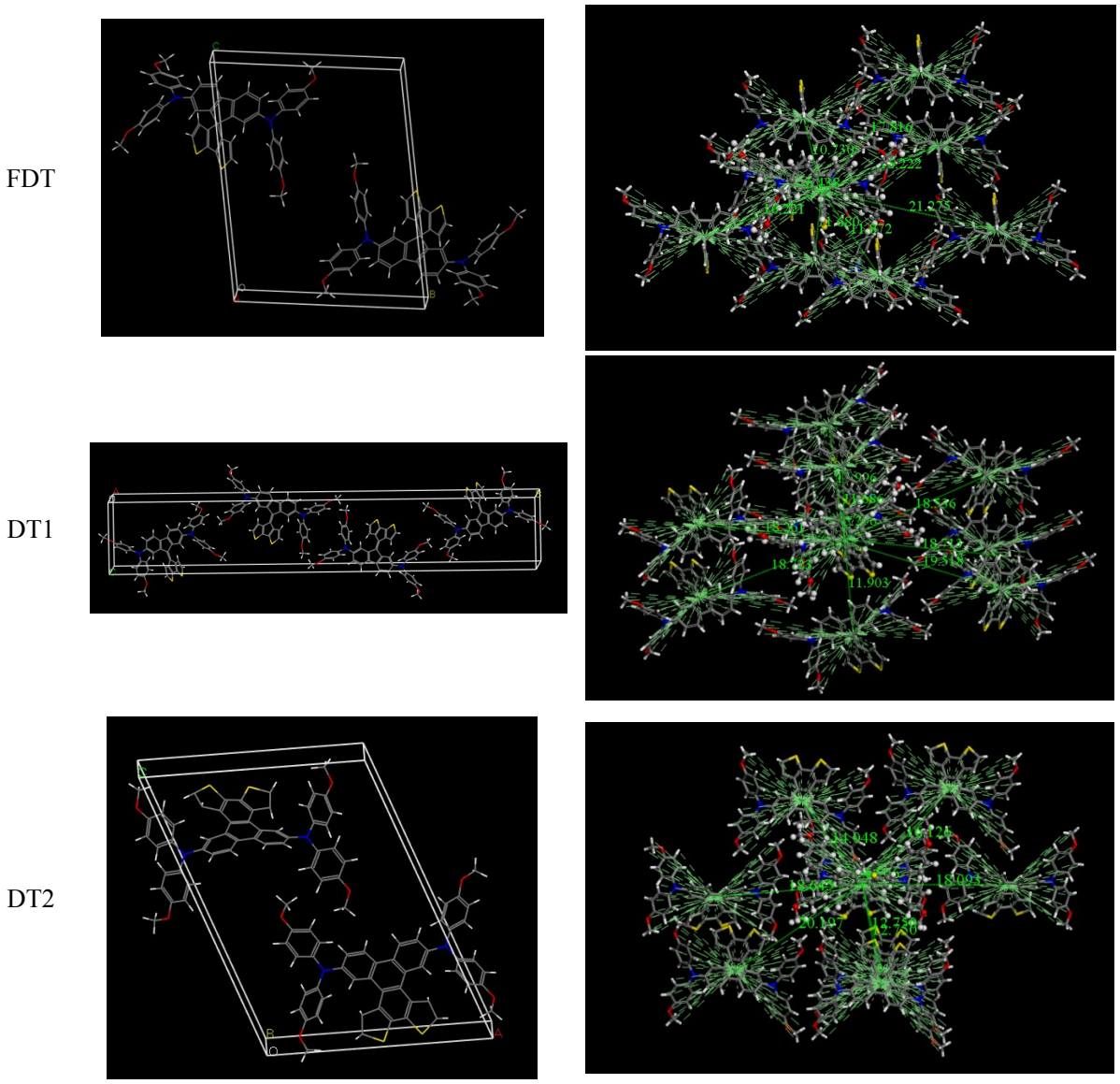


Fig. S2 The crystal structures of FDT, DT1 and DT2 and centroid-to-centroid distances of the correlated dimers.

Crystal structure data of FDT, DT1 and DT2 (in XYZ)

FDT:

S	4.99380000	17.81520000	5.47830000
S	1.65080000	15.91780000	6.85010000
O	4.98490000	10.68650000	8.87000000
O	6.76740000	7.04500000	0.21170000
O	-4.37580000	20.85580000	-2.77900000
O	2.52390000	23.54230000	2.93020000
N	4.73480000	11.26670000	3.27800000
N	-0.01270000	19.24270000	0.38330000
C	2.59900000	15.84620000	3.01670000
C	3.74960000	16.71020000	3.50470000
C	4.86200000	17.36270000	2.92550000
H	5.06630000	17.35350000	1.99810000
C	5.60530000	18.00730000	3.87330000
H	6.38360000	18.51220000	3.66850000
C	3.68600000	16.87340000	4.88210000
C	2.45330000	16.23690000	5.36520000
C	0.42320000	15.00720000	6.01960000
H	-0.31250000	14.59630000	6.45790000
C	0.62680000	14.94360000	4.66600000
H	0.06170000	14.48490000	4.05650000
C	1.79400000	15.65680000	4.30290000
C	3.00950000	14.45650000	2.50670000
C	3.74200000	13.51740000	3.18460000
H	4.08690000	13.71530000	4.04900000
C	3.98440000	12.25240000	2.59580000
C	3.49190000	12.02470000	1.29310000
H	3.66940000	11.19270000	0.86890000
C	2.75110000	12.99030000	0.61050000
H	2.42020000	12.80870000	-0.26220000
C	2.50040000	14.21750000	1.21390000
C	1.75330000	15.42290000	0.78310000
C	1.03220000	15.71710000	-0.38240000
H	0.95900000	15.07520000	-1.07910000
C	0.42320000	16.96770000	-0.50620000
H	-0.08210000	17.16500000	-1.28550000
C	0.54280000	17.94730000	0.50860000
C	1.25240000	17.63330000	1.67640000
H	1.33770000	18.27570000	2.37150000
C	1.82640000	16.38440000	1.80890000
C	4.74680000	11.17080000	4.71090000
C	3.66180000	11.54340000	5.50990000
H	2.87080000	11.87460000	5.10070000
C	3.72730000	11.43310000	6.90500000
H	3.00250000	11.73570000	7.43890000
C	4.84870000	10.88370000	7.51070000
C	5.93560000	10.49480000	6.72190000
H	6.71140000	10.12810000	7.13010000
C	5.88470000	10.64560000	5.32920000
H	6.63120000	10.38760000	4.80020000
C	3.90680000	11.06170000	9.70430000
H	3.72730000	12.01910000	9.59700000
H	4.13650000	10.87530000	10.63760000
H	3.10880000	10.55060000	9.45610000
C	5.30810000	10.17840000	2.52110000
C	4.74240000	8.90250000	2.57770000

H	4.00350000	8.73760000	3.15220000
C	5.25280000	7.88260000	1.80520000
H	4.86200000	7.01780000	1.84410000
C	6.34800000	8.11760000	0.96020000
C	6.94050000	9.37330000	0.92530000
H	7.69590000	9.53350000	0.37160000
C	6.40720000	10.40170000	1.72000000
H	6.81000000	11.26220000	1.70660000
C	7.88930000	7.21650000	-0.66850000
H	7.69140000	7.92350000	-1.31830000
H	8.06370000	6.37680000	-1.14210000
H	8.67970000	7.46500000	-0.14500000
C	-1.12640000	19.56180000	-0.45930000
C	-2.22740000	18.71080000	-0.62970000
H	-2.23500000	17.86050000	-0.20460000
C	-3.31620000	19.10140000	-1.42080000
H	-4.03850000	18.49990000	-1.56030000
C	-3.34490000	20.36450000	-2.00640000
C	-2.25160000	21.21780000	-1.82310000
H	-2.26110000	22.08240000	-2.21530000
C	-1.16710000	20.82110000	-1.08760000
H	-0.42640000	21.40970000	-0.99770000
C	-5.50220000	19.98790000	-3.01080000
H	-5.19800000	19.17160000	-3.46050000
H	-6.15640000	20.44780000	-3.57930000
H	-5.91780000	19.75630000	-2.15460000
C	0.64150000	20.33060000	1.05720000
C	1.96140000	20.66860000	0.78250000
H	2.46090000	20.16350000	0.15350000
C	2.55070000	21.75280000	1.43520000
H	3.45560000	21.97790000	1.25550000
C	1.81560000	22.50430000	2.35020000
C	0.50340000	22.18490000	2.63140000
H	0.00130000	22.70470000	3.24850000
C	-0.07890000	21.07760000	1.98920000
H	-0.97370000	20.83380000	2.19470000
C	1.83280000	24.27370000	3.95420000
H	1.02590000	24.67700000	3.57770000
H	2.42150000	24.97750000	4.30100000
H	1.58970000	23.66340000	4.68050000
S	1.37020000	-2.34390000	11.81500000
S	4.71310000	-0.44650000	10.44310000
O	1.37910000	4.78480000	8.42330000
O	-0.40350000	8.42630000	17.08160000
O	10.73970000	-5.38440000	20.07230000
O	3.84000000	-8.07090000	14.36310000
N	1.62920000	4.20470000	14.01530000
N	6.37660000	-3.77130000	16.91000000
C	3.76490000	-0.37480000	14.27650000
C	2.61430000	-1.23890000	13.78860000
C	1.50190000	-1.89130000	14.36780000
H	1.29760000	-1.88220000	15.29520000
C	0.75860000	-2.53590000	13.42000000
H	-0.01970000	-3.04080000	13.62480000
C	2.67790000	-1.40210000	12.41120000
C	3.91060000	-0.76550000	11.92800000
C	5.94070000	0.46420000	11.27370000
H	6.67640000	0.87500000	10.83540000
C	5.73710000	0.52780000	12.62730000
H	6.30220000	0.98650000	13.23670000

C	4.56990000	-0.18540000	12.99030000
C	3.35440000	1.01490000	14.78650000
C	2.62190000	1.95400000	14.10870000
H	2.27700000	1.75610000	13.24430000
C	2.37950000	3.21900000	14.69740000
C	2.87200000	3.44670000	16.00020000
H	2.69450000	4.27870000	16.42430000
C	3.61280000	2.48110000	16.68280000
H	3.94370000	2.66270000	17.55550000
C	3.86350000	1.25390000	16.07930000
C	4.61070000	0.04850000	16.51020000
C	5.33170000	-0.24580000	17.67570000
H	5.40490000	0.39620000	18.37240000
C	5.94070000	-1.49630000	17.79950000
H	6.44600000	-1.69360000	18.57880000
C	5.82110000	-2.47590000	16.78470000
C	5.11150000	-2.16190000	15.61680000
H	5.02620000	-2.80430000	14.92180000
C	4.53750000	-0.91300000	15.48440000
C	1.61710000	4.30060000	12.58240000
C	2.70210000	3.92790000	11.78340000
H	3.49320000	3.59680000	12.19250000
C	2.63660000	4.03830000	10.38830000
H	3.36140000	3.73570000	9.85440000
C	1.51520000	4.58770000	9.78260000
C	0.42830000	4.97660000	10.57130000
H	-0.34750000	5.34330000	10.16320000
C	0.47920000	4.82580000	11.96410000
H	-0.26730000	5.08380000	12.49300000
C	2.45710000	4.40960000	7.58900000
H	2.63660000	3.45230000	7.69630000
H	2.22740000	4.59610000	6.65570000
H	3.25510000	4.92080000	7.83720000
C	1.05580000	5.29300000	14.77220000
C	1.62150000	6.56890000	14.71560000
H	2.36040000	6.73380000	14.14110000
C	1.11110000	7.58880000	15.48810000
H	1.50190000	8.45360000	15.44920000
C	0.01590000	7.35380000	16.33310000
C	-0.57660000	6.09810000	16.36800000
H	-1.33200000	5.93790000	16.92170000
C	-0.04330000	5.06960000	15.57320000
H	-0.44610000	4.20910000	15.58670000
C	-1.52540000	8.25490000	17.96180000
H	-1.32750000	7.54790000	18.61150000
H	-1.69980000	9.09450000	18.43530000
H	-2.31580000	8.00630000	17.43830000
C	7.49030000	-4.09040000	17.75260000
C	8.59130000	-3.23940000	17.92300000
H	8.59890000	-2.38910000	17.49790000
C	9.68010000	-3.63010000	18.71410000
H	10.40250000	-3.02850000	18.85350000
C	9.70880000	-4.89310000	19.29970000
C	8.61550000	-5.74640000	19.11630000
H	8.62500000	-6.61110000	19.50860000
C	7.53110000	-5.34970000	18.38090000
H	6.79030000	-5.93840000	18.29100000
C	11.86620000	-4.51650000	20.30410000
H	11.56200000	-3.70020000	20.75380000
H	12.52040000	-4.97640000	20.87260000

H	12.28170000	-4.28490000	19.44790000
C	5.72240000	-4.85920000	16.23610000
C	4.40260000	-5.19720000	16.51080000
H	3.90300000	-4.69210000	17.13980000
C	3.81330000	-6.28140000	15.85810000
H	2.90830000	-6.50660000	16.03780000
C	4.54830000	-7.03290000	14.94310000
C	5.86050000	-6.71350000	14.66190000
H	6.36260000	-7.23330000	14.04480000
C	6.44280000	-5.60620000	15.30400000
H	7.33760000	-5.36250000	15.09860000
C	4.53110000	-8.80230000	13.33900000
H	5.33810000	-9.20560000	13.71560000
H	3.94240000	-9.50610000	12.99230000
H	4.77420000	-8.19210000	12.61280000

DT1:

C	0.72910000	47.34840000	10.91980000
C	0.59730000	46.47780000	12.02960000
C	0.33980000	45.11300000	11.84250000
C	0.25250000	44.62450000	10.54210000
C	0.47980000	45.43170000	9.44090000
C	0.66810000	46.80930000	9.61210000
C	-0.18800000	43.31610000	10.08210000
C	-0.50410000	42.17380000	10.81560000
C	-0.81200000	40.99650000	10.11590000
C	-0.75810000	40.96300000	8.69980000
C	-0.43250000	42.14170000	7.99590000
C	-0.22150000	43.32530000	8.70130000
N	-1.00460000	39.73370000	7.97570000
C	-1.64790000	39.78430000	6.68330000
C	-0.53390000	38.47580000	8.50090000
C	-1.09700000	39.10900000	5.58430000
C	-1.61670000	39.30660000	4.30110000
C	-2.70250000	40.18720000	4.09440000
C	-3.29760000	40.79040000	5.20770000
C	-2.77470000	40.59500000	6.48780000
C	-1.34660000	37.33420000	8.44340000
C	0.31860000	36.06430000	9.69290000
C	1.15140000	37.18810000	9.68650000
C	0.73050000	38.38460000	9.10390000
C	-0.93140000	36.13920000	9.03690000
O	-3.22140000	40.50880000	2.82290000
C	-2.45180000	40.14650000	1.67570000
H	-2.93880000	40.55940000	0.77020000
O	0.77750000	34.91980000	10.37530000
C	-0.18440000	33.91800000	10.70040000
H	0.29380000	33.15360000	11.34540000
N	0.83620000	48.78090000	11.11780000
C	0.16390000	49.68940000	10.21740000
C	1.57190000	49.32640000	12.23450000
C	0.79130000	50.87020000	9.79320000
C	0.14240000	51.75150000	8.92550000
C	-1.15410000	51.45560000	8.45150000
C	-1.77110000	50.27620000	8.88300000
C	-1.13710000	49.42130000	9.78260000
C	1.10080000	50.47020000	12.89950000
C	1.84460000	51.05270000	13.92180000
C	3.05650000	50.49230000	14.33230000

C	3.52500000	49.33140000	13.67840000
C	2.79190000	48.76240000	12.63420000
O	-1.87530000	52.28280000	7.56650000
C	-1.27930000	53.51060000	7.15100000
H	-1.98880000	54.04050000	6.48770000
O	3.74070000	51.14120000	15.37750000
C	4.92400000	50.53510000	15.88920000
H	5.30360000	51.16260000	16.71370000
H	0.63230000	46.86780000	13.03870000
H	0.17440000	44.46200000	12.68880000
H	0.69360000	47.46960000	8.76020000
H	-0.49450000	42.18520000	11.89730000
H	-1.06090000	40.10450000	10.67590000
H	-0.31130000	42.11530000	6.92620000
H	-0.22890000	38.47440000	5.71170000
H	-1.14730000	38.78890000	3.48030000
H	-4.14570000	41.45070000	5.07540000
H	-3.21740000	41.11060000	7.32640000
H	-2.32160000	37.38200000	7.97430000
H	2.12170000	37.14390000	10.16450000
H	1.38640000	39.24450000	9.13110000
H	-1.60210000	35.29280000	8.99170000
H	-1.42730000	40.57150000	1.74190000
H	-2.41060000	39.04410000	1.56440000
H	-1.03460000	34.36290000	11.25910000
H	-0.55070000	33.41810000	9.78180000
H	1.79520000	51.09910000	10.12210000
H	0.67170000	52.64210000	8.62110000
H	-2.76330000	50.02310000	8.54400000
H	-1.66470000	48.55560000	10.15440000
H	0.15560000	50.91730000	12.62060000
H	1.47170000	51.94480000	14.40780000
H	4.45930000	48.86940000	13.94840000
H	3.18330000	47.89320000	12.12470000
H	-1.06970000	54.15740000	8.02740000
H	-0.34730000	53.32600000	6.57740000
H	4.70930000	49.52390000	16.28510000
H	5.71170000	50.48230000	15.11590000
C	0.19380000	44.65230000	8.21200000
C	0.25610000	45.06950000	6.93300000
C	-0.50390000	44.60240000	5.75130000
C	1.06820000	46.15480000	6.36330000
C	0.80810000	46.31880000	5.04640000
C	-0.16790000	45.32620000	4.65390000
C	2.21120000	46.78790000	6.74480000
S	1.85900000	47.34060000	4.19220000
C	-1.66080000	43.89720000	5.55870000
C	-2.08780000	44.04270000	4.24450000
S	-1.15520000	45.13720000	3.28600000
C	2.71580000	47.52100000	5.68200000
H	2.69570000	46.66600000	7.69970000
H	-2.21960000	43.38450000	6.32750000
H	-2.98950000	43.57490000	3.87360000
H	3.62750000	48.09000000	5.76470000
C	4.06450000	11.69560000	5.68930000
C	4.19630000	10.82490000	4.57960000
C	4.45390000	9.46010000	4.76670000
C	4.54110000	8.97170000	6.06710000
C	4.31380000	9.77890000	7.16830000
C	4.12550000	11.15650000	6.99700000

C	4.98160000	7.66320000	6.52700000
C	5.29770000	6.52090000	5.79350000
C	5.60570000	5.34360000	6.49330000
C	5.55170000	5.31010000	7.90940000
C	5.22620000	6.48880000	8.61320000
C	5.01510000	7.67250000	7.90780000
N	5.79830000	4.08080000	8.63340000
C	6.44150000	4.13150000	9.92580000
C	5.32750000	2.82300000	8.10820000
C	5.89060000	3.45620000	11.02490000
C	6.41040000	3.65370000	12.30810000
C	7.49610000	4.53430000	12.51470000
C	8.09130000	5.13760000	11.40150000
C	7.56830000	4.94220000	10.12130000
C	6.14020000	1.68140000	8.16580000
C	4.47500000	0.41140000	6.91630000
C	3.64220000	1.53520000	6.92260000
C	4.06310000	2.73170000	7.50520000
C	5.72510000	0.48630000	7.57220000
O	8.01500000	4.85590000	13.78620000
C	7.24550000	4.49370000	14.93340000
H	7.73240000	4.90650000	15.83900000
O	4.01610000	-0.73300000	6.23390000
C	4.97800000	-1.73490000	5.90880000
H	4.49990000	-2.49930000	5.26370000
N	3.95740000	13.12810000	5.49140000
C	4.62970000	14.03650000	6.39170000
C	3.22170000	13.67360000	4.37460000
C	4.00230000	15.21730000	6.81600000
C	4.65130000	16.09870000	7.68360000
C	5.94770000	15.80280000	8.15760000
C	6.56480000	14.62340000	7.72620000
C	5.93070000	13.76840000	6.82660000
C	3.69290000	14.81730000	3.70960000
C	2.94900000	15.39990000	2.68740000
C	1.73720000	14.83940000	2.27690000
C	1.26860000	13.67860000	2.93070000
C	2.00170000	13.10960000	3.97490000
O	6.66890000	16.62990000	9.04270000
C	6.07290000	17.85780000	9.45810000
H	6.78240000	18.38760000	10.12150000
O	1.05300000	15.48830000	1.23160000
C	-0.13030000	14.88220000	0.72000000
H	-0.50990000	15.50970000	-0.10460000
H	4.16130000	11.21500000	3.57050000
H	4.61920000	8.80910000	3.92030000
H	4.10000000	11.81680000	7.84890000
H	5.28810000	6.53230000	4.71190000
H	5.85450000	4.45160000	5.93330000
H	5.10490000	6.46240000	9.68290000
H	5.02250000	2.82160000	10.89740000
H	5.94090000	3.13600000	13.12880000
H	8.93930000	5.79790000	11.53370000
H	8.01100000	5.45770000	9.28280000
H	7.11520000	1.72920000	8.63490000
H	2.67200000	1.49100000	6.44470000
H	3.40730000	3.59170000	7.47810000
H	6.39570000	-0.36010000	7.61740000
H	6.22100000	4.91870000	14.86720000
H	7.20420000	3.39130000	15.04470000

H	5.82820000	-1.28990000	5.35010000
H	5.34430000	-2.23470000	6.82730000
H	2.99850000	15.44620000	6.48710000
H	4.12190000	16.98930000	7.98810000
H	7.55700000	14.37020000	8.06510000
H	6.45840000	12.90280000	6.45470000
H	4.63800000	15.26440000	3.98850000
H	3.32190000	16.29190000	2.20130000
H	0.33430000	13.21650000	2.66080000
H	1.61040000	12.24030000	4.48440000
H	5.86340000	18.50450000	8.58170000
H	5.14090000	17.67310000	10.03180000
H	0.08430000	13.87110000	0.32400000
H	-0.91810000	14.82940000	1.49320000
C	4.59980000	8.99950000	8.39710000
C	4.53750000	9.41660000	9.67610000
C	5.29750000	8.94960000	10.85790000
C	3.72540000	10.50190000	10.24590000
C	3.98550000	10.66590000	11.56280000
C	4.96150000	9.67330000	11.95520000
C	2.58240000	11.13510000	9.86440000
S	2.93460000	11.68770000	12.41690000
C	6.45440000	8.24440000	11.05040000
C	6.88140000	8.38980000	12.36470000
S	5.94880000	9.48440000	13.32320000
C	2.07780000	11.86810000	10.92720000
H	2.09790000	11.01320000	8.90950000
H	7.01330000	7.73170000	10.28170000
H	7.78310000	7.92210000	12.73560000
H	1.16610000	12.43710000	10.84440000
C	4.06450000	23.95730000	-0.26240000
C	4.19630000	24.82790000	-1.37210000
C	4.45390000	26.19270000	-1.18500000
C	4.54110000	26.68120000	0.11540000
C	4.31380000	25.87400000	1.21660000
C	4.12550000	24.49640000	1.04530000
C	4.98160000	27.98960000	0.57530000
C	5.29770000	29.13190000	-0.15820000
C	5.60570000	30.30920000	0.54160000
C	5.55170000	30.34270000	1.95770000
C	5.22620000	29.16400000	2.66150000
C	5.01510000	27.98040000	1.95610000
N	5.79830000	31.57200000	2.68170000
C	6.44150000	31.52140000	3.97410000
C	5.32750000	32.82990000	2.15650000
C	5.89060000	32.19670000	5.07320000
C	6.41040000	31.99910000	6.35640000
C	7.49610000	31.11850000	6.56300000
C	8.09130000	30.51530000	5.44980000
C	7.56830000	30.71070000	4.16960000
C	6.14020000	33.97150000	2.21410000
C	4.47500000	35.24140000	0.96460000
C	3.64220000	34.11760000	0.97090000
C	4.06310000	32.92110000	1.55350000
C	5.72510000	35.16650000	1.62050000
O	8.01500000	30.79690000	7.83450000
C	7.24550000	31.15920000	8.98170000
H	7.73240000	30.74630000	9.88730000
O	4.01610000	36.38590000	0.28220000
C	4.97800000	37.38770000	-0.04290000

H	4.49990000	38.15210000	-0.68800000
N	3.95740000	22.52480000	-0.46030000
C	4.62970000	21.61630000	0.44000000
C	3.22170000	21.97930000	-1.57710000
C	4.00230000	20.43550000	0.86430000
C	4.65130000	19.55420000	1.73190000
C	5.94770000	19.85010000	2.20590000
C	6.56480000	21.02950000	1.77450000
C	5.93070000	21.88440000	0.87490000
C	3.69290000	20.83550000	-2.24210000
C	2.94900000	20.25300000	-3.26430000
C	1.73720000	20.81340000	-3.67480000
C	1.26860000	21.97430000	-3.02100000
C	2.00170000	22.54330000	-1.97680000
O	6.66890000	19.02290000	3.09100000
C	6.07290000	17.79510000	3.50640000
H	6.78240000	17.26520000	4.16980000
O	1.05300000	20.16450000	-4.72010000
C	-0.13030000	20.77060000	-5.23170000
H	-0.50990000	20.14310000	-6.05630000
H	4.16130000	24.43790000	-2.38120000
H	4.61920000	26.84370000	-2.03140000
H	4.10000000	23.83610000	1.89720000
H	5.28810000	29.12050000	-1.23980000
H	5.85450000	31.20120000	-0.01840000
H	5.10490000	29.19040000	3.73120000
H	5.02250000	32.83130000	4.94570000
H	5.94090000	32.51680000	7.17710000
H	8.93930000	29.85500000	5.58200000
H	8.01100000	30.19510000	3.33110000
H	7.11520000	33.92370000	2.68320000
H	2.67200000	34.16180000	0.49300000
H	3.40730000	32.06120000	1.52640000
H	6.39570000	36.01290000	1.66570000
H	6.22100000	30.73420000	8.91550000
H	7.20420000	32.26160000	9.09300000
H	5.82820000	36.94280000	-0.60160000
H	5.34430000	37.88760000	0.87560000
H	2.99850000	20.20660000	0.53540000
H	4.12190000	18.66360000	2.03640000
H	7.55700000	21.28260000	2.11340000
H	6.45840000	22.75010000	0.50300000
H	4.63800000	20.38840000	-1.96320000
H	3.32190000	19.36090000	-3.75040000
H	0.33430000	22.43630000	-3.29090000
H	1.61040000	23.41250000	-1.46730000
H	5.86340000	17.14830000	2.63000000
H	5.14090000	17.97970000	4.08010000
H	0.08430000	21.78180000	-5.62770000
H	-0.91810000	20.82340000	-4.45850000
C	4.59980000	26.65340000	2.44540000
C	4.53750000	26.23620000	3.72440000
C	5.29750000	26.70330000	4.90620000
C	3.72540000	25.15090000	4.29420000
C	3.98550000	24.98690000	5.61110000
C	4.96150000	25.97950000	6.00350000
C	2.58240000	24.51780000	3.91270000
S	2.93460000	23.96510000	6.46520000
C	6.45440000	27.40850000	5.09870000
C	6.88140000	27.26300000	6.41300000

S	5.94880000	26.16850000	7.37150000
C	2.07780000	23.78470000	4.97550000
H	2.09790000	24.63970000	2.95780000
H	7.01330000	27.92120000	4.33000000
H	7.78310000	27.73080000	6.78390000
H	1.16610000	23.21570000	4.89270000
C	0.72910000	59.61010000	4.96810000
C	0.59730000	60.48080000	6.07790000
C	0.33980000	61.84560000	5.89080000
C	0.25250000	62.33400000	4.59040000
C	0.47980000	61.52680000	3.48920000
C	0.66810000	60.14920000	3.66040000
C	-0.18800000	63.64250000	4.13040000
C	-0.50410000	64.78480000	4.86390000
C	-0.81200000	65.96210000	4.16420000
C	-0.75810000	65.99560000	2.74810000
C	-0.43250000	64.81690000	2.04420000
C	-0.22150000	63.63320000	2.74960000
N	-1.00460000	67.22490000	2.02400000
C	-1.64790000	67.17420000	0.73160000
C	-0.53390000	68.48270000	2.54920000
C	-1.09700000	67.84950000	-0.36740000
C	-1.61670000	67.65200000	-1.65060000
C	-2.70250000	66.77140000	-1.85730000
C	-3.29760000	66.16810000	-0.74400000
C	-2.77470000	66.36350000	0.53610000
C	-1.34660000	69.62430000	2.49170000
C	0.31860000	70.89430000	3.74120000
C	1.15140000	69.77050000	3.73480000
C	0.73050000	68.57400000	3.15220000
C	-0.93140000	70.81940000	3.08520000
O	-3.22140000	66.44980000	-3.12880000
C	-2.45180000	66.81200000	-4.27600000
H	-2.93880000	66.39920000	-5.18150000
O	0.77750000	72.03870000	4.42360000
C	-0.18440000	73.04060000	4.74870000
H	0.29380000	73.80500000	5.39370000
N	0.83620000	58.17760000	5.16610000
C	0.16390000	57.26920000	4.26570000
C	1.57190000	57.63210000	6.28280000
C	0.79130000	56.08840000	3.84150000
C	0.14240000	55.20700000	2.97380000
C	-1.15410000	55.50290000	2.49980000
C	-1.77110000	56.68230000	2.93130000
C	-1.13710000	57.53730000	3.83090000
C	1.10080000	56.48840000	6.94780000
C	1.84460000	55.90580000	7.97010000
C	3.05650000	56.46630000	8.38060000
C	3.52500000	57.62710000	7.72670000
C	2.79190000	58.19610000	6.68250000
O	-1.87530000	54.67580000	1.61480000
C	-1.27930000	53.44790000	1.19930000
H	-1.98880000	52.91810000	0.53600000
O	3.74070000	55.81740000	9.42580000
C	4.92400000	56.42350000	9.93750000
H	5.30360000	55.79600000	10.76200000
H	0.63230000	60.09070000	7.08700000
H	0.17440000	62.49660000	6.73710000
H	0.69360000	59.48890000	2.80850000
H	-0.49450000	64.77340000	5.94560000

H	-1.06090000	66.85410000	4.72420000
H	-0.31130000	64.84330000	0.97450000
H	-0.22890000	68.48410000	-0.24000000
H	-1.14730000	68.16970000	-2.47140000
H	-4.14570000	65.50780000	-0.87630000
H	-3.21740000	65.84800000	1.37470000
H	-2.32160000	69.57650000	2.02260000
H	2.12170000	69.81470000	4.21280000
H	1.38640000	67.71400000	3.17940000
H	-1.60210000	71.66580000	3.04000000
H	-1.42730000	66.38700000	-4.20980000
H	-2.41060000	67.91440000	-4.38730000
H	-1.03460000	72.59560000	5.30740000
H	-0.55070000	73.54040000	3.83010000
H	1.79520000	55.85950000	4.17040000
H	0.67170000	54.31640000	2.66940000
H	-2.76330000	56.93550000	2.59230000
H	-1.66470000	58.40290000	4.20270000
H	0.15560000	56.04130000	6.66890000
H	1.47170000	55.01380000	8.45610000
H	4.45930000	58.08920000	7.99670000
H	3.18330000	59.06540000	6.17300000
H	-1.06970000	52.80120000	2.07570000
H	-0.34730000	53.63260000	0.62570000
H	4.70930000	57.43460000	10.33340000
H	5.71170000	56.47630000	9.16420000
C	0.19380000	62.30620000	2.26030000
C	0.25610000	61.88910000	0.98130000
C	-0.50390000	62.35610000	-0.20040000
C	1.06820000	60.80380000	0.41160000
C	0.80810000	60.63980000	-0.90530000
C	-0.16790000	61.63240000	-1.29780000
C	2.21120000	60.17060000	0.79310000
S	1.85900000	59.61800000	-1.75950000
C	-1.66080000	63.06130000	-0.39300000
C	-2.08780000	62.91590000	-1.70720000
S	-1.15520000	61.82130000	-2.66570000
C	2.71580000	59.43760000	-0.26970000
H	2.69570000	60.29250000	1.74800000
H	-2.21960000	63.57400000	0.37580000
H	-2.98950000	63.38360000	-2.07810000
H	3.62750000	58.86860000	-0.18700000

DT2:

C	8.37740000	0.25250000	4.23560000
C	9.12840000	1.25960000	4.82420000
C	10.42490000	1.50990000	4.40170000
C	11.00870000	0.79220000	3.32610000
C	10.20570000	-0.15080000	2.61080000
C	8.93120000	-0.45750000	3.16090000
C	12.38130000	0.94920000	2.99180000
C	13.27060000	1.72540000	3.77670000
C	14.63800000	1.73690000	3.52990000
C	15.18570000	0.93160000	2.53470000
C	14.31850000	0.16420000	1.74890000
C	12.91140000	0.25070000	1.88270000
N	16.61980000	0.89570000	2.31270000
C	17.13510000	0.81190000	0.95790000
C	17.53020000	0.95110000	3.44210000

C	16.48250000	1.46250000	-0.10340000
C	16.91990000	1.29910000	-1.42030000
C	18.03510000	0.48340000	-1.70720000
C	18.71240000	-0.12130000	-0.64410000
C	18.27580000	0.04660000	0.67070000
C	18.73410000	1.66900000	3.35750000
C	19.24830000	1.15930000	5.68200000
C	18.07820000	0.40060000	5.74910000
C	17.21990000	0.30640000	4.65190000
C	19.58000000	1.78670000	4.46180000
O	18.51570000	0.23800000	-3.01010000
C	17.79620000	0.79550000	-4.10920000
H	18.29420000	0.49970000	-5.05320000
O	20.02390000	1.25360000	6.85390000
C	21.18120000	2.08330000	6.82250000
H	21.67230000	2.05840000	7.81260000
N	7.03190000	-0.03650000	4.70260000
C	6.01370000	-0.39390000	3.73300000
C	6.71720000	-0.01360000	6.12300000
C	5.07720000	-1.39720000	4.01410000
C	4.12900000	-1.77440000	3.06330000
C	4.11980000	-1.19500000	1.79130000
C	5.05050000	-0.17350000	1.50580000
C	5.97210000	0.22780000	2.47440000
C	5.42840000	0.33220000	6.57430000
C	5.12010000	0.32480000	7.93580000
C	6.07890000	-0.03530000	8.88620000
C	7.37560000	-0.36860000	8.44450000
C	7.68640000	-0.35870000	7.08250000
O	3.17200000	-1.67580000	0.86740000
C	3.26770000	-1.22820000	-0.48260000
H	2.49230000	-1.74360000	-1.07920000
O	5.68910000	-0.03000000	10.24080000
C	6.56890000	-0.62680000	11.19320000
H	6.11250000	-0.55330000	12.19800000
H	8.71150000	1.84710000	5.62840000
H	10.92720000	2.30730000	4.91970000
H	8.34620000	-1.28380000	2.83960000
H	12.95390000	2.30390000	4.61990000
H	15.27660000	2.34050000	4.15540000
H	14.76340000	-0.53970000	1.06770000
H	15.61820000	2.08200000	0.08220000
H	16.37190000	1.80430000	-2.20080000
H	19.57590000	-0.74160000	-0.83630000
H	18.82600000	-0.42850000	1.46370000
H	19.02380000	2.13790000	2.43280000
H	17.81840000	-0.09130000	6.67530000
H	16.30510000	-0.25540000	4.75640000
H	20.48350000	2.36900000	4.34580000
H	16.76090000	0.39830000	-4.12930000
H	17.79520000	1.90550000	-4.05480000
H	21.90850000	1.70090000	6.07980000
H	20.89760000	3.13370000	6.60160000
H	5.08650000	-1.89200000	4.97070000
H	3.42080000	-2.55360000	3.30610000
H	5.07110000	0.32940000	0.54910000
H	6.64470000	1.03930000	2.24960000
H	4.64780000	0.59380000	5.87480000
H	4.11990000	0.58510000	8.25350000
H	8.15680000	-0.63230000	9.14030000

H	8.68980000	-0.62490000	6.78080000
H	3.08110000	-0.13550000	-0.55000000
H	4.26150000	-1.48660000	-0.90730000
H	6.73120000	-1.69830000	10.95150000
H	7.53320000	-0.08860000	11.23710000
C	10.69090000	-0.69820000	1.36460000
C	12.03500000	-0.38440000	0.96310000
C	12.43520000	-0.65500000	-0.38200000
C	9.89570000	-1.46340000	0.43340000
C	10.38380000	-1.79940000	-0.81790000
C	11.62110000	-1.35630000	-1.23720000
C	8.51870000	-1.99770000	0.63470000
S	9.29090000	-2.73000000	-1.88850000
C	13.63980000	-0.08610000	-1.06020000
C	13.70170000	-0.56980000	-2.50160000
S	12.21000000	-1.54750000	-2.91880000
C	7.94520000	-2.50900000	-0.67680000
H	8.60260000	-2.86860000	1.30830000
H	13.59250000	1.02090000	-1.04530000
H	14.60580000	-1.19150000	-2.65030000
H	7.20430000	-1.78600000	-1.07710000
C	8.68380000	2.50550000	15.32480000
C	7.93280000	3.51260000	14.73620000
C	6.63630000	3.76290000	15.15870000
C	6.05250000	3.04520000	16.23430000
C	6.85550000	2.10220000	16.94960000
C	8.13000000	1.79550000	16.39950000
C	4.67990000	3.20220000	16.56860000
C	3.79070000	3.97840000	15.78370000
C	2.42320000	3.98990000	16.03050000
C	1.87550000	3.18460000	17.02580000
C	2.74280000	2.41720000	17.81150000
C	4.14980000	2.50370000	17.67770000
N	0.44140000	3.14870000	17.24770000
C	-0.07390000	3.06490000	18.60250000
C	-0.46900000	3.20410000	16.11830000
C	0.57870000	3.71550000	19.66380000
C	0.14130000	3.55210000	20.98070000
C	-0.97390000	2.73640000	21.26760000
C	-1.65120000	2.13170000	20.20450000
C	-1.21460000	2.29960000	18.88980000
C	-1.67290000	3.92200000	16.20290000
C	-2.18710000	3.41230000	13.87840000
C	-1.01700000	2.65360000	13.81130000
C	-0.15870000	2.55940000	14.90850000
C	-2.51870000	4.03970000	15.09860000
O	-1.45450000	2.49100000	22.57050000
C	-0.73500000	3.04850000	23.66960000
H	-1.23300000	2.75270000	24.61360000
O	-2.96270000	3.50660000	12.70650000
C	-4.11990000	4.33630000	12.73790000
H	-4.61110000	4.31140000	11.74780000
N	10.02930000	2.21650000	14.85780000
C	11.04750000	1.85910000	15.82740000
C	10.34400000	2.23940000	13.43740000
C	11.98400000	0.85580000	15.54630000
C	12.93220000	0.47860000	16.49710000
C	12.94140000	1.05800000	17.76910000
C	12.01080000	2.07950000	18.05460000
C	11.08910000	2.48080000	17.08600000

C	11.63280000	2.58520000	12.98610000
C	11.94110000	2.57780000	11.62460000
C	10.98230000	2.21770000	10.67420000
C	9.68570000	1.88440000	11.11600000
C	9.37480000	1.89430000	12.47790000
O	13.88920000	0.57720000	18.69300000
C	13.79350000	1.02480000	20.04300000
H	14.56890000	0.50940000	20.63960000
O	11.37220000	2.22300000	9.31960000
C	10.49230000	1.62620000	8.36720000
H	10.94870000	1.69970000	7.36240000
H	8.34980000	4.10010000	13.93210000
H	6.13400000	4.56030000	14.64070000
H	8.71500000	0.96920000	16.72080000
H	4.10730000	4.55690000	14.94050000
H	1.78460000	4.59350000	15.40500000
H	2.29780000	1.71330000	18.49270000
H	1.44300000	4.33500000	19.47820000
H	0.68930000	4.05730000	21.76120000
H	-2.51470000	1.51140000	20.39670000
H	-1.76480000	1.82450000	18.09670000
H	-1.96260000	4.39090000	17.12760000
H	-0.75720000	2.16170000	12.88510000
H	0.75620000	1.99760000	14.80400000
H	-3.42230000	4.62200000	15.21460000
H	0.30030000	2.65130000	23.68970000
H	-0.73400000	4.15850000	23.61530000
H	-4.84730000	3.95390000	13.48060000
H	-3.83640000	5.38670000	12.95880000
H	11.97480000	0.36100000	14.58970000
H	13.64040000	-0.30060000	16.25430000
H	11.99010000	2.58240000	19.01130000
H	10.41660000	3.29230000	17.31080000
H	12.41340000	2.84680000	13.68560000
H	12.94130000	2.83810000	11.30690000
H	8.90440000	1.62070000	10.42010000
H	8.37140000	1.62810000	12.77960000
H	13.98010000	2.11750000	20.11040000
H	12.79970000	0.76640000	20.46770000
H	10.33010000	0.55470000	8.60890000
H	9.52800000	2.16440000	8.32330000
C	6.37030000	1.55480000	18.19580000
C	5.02620000	1.86860000	18.59730000
C	4.62600000	1.59800000	19.94250000
C	7.16550000	0.78960000	19.12700000
C	6.67740000	0.45360000	20.37830000
C	5.44010000	0.89670000	20.79760000
C	8.54250000	0.25530000	18.92570000
S	7.77040000	-0.47700000	21.44890000
C	3.42150000	2.16690000	20.62060000
C	3.35950000	1.68320000	22.06200000
S	4.85120000	0.70550000	22.47920000
C	9.11600000	-0.25600000	20.23720000
H	8.45860000	-0.61560000	18.25210000
H	3.46870000	3.27390000	20.60570000
H	2.45540000	1.06150000	22.21070000
H	9.85690000	0.46700000	20.63750000