

## †Electronic Supporting Information

# TD-DFT benchmark for UV-visible spectra of fused- ring electron acceptors applying global and range- separated hybrids

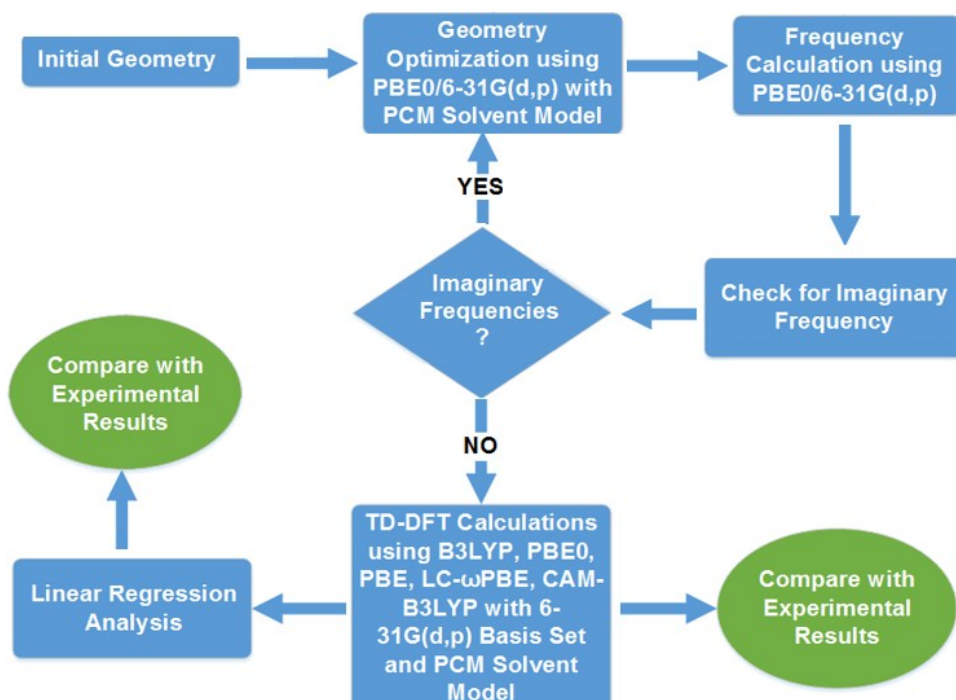
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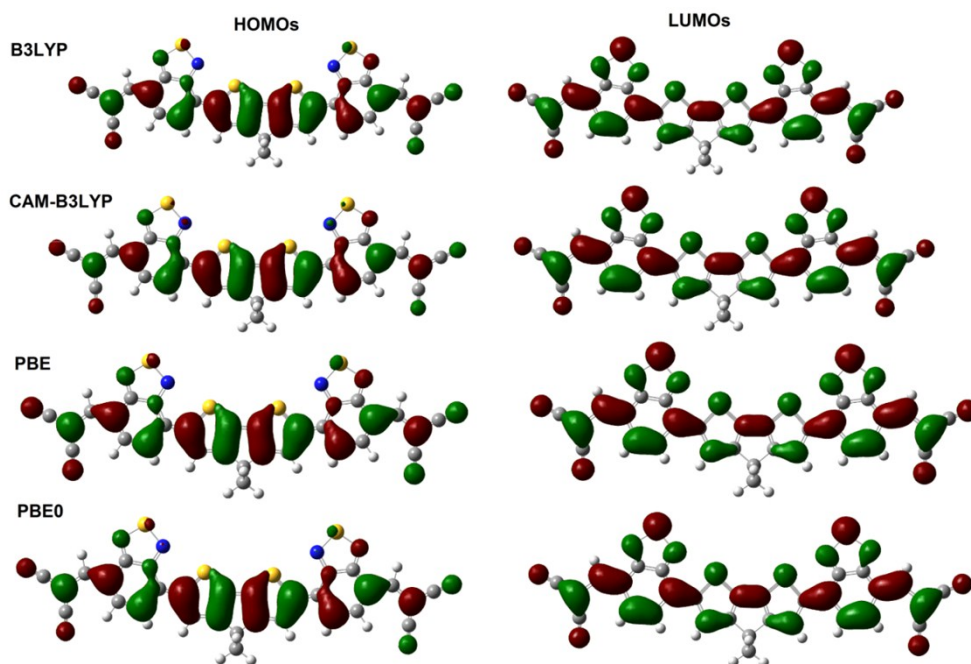
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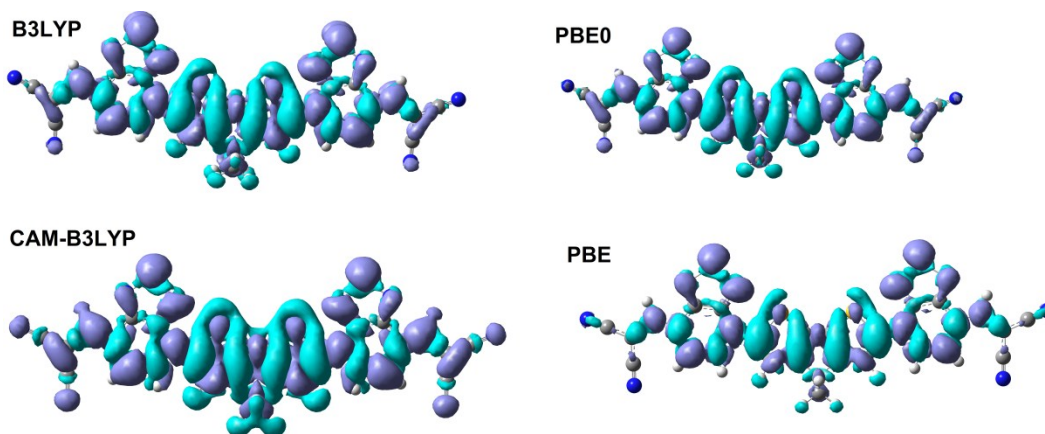
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**Scheme S1.** Flow diagram of simulation process.



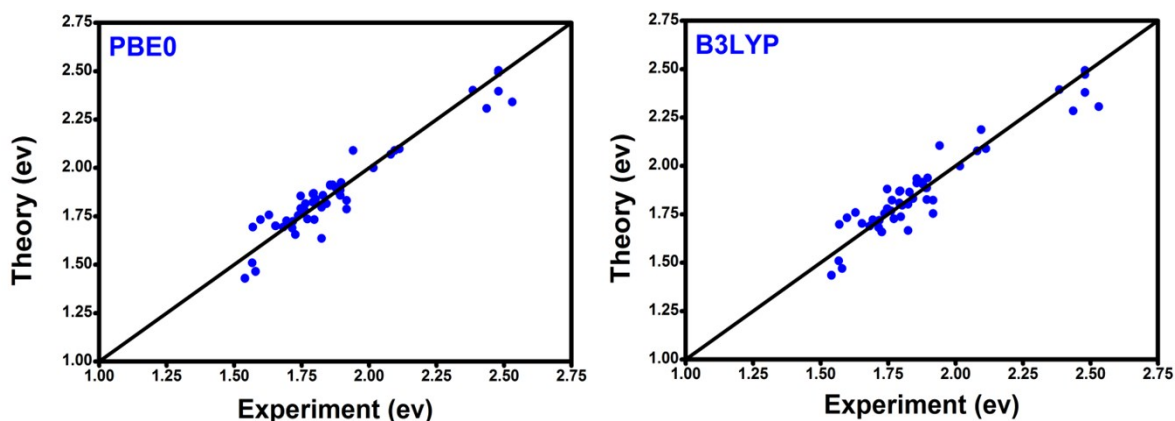
**Fig. S1.** HOMOs and LUMOs of CDTBM FREA using different functionals (contour threshold: 0.02 a.u.)



**Fig. S2.** Plot of the density difference between the ground and excited states computed for CDTBM (contour threshold: 0.0002 a.u.).

**Table S1.** Solvents used in the in simulation process

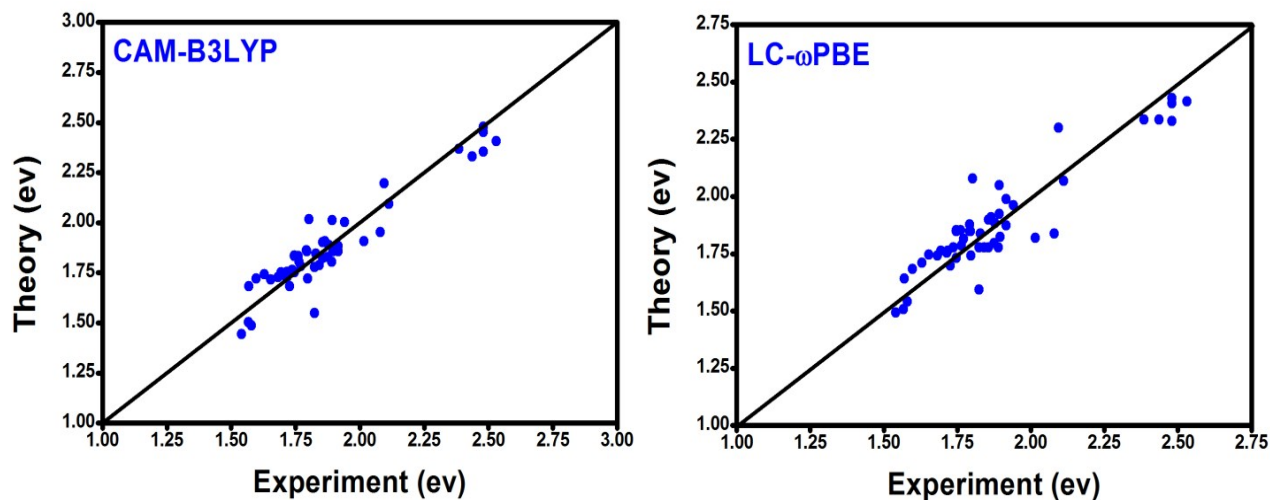
SN.	FREAs	Solvent	SN.	FREAs	Solvent
1	DBS-2DPP	Chlorobenzene	26	IDTOT2F	Chloroform
2	F(DPP)2B2	Chloroform	27	ITOIC-F	Chloroform
3	F8IDT	Chlorobenzene	28	ITOIC-2F	Chloroform
4	FEHIDT	Dichloromethane	29	IEICO	Chloroform
5	Cz-RH	Chloroform	30	ATT-2	Chloroform
6	Flu-RH	Chloroform	31	IEICO-4F	Chloroform
7	FBM	Chloroform	32	DTCCIC-C17	Chlorobenzene
8	CDTBM	Chloroform	33	m-ITIC	Chloroform
9	DICH2TF	Dichloromethane	34	IT-DM	Chloroform
10	FRd2	Chloroform	35	IT-M	Chloroform
11	ITDI	Chloroform	36	ITCPTC	Chloroform
12	IDT-BC6	Chloroform	37	C8-ITIC	Chlorobenzene
13	IDT-2B	Chlorobenzene	38	Cl-ITIC	Chloroform
14	SiIDT-IC	Chloroform	39	Br-ITIC	Chloroform
15	IFBR-d	Chlorobenzene	40	NFBBDT	Chloroform
16	IDIDT-C8	Chloroform	41	ITIC2	Chloroform
17	IC-1IDT-IC	Dichloromethane	42	BT-IC	Dichloromethane
18	IDT-OB	Chlorobenzene	43	ITVffIC	Chloroform
19	IDT-2O	Chlorobenzene	44	INIC	Chloroform
20	CO5IC	Chlorobenzene	45	INIC2	Chloroform
21	IDT-BOC6	Chloroform	46	INIC1	Chloroform
22	ATT-1	Chloroform	47	INIC3	Chloroform
23	DC-IDT2T	Chloroform	48	IPIC	Chloroform
24	BZIC	Chloroform	49	IPIC-4F	Chloroform
25	ITOIC	Chloroform	50	IPIC-4Cl	Chloroform



**Fig. S3.** Comparison between experimental  $\lambda_{\max}$  and the corrected theoretical vertical absorption wavelength values ( $\lambda_{\text{ver-abs}}$ ) using PBE0 and B3LYP. The solid line shows the theory-experiment perfect match.

**Table S2.** Charge transfer calculated with different functionals

FREAs	B3LYP	PBE0	CAM-B3LYP	PBE
BT-IC	0.602	0.613	0.638	0.545
C8-ITIC	0.554	0.568	0.622	0.439
F8IDT	0.547	0.553	0.558	0.447
IC-IDT-IC	0.525	0.542	0.618	0.413
CO5IC	0.557	0.571	0.633	0.455
IDT-2B	0.542	0.555	0.615	0.45
IDT-2O	0.507	0.522	0.59	0.393
IDT-OB	0.536	0.549	0.609	0.467
NFBDT	0.553	0.566	0.61	0.472
ITOIC-2F	0.637	0.648	0.664	0.497
INIC2	0.647	0.656	0.665	0.519
IEICO-4F	0.6	0.626	0.715	0.411
CDTBM	0.437	0.465	0.589	0.298
CI-ITIC	0.588	0.6	0.645	0.482
DC-IDT2T	0.647	0.659	0.67	0.509
IPIC	0.598	0.609	0.645	0.477
IPIC-4F	0.6	0.611	0.648	0.483
IT-DM	0.593	0.605	0.646	0.482
ITVFFIC	0.605	0.622	0.671	0.451
Flu-RH	0.521	0.527	0.547	0.397



**Fig. S4.** Comparison between the experimental  $\lambda_{\max}$  and corrected data for computed vertical absorption wavelength values ( $\lambda_{\text{ver-abs}}$ ) using LC- $\omega$ PBE and CAM-B3LYP. The solid line shows the theory-experiment perfect match.

**Table S3.** Theoretical vertical excitation energy ( $\lambda_{\text{ver-abs}}$ ) comparison with experimental maximum wavelength ( $\lambda_{\max}$ ) using B3LYP, PBE0, CAM-B3LYP and PBE for a subset of 20 FREAs

FREAs	Theoretical Vertical Excitation Energy (eV)				Exp. Transition Energy (eV)	Deviation (Exp.-Theoretical) (eV)			
	B3LYP	PBE0	CAM-B3LYP	PBE		B3LYP	PBE0	CAM-B3LYP	PBE
BT-IC	1.6	1.687	2.049	1.224	1.727	0.127	0.04	-0.322	0.503
C8-ITIC	1.717	1.805	2.138	1.39	1.824	0.107	0.019	-0.314	0.434
F8IDT	2.202	2.309	2.678	1.781	2.385	0.183	0.076	-0.293	0.604
IC-1IDT-IC	1.787	1.865	2.16	1.494	1.89	0.103	0.025	-0.27	0.396
CO5IC	1.742	1.821	2.145	1.405	1.842	0.1	0.021	-0.303	0.437
IDT-2B	1.829	1.91	2.21	1.519	1.896	0.067	-0.014	-0.314	0.377
IDT-2O	1.826	1.902	2.179	1.542	1.856	0.03	-0.046	-0.323	0.314
IDT-OB	1.81	1.89	2.183	1.501	1.876	0.066	-0.014	-0.307	0.375
NFBDT	1.734	1.821	2.16	1.379	1.764	0.03	-0.057	-0.396	0.385
ITOIC-2F	1.625	1.719	2.091	1.264	1.682	0.057	-0.037	-0.409	0.418
INIC2	1.689	1.792	2.187	1.301	1.761	0.072	-0.031	-0.426	0.46
IEICO-4F	1.417	1.499	1.828	1.1242	1.54	0.123	0.041	-0.288	0.4158
CDTBM	1.606	1.671	1.925	1.43	1.823	0.217	0.152	-0.102	0.393
CI-ITIC	1.773	1.864	2.21	1.425	1.795	0.022	-0.069	-0.415	0.37
DC-IDT2T	1.655	1.754	2.142	1.282	1.771	0.116	0.017	-0.371	0.489
IPIC	1.682	1.771	2.105	1.316	1.629	-0.053	-0.142	-0.476	0.313
IPIC-4F	1.659	1.751	2.084	1.299	1.597	-0.062	-0.154	-0.487	0.298
IT-DM	1.81	1.901	2.254	1.457	1.864	0.054	-0.037	-0.39	0.407
ITVffIC	1.635	1.724	2.0805	1.301	1.653	0.018	-0.071	-0.4275	0.352

## Cartesian Coordinates

Below are the Cartesian coordinates of all FREAs chemical structures optimized in solution (See Table S1) using DFT-PBE0/6-31G(d,p) and PCM solvent model. All data is in Å.

### FBM

0 1			
C	1.17269300	0.17346200	-0.00400900
C	0.72905100	-1.16094400	-0.00646400
C	-0.72904600	-1.16094300	0.00646100
C	-1.17268700	0.17346300	0.00400500
C	0.00000300	1.14064000	-0.00000300
C	-1.64624700	-2.21077900	0.02822400
C	-3.00327600	-1.92018300	0.04921700
C	-3.46241200	-0.58997300	0.03522500
C	-2.52487700	0.46000400	0.01383300
C	2.52488300	0.46000300	-0.01383700
C	3.46241800	-0.58997500	-0.03522800
C	3.00328100	-1.92018500	-0.04921900
C	1.64625200	-2.21077900	-0.02822700
C	0.00406700	2.01934600	1.25951100
C	-0.00406100	2.01934400	-1.25951800
C	-4.89804900	-0.28152600	0.00876200
C	4.89805400	-0.28152900	-0.00876400
C	-5.39213200	0.80680900	-0.69308700
C	-6.75793000	1.14497200	-0.75168600
C	-7.74091100	0.40948200	-0.10389600
C	-7.27743900	-0.72354600	0.64771500
C	-5.87759300	-1.06751200	0.70254600
C	5.87759900	-1.06751700	-0.70254500
C	7.27744500	-0.72355000	-0.64771500
C	7.74091600	0.40948100	0.10389200
C	6.75793400	1.14497100	0.75168200
C	5.39213700	0.80680800	0.69308300
N	-8.05213500	-1.54133300	1.35841600
S	-7.06611500	-2.64275500	2.03638300
N	-5.63480600	-2.13647200	1.46645000
N	5.63481200	-2.13647600	-1.46645000
S	7.06612300	-2.64277000	-2.03636800
N	8.05214100	-1.54133600	-1.35841700
C	-9.15459200	0.66573500	-0.11167000
C	9.15459500	0.66573900	0.11166800
C	-9.87888600	1.64608100	-0.72977300
C	9.87887800	1.64609100	0.72977400
C	-11.29859100	1.67245800	-0.57204000
N	-12.45362400	1.69722800	-0.44593900
C	-9.33675500	2.68161900	-1.54697000
N	-8.91323500	3.53300900	-2.21593600
C	11.29858300	1.67248300	0.57204800
N	12.45361700	1.69726400	0.44595200
C	9.33673000	2.68162300	1.54696800
N	8.91317600	3.53300000	2.21592900
H	-1.31377800	-3.24469600	0.02802100
H	-3.72335800	-2.72951700	0.06408200
H	-2.86977500	1.49038700	0.03840800
H	2.86978100	1.49038600	-0.03841200
H	3.72336200	-2.72951900	-0.06408400
H	1.31378200	-3.24469700	-0.02802200
H	-0.88122700	2.66266800	1.28090400
H	0.00854500	1.40890900	2.16673700
H	0.88797400	2.66489000	1.27289900
H	0.88123400	2.66266600	-1.28091100
H	-0.00853900	1.40890500	-2.16674300
H	-0.88796800	2.66488800	-1.27290700
H	-4.69915000	1.42039100	-1.25923200
H	-7.03122600	2.01093600	-1.34280700
H	7.03123200	2.01093800	1.34280000
H	4.69915500	1.42039200	1.25922700
H	-9.73821400	-0.04187900	0.47229600
H	9.73822300	-0.04187200	-0.47229700

### FEHDT

0 1

C	0.72118300	0.16286200	0.07644100
C	1.17444800	1.49452500	0.11164700
C	0.00000300	2.48368300	0.00015700
C	-1.17445000	1.49454700	-0.11144500
C	-0.72119500	0.16287700	-0.07639300
C	-2.53283300	1.73066800	-0.27275400
C	-3.43779800	0.65917200	-0.39916400
C	-2.95484000	-0.65975000	-0.35297500
C	-1.60271600	-0.91128400	-0.18981500
C	1.60269400	-0.91131900	0.18974300
C	2.95482100	-0.65981500	0.35293800
C	3.43778700	0.65909800	0.39928200
C	2.53283200	1.73061700	0.27299000
C	-0.07599700	3.29635000	1.35460300
C	0.07601500	3.29651300	-1.35418900
C	-4.86079800	0.93364500	-0.57516100
C	4.86078700	0.93354200	0.57532300
C	-5.44497800	2.09457800	-1.05954600
C	-6.83997800	2.02059700	-1.10467100
C	-7.35685800	0.80741300	-0.65809300
S	-6.05742300	-0.24853800	-0.16497000
S	6.05741400	-0.24856500	0.16492400
C	7.35684700	0.80730400	0.65823100
C	6.83996300	2.02041000	1.10501900
C	5.44496300	2.09439300	1.05990900
C	-8.75083100	0.53753400	-0.63299700
C	8.75082100	0.53743600	0.63308700
C	9.48732600	-0.54662000	0.26165400
C	-9.48733200	-0.54658700	-0.26174500
C	-10.96560200	-0.52310000	-0.36119600
C	-11.44087000	-1.85264500	0.10924600
C	-10.33885900	-2.63330200	0.47150900
C	-9.08175200	-1.86071700	0.25971000
C	10.96559500	-0.52314400	0.36111400
C	11.44086700	-1.85262500	-0.10950600
C	10.33886000	-2.63322500	-0.47190600
C	9.08175200	-1.86066300	-0.26002400
C	-12.73495700	-2.34329600	0.21118400
C	-12.90101500	-3.64346000	0.68727500
C	-11.79765900	-4.42513600	1.05006500
C	-10.49915700	-3.92741800	0.94648300
C	12.73495300	-2.34326900	-0.21148200
C	12.90101500	-3.64336600	-0.68775300
C	11.79766400	-4.42498500	-1.05068200
C	10.49916100	-3.92727300	-0.94706000
O	7.95151900	-2.26979200	-0.48596400
O	11.66180500	0.39976400	0.75219300
O	-7.95151800	-2.26988100	0.48558200
O	-11.66181700	0.39987400	-0.75210900
C	-1.45298100	3.83726900	1.75421000
C	0.94385900	4.43033300	1.48927800
C	-0.94378400	4.43056600	-1.48870600
C	1.45301800	3.83740900	-1.75375900
H	-2.92911700	2.73766900	-0.27021500
H	-3.64341900	-1.49178500	-0.46901900
H	-1.23858700	-1.93409200	-0.16528200
H	1.23855600	-1.93412000	0.16509300
H	3.64339400	-1.49186700	0.46889100
H	2.92912700	2.73761500	0.27057000
H	0.18060000	2.55111200	2.12040900
H	-0.18063400	2.55138100	-2.12008100
H	-4.87664100	2.95260600	-1.39795800
H	-7.48163900	2.81795000	-1.46437500
H	7.48162200	2.81770000	1.46486200
H	4.87661900	2.95235600	1.39847200
H	-9.35677700	1.37452900	-0.98691000
H	9.35676300	1.37437400	0.98714000
H	-13.58444800	-1.72973000	-0.07229200
H	-13.89975900	-4.05958600	0.77947400
H	-11.95974200	-5.43401100	1.41755700
H	-9.63729600	-4.52561800	1.22550600
H	13.58444100	-1.72974800	0.07210200
H	13.89975900	-4.05948500	-0.77998800
H	11.95974900	-5.43380800	-1.41831300
H	9.63730400	-4.52542900	-1.22618800
H	-1.36131900	4.34159900	2.72194300
H	-2.19215600	3.04341300	1.87365800
H	-1.84401400	4.57194400	1.04527700
H	0.90401400	4.82465100	2.50989200
H	1.97210500	4.11214300	1.31229700

H	0.72419500	5.26258300	0.81439800
H	-0.90393100	4.82501000	-2.50927200
H	-1.97204500	4.11241000	-1.31175200
H	-0.72406700	5.26271800	-0.81372400
H	1.36136400	4.34185000	-2.72143600
H	2.19215300	3.04353100	-1.87330800
H	1.84409900	4.57198900	-1.04475300

## Cz-RH

0 1			
C	-1.10965700	-2.20947800	0.12249400
C	-0.70982400	-3.56983600	0.08260400
C	0.71252000	-3.57044500	-0.11732300
C	1.10952100	-2.21043300	-0.18593600
N	-0.00325700	-1.40518500	-0.05647400
C	1.67983900	-4.57176000	-0.24160800
C	3.00344100	-4.21529300	-0.42532000
C	3.39690600	-2.85774900	-0.49287600
C	2.43867900	-1.84428600	-0.36971700
C	-2.43521800	-1.84226000	0.32923100
C	-3.39062900	-2.85497100	0.47797300
C	-2.99674300	-4.21287000	0.42311500
C	-1.67443100	-4.57035100	0.23198000
C	-0.00045600	0.03695400	-0.04118100
C	4.80662600	-2.53026000	-0.68733500
C	-4.79647000	-2.52529000	0.69522300
S	5.45359400	-1.01113700	-0.16562700
C	7.04724900	-1.41694300	-0.75113500
C	7.03393200	-2.69269000	-1.30812700
C	5.78321500	-3.31805200	-1.27310900
C	-5.76147600	-3.30386300	1.31165900
C	-7.01103200	-2.67717100	1.36217600
C	-7.03497700	-1.40988100	0.78645400
S	-5.45335900	-1.01422800	0.16278700
C	8.24364100	-0.64306300	-0.70779500
C	-8.23134400	-0.63525200	0.75676300
C	8.54283700	0.60108200	-0.24155000
C	-8.53926000	0.60182300	0.27759000
C	7.65131300	1.56776800	0.39103800
N	8.35404900	2.73321100	0.72634900
C	9.67957100	2.77433200	0.41077000
S	10.16662800	1.27685100	-0.34974000
S	-10.15932400	1.28199200	0.41124200
C	-9.68811500	2.76521500	-0.38626000
N	-8.37020600	2.71656100	-0.73128700
C	-7.66114000	1.55639900	-0.39116200
O	-6.47543900	1.42023500	-0.64630900
O	6.46011700	1.43695200	0.62223500
C	-7.67607600	3.81641000	-1.39631500
C	7.64619100	3.84605800	1.35423500
C	7.06954300	4.80642400	0.32726300
C	-7.07341400	4.79467100	-0.40169700
S	-10.74307200	4.00752700	-0.65707600
S	10.73011400	4.01976500	0.68440300
H	1.40032500	-5.61956500	-0.18306200
H	3.76070300	-4.98936000	-0.48972200
H	2.72927500	-0.80046200	-0.43622000
H	-2.72331900	-0.79861500	0.40715400
H	-3.75205100	-4.98667100	0.50980300
H	-1.39318300	-5.61856300	0.19181300
H	-0.94891300	0.40877400	-0.43312200
H	0.14908800	0.43420200	0.96860800
H	0.79456500	0.40879400	-0.69018900
H	7.92435700	-3.13929400	-1.73789800
H	5.58695600	-4.29896100	-1.68917200
H	-5.55714600	-4.27842400	1.73865600
H	-7.89274500	-3.11640400	1.81679000
H	9.08106700	-1.18497900	-1.14657100
H	-9.05966800	-1.16913400	1.22191800
H	-6.90040900	3.35478200	-2.01085600
H	-8.40431900	4.30660800	-2.04538300
H	6.85503700	3.39705500	1.95827800
H	8.35943700	4.34731300	2.01144500
H	6.54415300	5.61745000	0.83904700
H	7.86161400	5.24429100	-0.28559500
H	6.35675800	4.29499400	-0.32492600
H	-6.55958800	5.59505200	-0.94122300
H	-7.84972700	5.24532500	0.22199600
H	-6.34561600	4.29424500	0.24237900



# Flu-RH

0 1			
C	-1.17353200	-2.01317500	-0.01464600
C	-0.72823000	-0.67892900	-0.00992100
C	0.72822400	-0.67892700	0.00952100
C	1.17352300	-2.01317400	0.01461800
C	-0.00000600	-2.97990300	0.00012700
C	1.65003500	0.36735000	0.02307800
C	3.00448600	0.06957100	0.03968700
C	3.46843800	-1.26007600	0.04296400
C	2.52349300	-2.30523100	0.03062000
C	-2.52350300	-2.30523400	-0.03056200
C	-3.46844500	-1.26008000	-0.04320700
C	-3.00449000	0.06956800	-0.04030200
C	-1.65003900	0.36734700	-0.02376800
C	-0.01557300	-3.85819600	1.25962300
C	0.01555800	-3.85856100	-1.25911600
C	4.89706600	-1.56039800	0.05890100
C	-4.89707300	-1.56040200	-0.05906700
S	6.08134500	-0.29322000	0.06192400
C	7.40064400	-1.43396000	0.08268800
C	6.90045600	-2.73273700	0.08571200
C	5.50477200	-2.80630900	0.07242700
C	-5.50477700	-2.80631300	-0.07261100
C	-6.90046300	-2.73274400	-0.08580600
C	-7.40065200	-1.43396800	-0.08269800
S	-6.08135400	-0.29322700	-0.06195300
C	8.80364500	-1.18268900	0.09723200
C	-8.80365400	-1.18269700	-0.09715300
C	9.55707300	-0.04809000	0.10163600
C	-9.55708200	-0.04809700	-0.10148000
C	9.10322500	1.33915200	0.08903900
N	10.19995300	2.21168600	0.11156700
C	11.44220600	1.65104600	0.12519500
S	11.31837500	-0.09341700	0.12488700
S	-11.31838600	-0.09342000	-0.12463600
C	-11.44221300	1.65104400	-0.12486600
N	-10.19995800	2.21168000	-0.11139400
C	-9.10323000	1.33914500	-0.08889300
O	7.95173400	1.74204200	0.06484400
S	12.89219700	2.44250300	0.14634600
C	9.97330200	3.65461100	0.08739500
C	9.91799700	4.20027900	-1.32974800
S	-12.89219900	2.44250400	-0.14625700
O	-7.95173600	1.74203200	-0.06480600
C	-9.97330200	3.65460800	-0.08737600
C	-9.91786700	4.20040400	1.32971300
H	1.32356400	1.40313900	0.02150800
H	3.71785700	0.88891700	0.05081400
H	2.85454600	-3.33942900	0.03300700
H	-2.85456000	-3.33943100	-0.03262600
H	-3.71786000	0.88891100	-0.05168500
H	-1.32356400	1.40313600	-0.02249000
H	-0.90053300	-4.50249000	1.26687300
H	0.86897500	-4.50240500	1.28878700
H	-0.02683500	-3.24713300	2.16636400
H	0.90052200	-4.50285200	-1.26618900
H	-0.86898500	-4.50278600	-1.28808900
H	0.02681000	-3.24775800	-2.16603300
H	7.55322900	-3.59924300	0.09806800
H	4.96073200	-3.74267700	0.07346400
H	-4.96073400	-3.74268000	-0.07374900
H	-7.55323400	-3.59925100	-0.09817400
H	9.37091200	-2.11284500	0.10880600
H	-9.37092300	-2.11285200	-0.10872200
H	9.02739400	3.81878200	0.60769300
H	10.78217900	4.11376900	0.65909500
H	9.74043700	5.27881700	-1.29925000
H	10.86083000	4.02300700	-1.85358500
H	9.10483200	3.73574400	-1.89356600
H	-9.02744000	3.81872800	-0.60777300
H	-10.78222800	4.11371800	-0.65904600
H	-9.74031100	5.27894000	1.29909900
H	-10.86065000	4.02317900	1.85365300
H	-9.10464800	3.73592200	1.89349800

FR-d2

0	1			
C		-0.72674600	-2.52718200	-0.30557000
C		-1.39870900	-1.30622400	-0.48530600
C		-0.42614600	-0.19846700	-0.85764300
C		0.89125300	-0.95735800	-0.86897000
C		0.69644500	-2.31073400	-0.54329800
C		2.16103100	-0.47757500	-1.13462600
C		3.26638800	-1.34720100	-1.08195000
C		3.05505600	-2.69816400	-0.75246200
C		1.78120900	-3.18372400	-0.48651800
C		-1.43535800	-3.67375100	0.04993000
C		-2.81117300	-3.58692100	0.21366400
C		-3.49992600	-2.37420300	0.02671500
C		-2.77017000	-1.22349300	-0.32187100
C		-0.74676800	0.38723700	-2.24050100
C		-0.42209900	0.91530000	0.19973300
C		4.61006000	-0.83645800	-1.40271900
C		-7.88049500	-2.35434900	0.40620300
C		4.80234200	0.13774700	-2.36310400
C		6.06791100	0.67607800	-2.68447100
C		7.23647900	0.26462000	-2.07391700
C		7.10285300	-0.76029100	-1.08239000
C		5.80001600	-1.29968300	-0.74882800
C		-7.11707800	-1.21470200	0.81881100
C		-5.67361800	-1.20979000	0.69425600
C		-4.96515500	-2.34171300	0.16932100
C		-5.75160500	-3.41915500	-0.19059300
C		-7.15920900	-3.42783600	-0.07802200
N		8.09905300	-1.32417900	-0.39880000
S		7.42201900	-2.41615100	0.59317800
N		5.85607200	-2.23836400	0.20006400
N		-7.60389200	-0.10403600	1.37382800
S		-6.33150200	0.85391500	1.68781500
N		-5.11799700	-0.08528500	1.15467400
C		-9.32337500	-2.42027700	0.49539000
C		10.59014200	1.44092200	-2.16896100
C		10.25324300	1.78710900	-3.46649700
C		8.91428800	1.41022100	-3.65171600
C		8.50724300	0.83878500	-2.46215600
O		9.51908600	0.86058300	-1.56848700
O		-10.03281200	-1.27472300	0.42532700
C		-11.34834500	-1.59375700	0.52550000
C		-11.47516600	-2.96491500	0.66994400
C		-10.17639700	-3.49672200	0.64012000
C		11.85061400	1.61307000	-1.53876700
C		12.29420800	1.42895500	-0.26536000
C		-12.38883100	-0.62817000	0.50945100
C		-12.41183100	0.70792400	0.25098100
S		-13.89413000	1.64265800	0.44381600
C		-13.12196700	3.13113200	-0.05342200
N		-11.82038800	2.90211800	-0.36971700
C		-11.33826800	1.58266700	-0.24494800
S		13.99903200	1.63371400	0.13563200
C		13.73727800	1.24866000	1.82156100
N		12.42085000	0.99753300	2.04682300
C		11.53768900	1.10448000	0.95318200
O		10.33877000	0.96820000	1.08319400
O		-10.20378500	1.28362400	-0.55554700
S		-13.92928900	4.57294100	-0.11165900
S		14.96793900	1.21038500	2.92488200
C		-10.91027000	3.95212400	-0.81782200
C		11.88186300	0.69034500	3.36872500
C		11.48963000	1.94510600	4.13112200
C		-10.16954300	4.59476500	0.34313200
H		2.31623400	0.57576100	-1.35458300
H		3.90305600	-3.37131700	-0.71102100
H		1.64215900	-4.23271300	-0.24053800
H		-0.92678300	-4.62025100	0.20980500
H		-3.36453400	-4.46901300	0.52151800
H		-3.29001400	-0.28219300	-0.46428700
H		-0.00204000	1.13941000	-2.52042300
H		-0.75374500	-0.39248300	-3.00736700
H		-1.72836000	0.87184700	-2.23312000
H		-1.40105600	1.40295400	0.24579000
H		-0.19052200	0.51628900	1.19115600
H		0.32392100	1.67725100	-0.04818300
H		3.94256400	0.50732500	-2.91286200
H		6.11349000	1.45847700	-3.43583000

H	-5.27594600	-4.29360900	-0.62310600
H	-7.69359900	-4.30635200	-0.42633100
H	10.91386900	2.25125100	-4.18552400
H	8.32200300	1.50575900	-4.54989900
H	-12.40590600	-3.50238900	0.78683900
H	-9.88654000	-4.53187500	0.74607100
H	12.59666400	1.95548300	-2.25378200
H	-13.34538900	-1.07950500	0.76661100
H	-10.21409600	3.47231400	-1.50882700
H	-11.51001400	4.68467600	-1.36130200
H	11.01413500	0.04979800	3.19847100
H	12.64848000	0.12455300	3.90192900
H	11.08760500	1.66853400	5.10974700
H	12.35566900	2.59342300	4.28728700
H	10.72032700	2.50208800	3.59007500
H	-9.49579500	5.36875500	-0.03485900
H	-10.86904000	5.06070500	1.04215400
H	-9.57183100	3.85309900	0.87978900

## F8IDT

0 1			
C	0.72818000	-0.54778700	-0.00040600
C	1.17353600	-1.88205100	-0.00020000
C	0.00000000	-2.84890000	0.00020300
C	-1.17353500	-1.88205100	0.00018000
C	-0.72817900	-0.54778700	-0.00017600
C	-2.52387500	-2.17339500	0.00044800
C	-3.46757600	-1.12698700	0.00034700
C	-3.00334000	0.20269800	-0.00000400
C	-1.64893000	0.49971700	-0.00025700
C	1.64893100	0.49971700	-0.00076700
C	3.00334100	0.20269800	-0.00091000
C	3.46757700	-1.12698700	-0.00070300
C	2.52387600	-2.17339600	-0.00034600
C	-0.00020500	-3.72765500	-1.25913900
C	0.00020600	-3.72710000	1.25993200
C	-4.89669000	-1.42466700	0.00059100
C	4.89669000	-1.42466700	-0.00084300
C	-5.50536300	-2.67227500	0.00103500
C	-6.90023000	-2.59818500	0.00115100
C	-7.39788200	-1.29809700	0.00078300
S	-6.07857000	-0.15653200	0.00030100
S	6.07857100	-0.15653300	-0.00040300
C	7.39788200	-1.29809700	-0.00084800
C	6.90023100	-2.59818600	-0.00129900
C	5.50536400	-2.67227600	-0.00128700
C	-8.78912100	-1.01442700	0.00080900
C	8.78912100	-1.01442700	-0.00077600
C	9.50805500	0.14297400	-0.00031900
C	-9.50805600	0.14297400	0.00043000
C	-10.98955900	0.11042800	0.00057100
C	-11.44245200	1.52837800	0.00001500
C	-10.32443500	2.36794500	-0.00043300
C	-9.07868100	1.54980400	-0.00019100
C	10.98955800	0.11042900	-0.00038100
C	11.44245100	1.52837900	0.00023400
C	10.32443400	2.36794600	0.00063900
C	9.07868000	1.54980400	0.00031300
C	-12.73029400	2.04570800	-0.00010400
C	-12.87328700	3.43287500	-0.00068800
C	-11.75363100	4.27336700	-0.00113700
C	-10.46153000	3.74882300	-0.00101300
C	12.73029300	2.04570900	0.00043400
C	12.87328600	3.43287600	0.00105400
C	11.75363000	4.27336800	0.00145900
C	10.46152800	3.74882400	0.00125500
O	7.93930100	1.99436100	0.00055700
O	11.70346800	-0.87939300	-0.00083700
O	-7.93930200	1.99436100	-0.00047800
O	-11.70346900	-0.87939400	0.00105100
H	-2.85571300	-3.20725600	0.00071900
H	-3.71649800	1.02224300	-0.00007500
H	-1.32160700	1.53517000	-0.00051600
H	1.32160800	1.53516900	-0.00094900
H	3.71649900	1.02224200	-0.00122500
H	2.85571400	-3.20725700	-0.00013800
H	0.88458000	-4.37189100	-1.27695800
H	-0.88499600	-4.37189200	-1.27666900

H	-0.00035400	-3.11704400	-2.16626700
H	-0.88458000	-4.37132700	1.27803100
H	0.88499700	-4.37132800	1.27774200
H	0.00035500	-3.11609200	2.16679200
H	-4.96064300	-3.60814300	0.00127300
H	-7.55613300	-3.46222600	0.00148500
H	7.55613400	-3.46222700	-0.00163400
H	4.96064400	-3.60814400	-0.00164000
H	-9.41007500	-1.91300100	0.00120100
H	9.41007600	-1.91300000	-0.00115700
H	-13.59260700	1.38625500	0.00024400
H	-13.86657900	3.87159400	-0.00079900
H	-11.89762600	5.34965600	-0.00158700
H	-9.58710800	4.39215000	-0.00135800
H	13.59260600	1.38625600	0.00011800
H	13.86657700	3.87159600	0.00122700
H	11.89762400	5.34965700	0.00193900
H	9.58710700	4.39215000	0.00156700

## DICTF

0 1

C	1.41350100	-1.78451200	-0.34210500
C	1.02721400	-0.43672700	-0.22468000
C	-0.41945600	-0.38511700	-0.06028100
C	-0.91505100	-1.70190000	-0.06932800
C	0.20990600	-2.70773100	-0.24852400
C	-1.28814000	0.69632300	0.08679400
C	-2.64606600	0.45090100	0.22528300
C	-3.15766000	-0.86104000	0.21628900
C	-2.26881700	-1.94321400	0.06463400
C	2.74323300	-2.12216800	-0.50598500
C	3.71708200	-1.10632500	-0.55956600
C	3.31578800	0.23742700	-0.43899000
C	1.98213000	0.57901000	-0.27148100
C	0.03030000	-3.52589200	-1.53582800
C	0.31795600	-3.64479100	0.96375100
C	-4.58676100	-1.11143700	0.35934000
C	5.11961400	-1.45958500	-0.74074200
S	-5.75254800	0.11270900	-0.00803600
C	-7.08202900	-0.94273000	0.40950200
C	-6.58609400	-2.19015500	0.80289200
C	-5.19713100	-2.28847100	0.77539600
C	5.63926500	-2.62614100	-1.28342100
C	7.03562000	-2.62938600	-1.34369700
C	7.62398700	-1.48297200	-0.81598400
S	6.38901700	-0.38304300	-0.27027200
C	-8.47817900	-0.70437600	0.38714200
C	9.01688800	-1.21707500	-0.87477400
C	-9.25470600	0.38349300	0.06561600
C	9.81326100	-0.21309900	-0.39496200
C	-10.71184400	0.45279300	0.10232900
C	-11.09890200	1.82815100	-0.28314000
C	-9.93722400	2.56399400	-0.56116100
C	-8.75486700	1.70454600	-0.36394600
C	11.11138400	0.03031500	-1.09204300
C	11.51904100	1.40167700	-0.71452200
C	10.61411400	1.91275900	0.23255700
C	9.64563300	0.85141700	0.57533000
O	-7.59111700	2.03959300	-0.52786400
O	11.68060700	-0.72455900	-1.85920500
C	-11.60631300	-0.55043000	0.41919400
C	8.92298700	0.77976500	1.74799500
C	-12.34215900	2.45116900	-0.40223600
C	-12.38079000	3.78875700	-0.79574000
C	-11.21451300	4.50669100	-1.07039800
C	-9.97026200	3.89152500	-0.95351200
C	12.58836600	2.14543600	-1.18608000
C	12.74302900	3.44521600	-0.70793900
C	11.83842700	3.96937600	0.21902400
C	10.77173300	3.21395700	0.70624100
C	8.33970200	-0.43475300	2.20763500
N	7.90462900	-1.42410800	2.63784900
C	8.83733300	1.85634300	2.67592700
N	8.73501800	2.71984200	3.44879400
C	-13.01983600	-0.37492500	0.42156300
N	-14.18047800	-0.29370500	0.44143500
C	-11.23724000	-1.87940300	0.77407900
N	-10.99324600	-2.97871600	1.06888200
H	-0.91660000	1.71654700	0.10188400

H	-3.32326100	1.28874000	0.36444900
H	-2.65286100	-2.95864800	0.02909600
H	3.04393100	-3.16406200	-0.56853100
H	4.05997300	1.02672500	-0.49898600
H	1.69590000	1.62297700	-0.18582200
H	0.88036100	-4.19962200	-1.68263000
H	-0.87606300	-4.13664000	-1.47708000
H	-0.04874900	-2.87427400	-2.41046000
H	1.17275100	-4.31904500	0.85153100
H	0.44501100	-3.07856700	1.89058000
H	-0.58458500	-4.25740200	1.05415300
H	-7.24695700	-2.99389800	1.10989800
H	-4.64894300	-3.17304800	1.07571400
H	5.01873000	-3.42868300	-1.66270200
H	7.62545900	-3.43410500	-1.76884500
H	-9.01362500	-1.59583700	0.69933000
H	9.55605700	-1.89722000	-1.53725100
H	-13.27006000	1.93338800	-0.19883400
H	-13.34408500	4.28033300	-0.88956700
H	-11.28205300	5.54637300	-1.37484300
H	-9.04650400	4.42298800	-1.15952700
H	13.27618700	1.71734500	-1.90846100
H	13.56701200	4.05853500	-1.05873600
H	11.96612400	4.98844400	0.57047800
H	10.08523700	3.65039700	1.42124200

## DBS-2DPP

0	1		
C	1.58255100	0.00321800	0.59599400
C	0.63180700	1.05111900	0.58947100
C	-0.78038500	0.62085600	0.60775500
C	-0.98417500	-0.77970500	0.63998900
Si	0.68584700	-1.65437800	0.63571900
C	-1.88519900	1.47680200	0.59387800
C	-3.17057300	0.95569900	0.61843000
C	-3.39378800	-0.43027600	0.64972100
C	-2.27638800	-1.28520500	0.65488500
C	2.93708400	0.30658400	0.58956800
C	3.38668000	1.63870700	0.56937100
C	2.42708400	2.66477600	0.55373100
C	1.07027100	2.37877200	0.56853500
C	0.97480700	-2.70129800	-0.89715700
C	1.02057100	-2.63937700	2.20026600
C	-4.74370700	-0.98397200	0.67554400
C	4.80897500	1.96463900	0.56955600
S	-6.09695900	-0.07886900	0.09028800
C	-7.21266100	-1.36951400	0.46003500
C	-6.52820100	-2.44087000	1.01677200
C	-5.14664100	-2.22216200	1.13752300
C	5.41395200	3.13663200	0.98106900
C	6.81199400	3.11765000	0.85529700
C	7.30666100	1.92537900	0.34519900
S	5.99051900	0.82394500	0.02562500
C	-8.61240800	-1.20539600	0.18955400
C	8.65894900	1.51896900	0.09047100
N	9.74431300	2.38364900	0.08725600
C	10.96312200	1.69808200	-0.17547400
C	10.56303900	0.32122000	-0.32906900
C	9.15478700	0.24903800	-0.17952500
C	-9.31130100	-0.04795400	-0.13149400
C	-10.68570300	-0.36157000	-0.28544000
C	-10.85087800	-1.77935900	-0.08004400
N	-9.53724500	-2.23960300	0.21616600
C	-9.15347100	1.37606900	-0.29028700
N	-10.47872100	1.84635800	-0.51284300
C	-11.39876000	0.80905200	-0.50633100
C	11.07025000	-0.95993300	-0.49999400
N	9.98812900	-1.82712800	-0.48089000
C	8.76007000	-1.13273600	-0.28981800
O	-11.81720500	-2.52874000	-0.14262100
O	-8.17943400	2.11866300	-0.28590000
C	-12.81440000	0.98779700	-0.69021800
C	-13.57992900	2.14220100	-0.63964100
C	-14.95470900	1.91250100	-0.86185700
C	-15.23390900	0.58986400	-1.08386300
S	-13.83590500	-0.39285100	-1.00634800
O	12.04237700	2.27111600	-0.25486500
O	7.67430700	-1.69968400	-0.27045700

C	9.75105100	3.82294900	0.19166900
C	9.96446300	-3.24655500	-0.74101900
C	-9.30449900	-3.65397800	0.38269300
C	-10.69192100	3.23906100	-0.82572100
C	12.43712300	-1.37983000	-0.65843600
S	13.68142700	-0.19876200	-0.98690600
C	14.89386600	-1.40501900	-1.02175800
C	14.39236700	-2.65618000	-0.77763000
C	12.99596600	-2.64539000	-0.57239700
H	-1.75532200	2.55482000	0.57311700
H	-4.01705200	1.63722700	0.63302800
H	-2.43796300	-2.36024800	0.64929500
H	3.67056800	-0.49671800	0.62123300
H	2.75089700	3.70016900	0.50971300
H	0.35966800	3.20006400	0.55392200
H	0.31616200	-3.57612900	-0.89911100
H	0.78259400	-2.12687100	-1.80776900
H	2.00860300	-3.06048800	-0.93131100
H	2.05820000	-2.98866900	2.22086300
H	0.84768500	-2.03106900	3.09260100
H	0.37093300	-3.51918000	2.25426100
H	-7.00622300	-3.34633700	1.36185100
H	-4.46723700	-2.93946100	1.58282100
H	4.86512100	3.97446600	1.39485600
H	7.43504600	3.94412600	1.16530000
H	-13.17769600	3.12198900	-0.42579500
H	-15.70668600	2.69254300	-0.85440900
H	-16.19617000	0.13545600	-1.28022000
H	10.74806300	4.14695000	-0.11101100
H	9.00662800	4.26794200	-0.47277500
H	9.57775800	4.15812400	1.21900600
H	10.53519700	-3.48985500	-1.64024100
H	10.34690600	-3.82309200	0.10695400
H	8.91707700	-3.51274400	-0.89188600
H	-10.23064900	-4.15253500	0.09235600
H	-8.48976800	-3.99614900	-0.25985700
H	-9.08804900	-3.91131700	1.42415300
H	-11.29353200	3.34937000	-1.73084600
H	-11.16772100	3.77467800	0.00160100
H	-9.70353700	3.67108100	-0.98982700
H	15.92147200	-1.12420800	-1.21191300
H	15.00136600	-3.55167100	-0.74277100
H	12.43151000	-3.53826400	-0.34569600

## F(DPP)2B2

0 1			
C	-1.11560800	-1.79419100	-0.15507400
C	-0.52656100	-0.61462100	-0.64522300
C	0.92201600	-0.77371800	-0.61134100
C	1.21758900	-2.04969100	-0.09853300
C	-0.05496500	-2.80795000	0.24348500
C	1.95075300	0.09202800	-0.98012600
C	3.26600800	-0.32716200	-0.83730000
C	3.57735800	-1.59944700	-0.32326700
C	2.52859800	-2.46114700	0.05084000
C	-2.48997300	-1.91202800	-0.07068500
C	-3.30854400	-0.84446600	-0.48665200
C	-2.70498400	0.32884600	-0.97520400
C	-1.32496400	0.45262400	-1.05437100
C	-0.12656700	-3.12881600	1.74361800
C	-0.17598400	-4.09782900	-0.58056300
C	4.96297200	-2.03369500	-0.17449900
C	-4.75984900	-0.97131500	-0.40720000
S	6.25198200	-0.88816900	-0.03299800
C	7.45511900	-2.14694200	0.09401400
C	6.84498100	-3.39165100	0.02263500
C	5.45052600	-3.32533200	-0.12862900
C	-5.51975200	-2.12572200	-0.38960700
C	-6.90077900	-1.89280800	-0.30701500
C	-7.22943900	-0.54519800	-0.25743200
S	-5.78019400	0.42511200	-0.30657100
C	8.84046900	-1.79942000	0.23184400
C	-8.56851500	-0.04409400	-0.17453000
N	-8.93911300	1.28714700	-0.11095100
C	-10.35341600	1.43878100	-0.03394000

C	-10.85101700	0.08540500	-0.06168800
C	-9.74272900	-0.79369300	-0.14244000
C	9.45408900	-0.56255300	0.06828100
C	10.84729500	-0.70191200	0.28594400
C	11.11732300	-2.07577300	0.61804500
N	9.84267000	-2.70064400	0.56498200
C	9.18675700	0.80897700	-0.28830800
N	10.47114000	1.42495000	-0.27260400
C	11.46636500	0.52734400	0.07004600
C	-12.02592800	-0.65818800	-0.07462700
N	-11.65130900	-1.99308500	-0.14866600
C	-10.23927400	-2.14298100	-0.19178500
O	12.14199000	-2.68762200	0.91084000
O	8.16093100	1.42434200	-0.54929100
C	12.86535800	0.81770000	0.17597000
C	13.82990800	-0.10636700	0.55154700
C	15.12920400	0.42471500	0.57486900
C	15.19112400	1.75814000	0.22137500
S	13.61211100	2.35887900	-0.15731100
O	-10.89814700	2.53233900	0.04639900
O	-9.69218400	-3.24213500	-0.24691500
C	-8.09282800	2.45619800	-0.09575800
C	-12.48675000	-3.16885400	-0.10226000
C	9.71857100	-4.09025800	0.93395300
C	10.59228800	2.83312900	-0.56509600
C	-13.38611400	-0.20201300	-0.02800900
S	-13.73027600	1.47010600	0.33986000
C	-15.43624300	1.22502200	0.19955600
C	-15.71772900	-0.08753700	-0.12068700
C	-14.57136000	-0.88955400	-0.24821500
C	16.36818500	2.62117100	0.144416100
C	-16.37933100	2.32323000	0.40598600
C	16.26582600	4.01452900	0.27442100
C	17.39663400	4.81855600	0.20210600
C	18.65238600	4.24826200	0.00628400
C	18.76710400	2.86533900	-0.12295100
C	17.63819700	2.05861400	-0.06031800
C	-16.00005400	3.66020300	0.21235400
C	-16.91049800	4.69092100	0.41116500
C	-18.21803900	4.40832800	0.79966300
C	-18.60679400	3.08417500	0.99431500
C	-17.69746200	2.05138900	0.80522400
H	1.73693900	1.07804400	-1.38242700
H	4.06979800	0.33470300	-1.14780800
H	2.75657500	-3.43466900	0.47654900
H	-2.94299000	-2.81190600	0.33616500
H	-3.33066300	1.14831000	-1.31820700
H	-0.88360300	1.36750700	-1.43883800
H	-1.07690700	-3.61437900	1.98724700
H	0.68199200	-3.80944600	2.02879300
H	-0.03976800	-2.21996400	2.34542900
H	-1.12570800	-4.60013700	-0.37026000
H	-0.12800400	-3.88702700	-1.65252200
H	0.63368700	-4.79021200	-0.32865300
H	7.38336800	-4.32804100	0.04303400
H	4.82169000	-4.20132300	-0.23660600
H	-5.08588300	-3.11594900	-0.46493500
H	-7.66372800	-2.66675500	-0.29383600
H	13.57105900	-1.13142700	0.80320200
H	16.00182000	-0.14488700	0.87249200
H	-8.76347600	3.31441300	-0.02641700
H	-7.42486200	2.45859800	0.77018100
H	-7.50616800	2.53950400	-1.01493600
H	-13.17700900	-3.12717600	0.74376000
H	-13.04756200	-3.30626000	-1.03184600
H	-11.81274200	-4.01773800	0.02142200
H	10.68470600	-4.38488600	1.34625100
H	8.94299100	-4.22702600	1.69127200
H	9.50609100	-4.72428000	0.06756200
H	11.20210600	3.00821500	-1.45591700
H	9.57902900	3.19072700	-0.75623900
H	11.00918200	3.38482400	0.28212500
H	-16.72326300	-0.45392500	-0.29166300
H	-14.62055600	-1.93227800	-0.52570900
H	15.29582300	4.47010700	0.45525200
H	17.29689400	5.89459900	0.30881100
H	19.53587400	4.87716800	-0.04701200
H	19.74073400	2.41211900	-0.28420700
H	17.73597800	0.98534000	-0.19161500
H	-14.99037300	3.89297600	-0.11542500
H	-16.59846600	5.71896500	0.25313800

H	-18.92914000	5.21459800	0.95218100
H	-19.62149700	2.85443200	1.30589400
H	-18.00208500	1.02552000	0.98885500

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C	1.06458400	-2.12073000	-0.18799300
C	1.81095000	-0.96015400	0.12297100
C	3.20104300	-1.33576400	0.04759000
C	3.33504300	-2.66796100	-0.29432700
C	1.97702100	-3.30869500	-0.48375400
C	-0.31393500	-2.07455100	-0.20574900
C	-0.97966100	-0.86935800	0.09897100
C	-0.21936100	0.27304800	0.40742100
C	1.16786600	0.24042900	0.41879400
S	4.71343900	-0.56299400	0.28048200
C	5.56042900	-2.05045100	-0.09631700
C	4.67332700	-3.08094400	-0.37892600
C	1.78784000	-3.81525700	-1.92108200
C	1.74962600	-4.44932700	0.51925300
C	6.99368800	-2.12234300	-0.09154900
C	7.77640200	-3.27303400	-0.14825400
C	9.14287300	-3.00058600	-0.15142600
C	9.45397100	-1.64344300	-0.06174200
S	7.98478700	-0.70490700	-0.02750600
C	-2.43687700	-0.82684200	0.09614700
S	-3.29768000	0.66511700	-0.11407900
C	-4.84363800	-0.12281200	0.01904400
C	-4.67292800	-1.48242100	0.20397800
C	-3.32389200	-1.87580300	0.24601600
C	-8.45851600	1.34481300	-0.14250300
C	-7.54068800	2.39641800	-0.25311800
C	-6.20841200	2.00270200	-0.21007000
C	-6.06564800	0.62507000	-0.06495800
S	-7.60175400	-0.17377700	0.01434100
C	10.76907200	-1.12921000	-0.15442500
C	-9.84803700	1.60632400	-0.16410900
C	11.30869700	0.12832400	-0.06534500
C	-10.96931500	0.81358200	-0.07130600
C	12.61189100	0.36638600	-0.75152400
C	12.72484600	1.83470800	-0.90209100
C	11.64024700	2.45355400	-0.25640300
C	10.83966200	1.40983700	0.41847900
C	-12.35642400	1.26125900	-0.10451100
C	-13.21184100	0.06152700	0.04142000
C	-12.38905100	-1.06904800	0.15409500
C	-10.97517800	-0.65288800	0.08777400
C	9.99871400	1.62076200	1.49275800
C	-12.83583400	2.54923000	-0.24375300
O	13.38999600	-0.47841300	-1.15602300
O	-10.00683500	-1.39584700	0.15407100
C	13.69334500	2.56119100	-1.57459000
C	13.55997800	3.94783700	-1.61666500
C	12.47664400	4.57179500	-0.99349600
C	11.51070900	3.84033200	-0.30166900
C	-14.59735000	-0.10034800	0.08284600
C	-15.11203900	-1.38789700	0.23556200
C	-14.27869000	-2.50314800	0.34569000
C	-12.89485000	-2.34897400	0.30503400
C	9.59447700	0.56546400	2.35824100
N	9.29844600	-0.26612800	3.11607800
C	9.60129600	2.91736600	1.92603400
N	9.24584600	3.96183600	2.29550600
C	-14.22195400	2.87609700	-0.26459400
N	-15.33862700	3.20262900	-0.28878200
C	-12.01420000	3.70403100	-0.38354200
N	-11.38783400	4.67821900	-0.50053200
H	-0.89022500	-2.95520500	-0.47467700
H	-0.72616900	1.19885200	0.66478700
H	1.73356300	1.13374800	0.66474000
H	5.00298900	-4.07799100	-0.64774200
H	0.77843600	-4.21631300	-2.05573700
H	1.93965200	-3.01099400	-2.64593000
H	2.50045500	-4.61688000	-2.13905100
H	2.45802900	-5.26344800	0.33655500
H	1.87986200	-4.10209200	1.54773900
H	0.73778900	-4.85343100	0.41619900
H	7.35639600	-4.27074000	-0.17717100



H	9.91428500	-3.76098300	-0.20597900
H	-5.50246000	-2.17135600	0.32104200
H	-3.00551100	-2.89761200	0.41498900
H	-7.86689600	3.42555700	-0.35941800
H	-5.37062200	2.68736800	-0.27675900
H	11.49853600	-1.87249300	-0.48250700
H	-10.02618500	2.67142400	-0.27628800
H	14.52433700	2.05177500	-2.05232600
H	14.29761600	4.54916000	-2.13881200
H	12.38117200	5.65190800	-1.04639100
H	10.68112300	4.35384700	0.16850400
H	-15.27935800	0.73564100	0.00141700
H	-16.18885600	-1.52148400	0.26908100
H	-14.71417100	-3.49050400	0.46335300
H	-12.22008500	-3.19517000	0.38832600

## CDTBM

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C	-1.16192400	-1.69108900	-0.00016100
C	-0.71262400	-0.37244600	0.00001500
C	0.71262700	-0.37244400	-0.00000700
C	1.16192600	-1.69108900	-0.00019500
C	0.00000200	-2.66970400	-0.00032900
S	1.98545500	0.77089800	0.00004300
C	3.17501900	-0.52542400	-0.00012500
C	2.55331900	-1.77600300	-0.00025800
C	-2.55331800	-1.77600100	-0.00015600
C	-3.17501400	-0.52542000	0.00002200
S	-1.98545600	0.77089600	0.00019600
C	-0.00001300	-3.54422900	-1.26258500
C	0.00001800	-3.54465000	1.26163400
C	4.59308200	-0.27783500	-0.00006800
C	-4.59307800	-0.27783400	0.00003800
C	5.52596700	-1.31631800	0.00015700
C	6.91152600	-1.11495500	0.00021400
C	7.50054700	0.14846300	0.00006900
C	6.58319500	1.25303600	-0.00015400
C	5.15776000	1.04346400	-0.00022400
C	-5.15776000	1.04346500	0.00015500
C	-6.58319400	1.25303400	0.00016500
C	-7.50054500	0.14846000	0.00006800
C	-6.91152100	-1.11495700	-0.00005300
C	-5.52596100	-1.31631800	-0.00006500
N	-4.46229200	2.17904200	0.00034300
S	-5.53974500	3.39518600	0.00009000
N	-6.92315200	2.54068700	0.00035400
N	6.92315000	2.54068900	-0.00029600
S	5.53974000	3.39518500	-0.00056900
N	4.46229000	2.17903900	-0.00041200
C	-8.90039500	0.44401800	0.00008400
C	8.90039600	0.44402200	0.00015800
C	-9.99017300	-0.38673200	0.00008200
C	9.99017200	-0.38673100	0.00032700
C	-11.30048100	0.17958600	0.00008900
N	-12.36896100	0.63784900	0.00009600
C	-9.94048800	-1.81088400	0.00007800
N	-9.91767200	-2.97377000	0.00006400
C	11.30048200	0.17958300	0.00039000
N	12.36896300	0.63784500	0.00044300
C	9.94048300	-1.81088300	0.00044900
N	9.91765200	-2.97376800	0.00056000
H	3.10535200	-2.70829000	-0.00041800
H	-3.10535300	-2.70828700	-0.00029000
H	-0.88531100	-4.18717900	-1.27852200
H	-0.00002300	-2.93136600	-2.16776200
H	0.88528300	-4.18718100	-1.27854300
H	0.88531700	-4.18760500	1.27735600
H	0.00002400	-2.93209000	2.16701500
H	-0.88527600	-4.18761200	1.27737400
H	5.17769200	-2.34238400	0.00033400
H	7.53840600	-1.99877700	0.00040500
H	-7.53839900	-1.99878000	-0.00012900
H	-5.17768600	-2.34238400	-0.00014200
H	-9.13214500	1.50644700	0.00010600
H	9.13214700	1.50645000	0.00007400

# IDTBC6

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C		-0.53514600	-1.34068800	-0.06172200
C		0.83339100	-1.13444700	-0.07801900
C		1.36425600	0.17706500	-0.07703000
C		0.53701000	1.30363000	-0.06774100
C		1.95043300	-2.18955400	-0.07367000
C		3.17416900	-1.28706200	-0.05699500
C		2.80203900	0.03788700	-0.07811200
C		4.57008800	-1.47210900	-0.04247000
C		5.26483000	-0.27551300	-0.05348100
S		4.15524200	1.08922900	-0.08358300
C		-1.94858000	2.15256800	-0.04575000
C		-3.17242800	1.24995600	-0.05162200
C		-2.80015200	-0.07509600	-0.04643300
C		-4.56809200	1.43522200	-0.02139800
C		-5.26271100	0.23860000	-0.00803000
S		-4.15317800	-1.12632100	-0.01227200
C		-1.81860900	3.00581300	-1.31237100
C		-1.98255300	2.99887400	1.23272700
C		1.81191500	-3.03968900	1.19451000
C		1.99220900	-3.03784000	-1.35035700
C		-0.98071600	4.12567300	-1.33316300
C		-0.79336400	4.85592100	-2.50133700
C		-1.43644500	4.50042700	-3.69054800
C		-2.26855400	3.37919800	-3.66609000
C		-2.45712600	2.64354100	-2.49989300
C		-2.78054600	4.14799100	1.28173600
C		-2.89676800	4.88900100	2.45113400
C		-2.22200800	4.51374800	3.61741400
C		-1.43551500	3.36202400	3.56689900
C		-1.31627500	2.61549000	2.39717200
C		0.98240400	-4.16581000	1.21027100
C		0.78660300	-4.89251100	2.37933500
C		1.41212300	-4.52683000	3.57475700
C		2.23505400	-3.39872100	3.55563600
C		2.43205500	-2.66663700	2.38860900
C		2.79005600	-4.18754200	-1.39319100
C		2.91202600	-4.93063400	-2.56038500
C		2.24343700	-4.55711700	-3.73102900
C		1.45707400	-3.40533500	-3.68661100
C		1.33203500	-2.65652500	-2.51870400
C		-1.26025600	5.31319900	-4.94206200
C		-2.32126100	5.33736100	4.87028400
C		1.22638000	-5.33531200	4.82763000
C		2.35139700	-5.38292500	-4.98174100
C		-12.01835900	-0.34329600	0.07599900
C		-13.33839500	-0.98073200	0.06351200
C		-14.35295800	0.07859800	-0.08436900
C		-13.70632000	1.32181000	-0.04149300
C		-12.24835600	1.13123300	0.11053300
C		-15.74023500	0.03425500	-0.23733100
C		-16.43399400	1.23891200	-0.33893500
C		-15.77636900	2.47102200	-0.28486200
C		-14.39305100	2.52133500	-0.13476500
O		-11.43570400	2.03520500	0.20126700
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C		6.70162200	-0.02336000	-0.06516700
C		-6.69995300	-0.01172500	-0.02299500
C		7.18033000	1.11811200	-0.73675800
C		8.51722600	1.47260800	-0.78243700
C		9.45851700	0.62357000	-0.13378700
C		8.97666100	-0.51086900	0.54607100
C		7.63390300	-0.85745600	0.60105600
C		-7.17665000	-1.16462700	-0.67633900
C		-8.51526500	-1.51100700	-0.73365700
C		-9.45954400	-0.63936400	-0.12147400
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C		-7.63498900	0.83939800	0.61714900
C		-10.84704400	-1.02322200	-0.13877000
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C		12.01826200	0.37723300	0.14871100
C		13.32497500	1.04217100	0.13956500
C		14.36518100	-0.00010700	0.07067500
C		13.74374800	-1.25328700	0.16341700
C		12.27873300	-1.08740000	0.26953500
C		15.75467800	0.06707100	-0.05009000

C	16.47577000	-1.12560100	-0.07056600
C	15.84285200	-2.36744400	0.03295400
C	14.45750000	-2.44054100	0.15161000
O	11.48478800	-2.00432000	0.39293500
C	13.56914000	2.39300100	0.26751800
C	-8.91947300	-2.76538500	-1.45708900
C	-7.24333900	2.06142400	1.39872900
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C	7.24088000	-2.07073900	1.39544600
C	-14.93517100	-2.85434100	0.22710600
N	-15.99217300	-3.34014700	0.21588100
C	-12.63058800	-3.31338000	0.52322400
N	-11.87754900	-4.16867300	0.75923200
C	14.87840300	2.95549700	0.25259500
N	15.92505300	3.46326600	0.24320400
C	12.55891000	3.37778900	0.47549100
N	11.78392500	4.22683900	0.65665500
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H	0.95549900	2.30586500	-0.07457100
H	5.05879000	-2.43718700	-0.06091700
H	-5.05691100	2.40006100	-0.04694600
H	-0.47638800	4.43819100	-0.42308800
H	-0.13527600	5.72168500	-2.48754200
H	-2.78034400	3.07359200	-4.57573200
H	-3.10881700	1.77490900	-2.51713900
H	-3.31088000	4.47233900	0.39047400
H	-3.52360700	5.77777400	2.45828100
H	-0.90353700	3.03852700	4.45851300
H	-0.69829800	1.72316000	2.39794400
H	0.49090000	-4.48576000	0.29580700
H	0.13516600	-5.76320800	2.36141200
H	2.73203700	-3.08429100	4.47046200
H	3.07447000	-1.79115300	2.41090800
H	3.31553400	-4.51047700	-0.49856200
H	3.53877700	-5.81950400	-2.56261000
H	0.92967300	-3.08346200	-4.58152100
H	0.71394200	-1.76426500	-2.52398800
H	-0.26164100	5.75630400	-4.99323400
H	-1.41086800	4.70440800	-5.83782100
H	-1.98324400	6.13670600	-4.98192700
H	-3.31517200	5.78105500	4.97907000
H	-2.11552000	4.73653800	5.76029600
H	-1.59818900	6.16160200	4.85769700
H	0.22701100	-5.77737100	4.87305000
H	1.94823500	-6.15940100	4.87534900
H	1.37092700	-4.72363600	5.72238100
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H	1.67396500	-6.24430100	-4.94466400
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H	-16.28505000	-0.89939800	-0.28858500
H	-17.51209400	1.21525400	-0.46366500
H	-16.34973800	3.38949800	-0.36225800
H	-13.85332100	3.46206500	-0.09106800
H	6.46638900	1.74428900	-1.26502900
H	9.69210800	-1.13876200	1.06091900
H	-6.45977000	-1.80671500	-1.18101600
H	-9.69703800	1.14418900	1.04081700
H	-10.98442000	-2.06743500	-0.39912400
H	10.97093100	2.05683400	-0.43622300
H	16.28099000	1.00862700	-0.13745400
H	17.55600900	-1.08473800	-0.16990500
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H	-8.04057200	-3.27235400	-1.86053600
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H	-9.59623300	-2.55614100	-2.29195500
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H	-6.32190000	1.90488600	1.96655700
H	-7.08145400	2.92631900	0.74503100
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H	9.41219200	3.44176900	-0.87255900
H	9.61505000	2.49089100	-2.34648600
H	8.03337300	-2.33271000	2.10007300
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C	1.36934000	-0.11489300	-0.00619000
C	0.61215600	-1.29134800	-0.00492000
C	1.81488600	2.28663100	-0.01391900
C	3.08599900	1.45442200	-0.04596500
C	2.79425800	0.09748800	-0.02510900
C	-1.81487500	-2.28662900	0.01388900
C	-3.08598800	-1.45442000	0.04595300
C	-2.79424600	-0.09748600	0.02509200
C	1.60763600	3.13144800	-1.27679900
C	1.82484800	3.13518800	1.26385900
C	-1.60761300	-3.13145900	1.27675900
C	-1.82485300	-3.13517600	-1.26389400
C	4.45452700	1.69577100	-0.05522600
C	5.22041200	0.51798500	-0.04922500
S	4.17913300	-0.90518000	-0.02069500
C	-4.45451700	-1.69576800	0.05523000
C	-5.22040100	-0.51798200	0.04923500
S	-4.17912100	0.90518300	0.02069200
C	6.63402300	0.59374400	-0.06758200
C	-6.63401200	-0.59374100	0.06760800
C	7.64215900	-0.34225500	-0.06899800
C	-7.64214900	0.34225700	0.06903200
C	9.07646600	-0.07596600	-0.09299200
C	9.76950400	-1.38393500	-0.07166700
C	8.80765300	-2.40467300	-0.04268600
C	7.45971800	-1.80634900	-0.04145500
C	-9.07645500	0.07596700	0.09304200
C	-9.76949500	1.38393400	0.07172700
C	-8.80764600	2.40467300	0.04273100
C	-7.45971000	1.80635100	0.04148400
C	11.12259000	-1.72618200	-0.07648400
C	11.46643800	-3.07781200	-0.05269100
C	10.49580500	-4.08180800	-0.02461900
C	9.14358100	-3.74763100	-0.01925100
C	-11.12258100	1.72617800	0.07656100
C	-11.46643200	3.07780800	0.05277100
C	-10.49580200	4.08180600	0.02468500
C	-9.14357600	3.74763100	0.01929900
O	6.40369400	-2.42130400	-0.02058700
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C	0.70867200	4.20270300	-1.27025600
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C	1.07455600	4.60218500	-3.63909100
C	1.96884400	3.52952200	-3.64083600
C	2.23106500	2.80436400	-2.48230400
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C	2.67613700	5.06560000	2.46241900
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C	1.27418600	3.49613900	3.59650700
C	1.17739500	2.73591700	2.43240700
C	-0.70865700	-4.20271600	1.27019500
C	-0.44700900	-4.92124500	2.43126200
C	-1.07451900	-4.60222500	3.63902900
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C	-2.23103100	-2.80438400	2.48227700
C	-2.58146600	-4.31310700	-1.29964500
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C	-2.01978300	-4.67427900	-3.63506900
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C	-1.17738000	-2.73592800	-2.43243200
C	-0.81621200	-5.40347400	4.88348800
C	-2.10305200	-5.50913900	-4.88145400
C	0.81623200	5.40342600	-4.88355200
C	2.10284500	5.50921500	4.88139000
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N	12.28347400	1.47450400	-0.17576900
C	9.05312200	2.40574400	-0.16237200
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H	4.92172300	2.67460100	-0.06611600
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H	11.90688600	-0.98122500	-0.09736800
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H	10.80012300	-5.12361000	-0.00671000
H	8.36537600	-4.50400000	0.00271200
H	-11.90687600	0.98122100	0.09745700
H	-12.51687100	3.35174000	0.05604800
H	-10.80012100	5.12360700	0.00677800
H	-8.36537300	4.50400100	-0.00267500
H	0.21491000	4.48667900	-0.34522500
H	-0.25759200	5.74875200	-2.39700400
H	2.47081900	3.25364800	-4.56515300
H	2.92907300	1.97333400	-2.52303400
H	3.09527000	4.65050900	0.40350900
H	3.27089100	5.97602400	2.46012200
H	0.75664500	3.16141000	4.49227300
H	0.59089100	1.82265400	2.44457800
H	-0.21490400	-4.48668500	0.34515700
H	0.25761300	-5.74878200	2.39692100
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H	-2.92903400	-1.97335000	2.52302000
H	-3.09530800	-4.65047400	-0.40354400
H	-3.27097100	-5.97597700	-2.46015700
H	-0.75662400	-3.16144400	-4.49229800
H	-0.59083400	-1.82269200	-2.44459700
H	0.20649900	-5.79032800	4.90374100
H	-0.97406200	-4.80392600	5.78413800
H	-1.49100500	-6.26570900	4.94285100
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H	-1.77296100	-4.94903600	-5.76005500
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H	1.49043300	6.26615200	-4.94249400
H	0.97488900	4.80411500	-5.78421500
H	-0.20674500	5.78956500	-4.90419300
H	3.12477400	5.85728300	5.06025000
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C	-0.89006900	-1.09257200	-0.00002600
C	0.47705900	-1.33076000	0.00000800
C	1.36861100	-0.22498200	-0.00005400
C	0.88986600	1.09283200	-0.00015400
Si	1.46006600	-2.95395300	0.00014600
C	3.07409700	-1.98785600	0.00010000
C	2.76845500	-0.62311300	-0.00000100
Si	-1.46027200	2.95421300	-0.00030000
C	-3.07430400	1.98811700	-0.00023100
C	-2.76865700	0.62337400	-0.00014900
C	-1.19524900	3.97094600	-1.55374700
C	1.19500700	-3.97067100	1.55359700
C	1.19507100	-3.97092600	-1.55315000
C	-1.19524100	3.97116800	1.55300100
C	4.45482900	-2.18386200	0.00013500
C	5.21362900	-1.00321100	0.00006800
S	4.15195300	0.39535200	-0.00004200
C	-4.45503600	2.18412500	-0.00022700
C	-5.21382300	1.00346500	-0.00014800
S	-4.15214900	-0.39509600	-0.00008300
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C	-6.62796700	1.06801400	-0.00008200
C	7.62876500	-0.12449700	0.00003700
C	-7.62879500	0.12450600	0.00000100
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C	-8.78025700	-1.94599600	-0.00011700
C	-7.43562600	-1.33904800	-0.00008100
C	9.06491200	-0.38157500	0.00005200
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C	8.78062800	1.94580600	0.00003300
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C	-9.05919000	2.86401200	0.00054800
N	-8.57280200	3.92156300	0.00072900
C	11.13283100	-1.73640000	0.00004800
N	12.28347000	-1.90977700	0.00006600
C	9.05907700	-2.86429400	-0.00001600
N	8.57288700	-3.92193600	-0.00007000
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H	1.59339000	1.92298600	-0.00020200
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H	-0.17720900	4.37268000	-1.58271500
H	-1.35122500	3.36764200	-2.45236300
H	1.89017200	-4.81588700	1.58272500
H	0.17695800	-4.37238300	1.58255600
H	1.35098600	-3.36736600	2.45221100
H	1.35104200	-3.36775700	-2.45185600
H	1.89027200	-4.81611700	-1.58213000
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H	-0.17719100	4.37287900	1.58192100
H	-1.89040300	4.81639200	1.58198400
H	-1.35124300	3.36800000	2.45170400
H	4.94197000	-3.15428300	0.00020500
H	-4.94218100	3.15454500	-0.00026700
H	6.95175600	-2.10412400	0.00014100
H	-6.95208000	2.10425500	-0.00010600
H	11.88908800	0.54156200	0.00013800
H	12.48396500	2.91644500	0.00013900
H	10.75560300	4.67781300	0.00007000
H	8.32463200	4.04238900	0.00000200
H	-11.88900700	-0.54240500	-0.00001600
H	-12.48338900	-2.91738900	-0.00021800
H	-10.75467300	-4.67840800	-0.00034600
H	-8.32383500	-4.04248700	-0.00028800

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C	1.39874600	-0.05815600	0.41782000
C	0.71986500	1.18366600	0.37436200
C	0.70862400	-1.27274600	0.47624400
C	-0.67389400	-1.22661000	0.48295100
C	-1.35364900	0.01510100	0.45347800
C	-0.66255700	1.22998800	0.40325600
C	-1.65861200	-2.40339000	0.55262700
C	-2.97732400	-1.64681300	0.57411200
C	-2.76427700	-0.28539300	0.50146100
C	-4.33659400	-1.98356300	0.60448000
C	-5.16520200	-0.86883900	0.56295800
S	-4.22324200	0.61200800	0.46253200
C	1.70654500	2.35983300	0.32978000
C	3.02656600	1.60618500	0.37393600
C	2.80842400	0.24549300	0.40507200
C	4.38846400	1.94935300	0.35287200
C	5.21387000	0.83500800	0.37285300
S	4.26933700	-0.64987600	0.40930800
C	1.47054200	3.24855400	1.55611600
C	1.65266800	3.15340600	-0.98218000
C	-1.63496800	-3.29276300	-0.69657700
C	-1.38836500	-3.19138300	1.83954500
C	0.51874900	4.27226100	1.51605700
C	0.23811100	5.03093200	2.64706700
C	0.89868600	4.80069800	3.85711700
C	1.84574100	3.77466300	3.89310400
C	2.12753700	3.01032800	2.76488600
C	2.35848100	4.35838700	-1.08384900
C	2.39905500	5.06511100	-2.27847600
C	1.73559200	4.59961700	-3.41906000
C	1.03839300	3.39578600	-3.31499800
C	0.99605600	2.68207200	-2.11886100

C	-2.31230000	-4.51822700	-0.68448000
C	-2.37938400	-5.30983200	-1.82377300
C	-1.77323100	-4.91163500	-3.02014500
C	-1.10600200	-3.68625800	-3.03004100
C	-1.03687200	-2.88824200	-1.89013200
C	-0.44271700	-4.22150900	1.85699500
C	-0.13101300	-4.88486400	3.03872100
C	-0.75201100	-4.54882100	4.24498600
C	-1.69157600	-3.51552900	4.22364400
C	-2.00486000	-2.84687400	3.04411900
C	0.62000400	5.64559500	5.06806900
C	1.75477600	5.38444500	-4.70029900
C	-1.81938200	-5.78670800	-4.24073800
C	-0.43964800	-5.29208500	5.51303700
C	-6.61122300	-0.87776100	0.60763400
C	6.65799600	0.77536800	0.36320600
C	-7.32298400	-2.03612900	0.87748500
C	-8.72571000	-2.05949600	0.89051800
C	-9.55508100	-0.98726000	0.61404600
C	-8.85910300	0.24472800	0.40254600
C	-7.41413900	0.29605500	0.39273500
C	7.48487300	1.95745300	0.33791600
C	8.92559700	1.84948000	0.32006700
C	9.60128800	0.58671500	0.30596000
C	8.75365900	-0.50261800	0.37408700
C	7.34913800	-0.42402400	0.39057100
N	-9.42398600	1.44091200	0.25857700
S	-8.21748100	2.51703200	0.09084600
N	-6.93559300	1.52410500	0.21090600
C	-10.99059000	-1.14378800	0.69728700
C	-11.94021700	-0.54979200	-0.06133500
S	-13.65889900	-0.66569100	0.29701300
C	-14.09951200	0.25925800	-1.12511700
N	-12.99016400	0.58787100	-1.84107300
C	-11.74856900	0.15826400	-1.34341500
S	-15.66652000	0.63502300	-1.48364000
C	-13.03634000	1.34833300	-3.08753200
C	-12.90627300	2.84238100	-2.84324900
O	-10.71374900	0.31467500	-1.95671700
N	7.06201900	3.21990100	0.33814300
S	8.38187300	4.16816000	0.32095400
N	9.54475500	3.02822200	0.30347500
C	11.04405000	0.55528000	0.36934500
C	11.90206700	-0.31868100	-0.20683100
S	13.63333400	-0.29694200	0.10923500
C	13.94528800	-1.55890800	-1.06539300
N	12.78777900	-1.94109900	-1.67170400
C	11.60398000	-1.30450800	-1.26505300
S	15.46056400	-2.14874400	-1.34853900
C	12.72901000	-2.96974100	-2.70771400
C	12.52085300	-4.35659400	-2.12264200
O	10.53178000	-1.53116600	-1.78667800
F	9.26163000	-1.72589500	0.49324300
F	-9.29455300	-3.23754700	1.17019000
H	1.24111000	-2.21835600	0.51876400
H	-1.19478400	2.17660200	0.39166500
H	-4.71278300	-2.99890600	0.63796600
H	4.78640200	2.95484900	0.32478700
H	-0.00267100	4.48670100	0.58744700
H	-0.50783500	5.82001200	2.58693700
H	2.37412100	3.56767300	4.82078500
H	2.86735000	2.21785600	2.82964900
H	2.87701700	4.75217600	-0.21390700
H	2.95668400	5.99752000	-2.32717300
H	0.51575200	3.00420600	-4.18451600
H	0.44486800	1.74786200	-2.07866700
H	-2.78504300	-4.86246500	0.23150800
H	-2.91243000	-6.25695500	-1.78366200
H	-0.62893700	-3.34500400	-3.94570700
H	-0.51090000	-1.93991600	-1.93829900
H	0.04905300	-4.51705800	0.93453200
H	0.60865100	-5.68195000	3.02206200
H	-2.18836400	-3.22593700	5.14668500
H	-2.73639400	-2.04436400	3.06519100
H	-0.40938900	6.01470100	5.06890100
H	0.78359200	5.08452000	5.99236100
H	1.27956500	6.52115000	5.09763800
H	2.72541900	5.86292700	-4.86049500
H	1.54116600	4.74694500	-5.56237300
H	1.00050900	6.18013900	-4.68571200
H	-1.04681300	-6.56355500	-4.19737100

H	-2.78361400	-6.29550200	-4.33094000
H	-1.65097000	-5.20831000	-5.15300400
H	0.59540000	-5.64506300	5.52410900
H	-0.59650100	-4.66296700	6.39353000
H	-1.08432300	-6.17238000	5.62211100
H	-6.82058700	-2.97157400	1.09272800
H	6.82323700	-1.37185800	0.44369100
H	-11.33280700	-1.82636800	1.47338900
H	-12.20965400	0.97653100	-3.69646900
H	-13.98099800	1.10418500	-3.57706300
H	-12.93424800	3.37324500	-3.79875700
H	-13.72728300	3.20962300	-2.22206200
H	-11.95807800	3.07357400	-2.35050700
H	11.47921900	1.36864600	0.94858500
H	11.89941900	-2.68996500	-3.36012200
H	13.66294200	-2.91118900	-3.26987600
H	12.47659100	-5.09115000	-2.93139500
H	13.34503000	-4.62784100	-1.45790800
H	11.58258600	-4.40655300	-1.56380200

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C	-4.18491500	-1.71369200	-0.02138900
C	-2.83441500	-1.45841900	0.08234400
C	-2.38077300	-0.19284500	0.51190400
C	-3.28832300	0.81534600	0.83751900
C	-4.64535300	0.54887700	0.73260300
C	-5.11775200	-0.70645100	0.30599600
C	-1.66816300	-2.39817600	-0.21453900
C	-0.48079400	-1.49101300	0.08649000
C	-0.94284000	-0.25230000	0.50653200
C	0.93697100	-1.53580800	0.07946800
C	1.48065100	-0.33181900	0.50278000
S	0.30754700	0.86883400	0.90480000
C	2.06162600	-2.50418300	-0.26782200
C	3.28767200	-1.65719200	0.06543100
C	2.91942900	-0.36876900	0.50900800
C	4.61790200	-2.00403000	-0.03543400
C	5.61483000	-1.06789100	0.31289700
C	5.22818100	0.21140800	0.75281200
C	3.89211100	0.57050800	0.85177600
C	-1.72800200	-3.60996000	0.72885200
C	-1.71128200	-2.86155800	-1.67726000
C	2.07389200	-2.86527600	-1.76190100
C	2.04320800	-3.77784300	0.58812900
C	-6.54384400	-0.97800900	0.20187400
C	7.01852700	-1.43797900	0.21811600
S	-7.69676600	0.30608100	0.07335800
C	-9.03480400	-0.81828700	0.01663700
C	-8.54952100	-2.12928300	0.08456900
C	-7.16477700	-2.22259800	0.18650700
C	7.56578300	-2.71437200	0.20641800
C	8.95720600	-2.71531200	0.08641900
C	9.51929300	-1.44161200	0.03356500
S	8.25942600	-0.23977600	0.08663400
C	-10.42559600	-0.57711900	-0.08576600
C	10.89729600	-1.19967900	-0.19504300
C	-11.19403300	0.56144400	-0.16062600
C	-12.64799600	0.62395500	-0.25759300
C	-13.02792800	2.05449200	-0.29083200
C	-11.86293400	2.83319000	-0.22746700
C	-10.68581800	1.94709600	-0.14775300
C	11.67218000	-0.07124700	-0.24043700
C	12.93851000	-0.13984400	-1.02789400
C	13.31762000	1.26405400	-1.30278500
C	12.42772900	2.12563400	-0.63789100
C	11.49982500	1.30760700	0.17112900
O	13.50538500	-1.14599200	-1.41320000
O	-9.52075900	2.30998200	-0.08391500
C	10.80862600	1.74960800	1.28024500
C	-13.54660100	-0.42340000	-0.31508600
C	-14.26723100	2.69161600	-0.36864500
C	-14.29812200	4.08608000	-0.38100000
C	-13.12840500	4.84667600	-0.31838900
C	-11.88815100	4.21742900	-0.24029800
C	14.34961400	1.73970700	-2.09472800
C	14.48161500	3.11945700	-2.23865800
C	13.59180900	3.98441900	-1.59696200



C	12.56294200	3.50484000	-0.78599100
C	10.27373800	0.85404900	2.24891000
N	9.87884000	0.14948400	3.08614200
C	10.71083000	3.12418700	1.63856800
N	10.59858200	4.23936500	1.95060000
C	-14.95687400	-0.24757400	-0.41074700
N	-16.11500500	-0.16580300	-0.48925200
C	-13.18284100	-1.80012300	-0.29016400
N	-12.93928500	-2.93830200	-0.27378400
H	-4.53574900	-2.67847000	-0.37631500
H	-2.94759000	1.78937800	1.17499700
H	-5.35644400	1.32258800	1.00779600
H	4.90447100	-2.98589800	-0.40182100
H	5.98927300	0.92837000	1.04767200
H	3.61761500	1.56092200	1.20152100
H	-0.89589700	-4.29215500	0.53931900
H	-1.68913900	-3.29725700	1.77573700
H	-2.65720400	-4.16588700	0.56936100
H	-0.89295500	-3.55474300	-1.88843600
H	-2.64919800	-3.38788700	-1.87995800
H	-1.63653000	-2.01451600	-2.36434900
H	1.19730000	-3.46162000	-2.02634700
H	2.08199300	-1.96656000	-2.38445900
H	2.96356000	-3.45676700	-1.99950900
H	1.17825600	-4.39925400	0.34270300
H	2.94171100	-4.37289100	0.39757800
H	2.00867500	-3.53829400	1.65422600
H	-9.21788800	-2.98395400	0.07084000
H	-6.62884300	-3.15936500	0.27907100
H	6.96901500	-3.61287500	0.30376800
H	9.56564300	-3.61248200	0.05093700
H	-10.96663300	-1.51822800	-0.10464400
H	11.44163100	-2.08977200	-0.51723400
H	-15.19733500	2.14113800	-0.41843300
H	-15.25844200	4.58880200	-0.44093800
H	-13.19024500	5.93036900	-0.33039400
H	-10.96104200	4.77974000	-0.18982300
H	15.02579200	1.04626200	-2.58481800
H	15.27609000	3.52799200	-2.85527300
H	13.70100600	5.05627900	-1.73004700
H	11.88767300	4.20158000	-0.30481000

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C	-1.37016900	0.10286900	0.00430600
C	-0.75424800	-1.17383900	-0.00098400
C	-0.62350600	1.28615200	0.00098100
C	0.75421000	1.17384500	0.00130900
C	1.37012900	-0.10286300	-0.00398700
C	0.62346700	-1.28614500	-0.00065600
C	1.79443400	2.30271100	-0.01741700
C	3.07288900	1.48169600	-0.04688000
C	2.79286500	0.12182100	-0.02210400
C	4.43881400	1.73502000	-0.05681600
C	5.21503500	0.56343600	-0.04679400
S	4.18598000	-0.86880500	-0.01389600
C	-1.79446900	-2.30271200	0.01766000
C	-3.07292400	-1.48170200	0.04704200
C	-2.79290700	-0.12182400	0.02233500
C	-4.43884500	-1.73504300	0.05684200
C	-5.21507700	-0.56346700	0.04680000
S	-4.18603400	0.86878700	0.01404300
C	-1.58051000	-3.14327300	1.28232100
C	-1.79585700	-3.15399600	-1.25845100
C	1.58039400	3.14326200	-1.28207300
C	1.79594200	3.15403500	1.25866300
C	-0.67310100	-4.20740200	1.27768700
C	-0.40563400	-4.92162600	2.44018700
C	-1.03554100	-4.60518300	3.64746300
C	-1.93818100	-3.53937800	3.64730300
C	-2.20628400	-2.81854900	2.48733500
C	-2.54570100	-4.33622100	-1.29359400
C	-2.63190800	-5.09260200	-2.45469600
C	-1.97323000	-4.70109400	-3.62595800
C	-1.23480400	-3.51823100	-3.58823400
C	-1.14657800	-2.75419400	-2.42594600
C	0.67311300	4.20751000	-1.27733300
C	0.40556600	4.92173000	-2.43980800

C	1.03525500	4.60516200	-3.64717500
C	1.93776000	3.53925500	-3.64711600
C	2.20595000	2.81842400	-2.48715900
C	2.54621700	4.33604000	1.29377700
C	2.63255000	5.09249400	2.45476500
C	1.97359300	4.70131000	3.62603600
C	1.23465600	3.51882200	3.58830000
C	1.14631800	2.75464500	2.42605400
C	-0.77080600	-5.40193600	4.89345900
C	-2.04461700	-5.54080600	-4.86981200
C	0.77037500	5.40192400	-4.89313600
C	2.04593400	5.54092700	4.86990100
C	6.62698900	0.64942200	-0.06540600
C	-6.62703300	-0.64946600	0.06529200
C	7.64582300	-0.27641700	-0.06381300
C	-7.64587500	0.27636400	0.06365100
C	9.07340300	0.03277600	-0.09035000
C	9.78251400	-1.24796600	-0.07195600
C	8.83556000	-2.31370700	-0.03792000
C	7.47680300	-1.75128600	-0.03276500
C	-9.07345400	-0.03284100	0.09006200
C	-9.78257400	1.24789600	0.07162600
C	-8.83562600	2.31364500	0.03769800
C	-7.47686400	1.75123600	0.03265600
C	11.07828200	-1.69638400	-0.07907500
S	11.11358300	-3.41661200	-0.04377200
C	9.39780200	-3.55379000	-0.01928000
C	-11.07834700	1.69630300	0.07863300
S	-11.11365900	3.41653200	0.04336000
C	-9.39787700	3.55372400	0.01903200
O	6.42147500	-2.36596900	-0.00787400
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C	-9.71065000	-1.25831600	0.12857700
C	9.71060600	1.25824600	-0.12893000
C	-9.05487200	-2.51929400	0.15185900
N	-8.55613500	-3.57107400	0.17260400
C	-11.13044900	-1.34333200	0.15067500
N	-12.29136000	-1.42362900	0.16924700
C	9.05483500	2.51923000	-0.15215700
N	8.55610400	3.57101300	-0.17285800
C	11.13040300	1.34325000	-0.15115500
N	12.29131300	1.42353800	-0.16983000
H	-1.11174800	2.25593200	-0.00234300
H	1.11171000	-2.25592400	0.00263800
H	4.89742700	2.71780600	-0.07132600
H	-4.89743900	-2.71784000	0.07126500
H	-0.17682100	-4.48915100	0.35333600
H	0.30550200	-5.74361400	2.40733800
H	-2.44209100	-3.26551100	4.57115100
H	-2.91076800	-1.99293400	2.52686400
H	-3.06128800	-4.67404700	-0.39866700
H	-3.22154900	-6.00631900	-2.45198200
H	-0.71604400	-3.18295900	-4.48308600
H	-0.56516300	-1.83769600	-2.43886200
H	0.17700100	4.48933600	-0.35291600
H	-0.30546000	5.74381000	-2.40687900
H	2.44150200	3.26530000	-4.57102800
H	2.91033000	1.99272300	-2.52676400
H	3.06195600	4.67362200	0.39884400
H	3.22246800	6.00603600	2.45200200
H	0.71553000	3.18391400	4.48307300
H	0.56447000	1.83842500	2.43898100
H	0.25383400	-5.78363900	4.91259000
H	-0.93032400	-4.80099400	5.79287000
H	-1.44111600	-6.26742500	4.95607700
H	-3.05631800	-5.92345800	-5.03483200
H	-1.74561600	-4.97146400	-5.75363400
H	-1.37990800	-6.40946000	-4.79598800
H	-0.25490600	5.78187800	-4.91311600
H	1.43922800	6.26860900	-4.95475900
H	0.93178400	4.80159300	-5.79261100
H	3.06078500	5.91232200	5.04147400
H	1.39168400	6.41702700	4.79114500
H	1.73487700	4.97544800	5.75201300
H	6.93839900	1.68998800	-0.08518300
H	-6.93843600	-1.69003500	0.08500400
H	12.00693700	-1.14457400	-0.10218900
H	8.92085300	-4.52404000	0.00676400
H	-12.00699900	1.14448500	0.10165000
H	-8.92093400	4.52397900	-0.00694900

# IDT-OB

0	1			
C		0.73220900	-1.09818400	0.44474500
C		1.37284100	0.08851800	0.00482800
C		0.64626600	1.19818700	-0.44151300
C		-0.73219600	1.09812100	-0.44473800
C		-1.37282800	-0.08858200	-0.00482200
C		-0.64625200	-1.19825000	0.44152000
C		-1.74581100	2.14713800	-0.90944700
C		-3.04039400	1.41318200	-0.62128300
C		-2.79111900	0.13906700	-0.12596100
C		1.74582400	-2.14720000	0.90945800
C		3.04040700	-1.41324500	0.62129400
C		2.79113200	-0.13913000	0.12597000
C		-1.63021500	3.43397100	-0.09006400
C		-1.59797400	2.37083300	-2.42257800
C		1.63022800	-3.43403700	0.09008000
C		1.59798500	-2.37089000	2.42258900
C		-4.39917100	1.67197700	-0.74450700
C		-5.20343400	0.59168100	-0.34224900
S		-4.20863000	-0.76221100	0.19616200
C		4.39918400	-1.67204000	0.74452100
C		5.20344500	-0.59174400	0.34226300
S		4.20864300	0.76214900	-0.19615000
C		-6.61299100	0.69654900	-0.40861400
C		6.61300100	-0.69659500	0.40863100
C		-7.65281500	-0.14942600	-0.09744800
C		7.65279600	0.14941100	0.09745900
C		-9.07647600	0.13721500	-0.23401400
C		-9.81527800	-1.05160400	0.24823300
C		-8.88974300	-2.02626100	0.65000400
C		-7.52141700	-1.51238400	0.45170500
C		9.07647600	-0.13715700	0.23401200
C		9.81520800	1.05168900	-0.24826700
C		8.88962100	2.02629700	-0.65003700
C		7.52132300	1.51235900	-0.45170200
C		-11.17950600	-1.32646800	0.35388900
C		-11.57069300	-2.56720300	0.85738800
C		-10.63593200	-3.52701800	1.25181800
C		-9.27274500	-3.25946100	1.14936300
C		11.17942200	1.32661100	-0.35395000
C		11.57054400	2.56735600	-0.85747600
C		10.63573200	3.52712300	-1.25190500
C		9.27255800	3.25950700	-1.14942200
O		-6.48756600	-2.11421100	0.70268200
O		6.48743700	2.11412700	-0.70267600
C		9.67443500	-1.28238500	0.72234800
C		-9.67434000	1.28249700	-0.72233800
C		-1.39355800	4.67870600	-0.66859300
C		-1.29517000	5.82610400	0.12026300
C		-1.42856500	5.76837900	1.50569400
C		-1.66522500	4.51397500	2.08399600
C		-1.76407400	3.37258400	1.30373200
C		1.39358600	-4.67877100	0.66861600
C		1.29520600	-5.82617400	-0.12023400
C		1.42858800	-5.76845300	-1.50566600
C		1.66524400	-4.51405100	-2.08397500
C		1.76408400	-3.37265500	-1.30371700
C		1.32548100	-7.00136300	-2.35811600
C		-1.32553600	7.00129600	2.35814200
C		-11.08496700	1.45861500	-0.81056600
N		-12.22713300	1.65964300	-0.90625400
C		-8.96586400	2.42160900	-1.20079500
N		-8.43642500	3.37642400	-1.60458600
C		11.08508100	-1.45838000	0.81053500
N		12.22727400	-1.65927200	0.90618000
C		8.96607500	-2.42154500	1.20086200
N		8.43676900	-3.37642600	1.60467300
H		1.14768200	2.10536200	-0.76675300
H		-1.14766900	-2.10542500	0.76676100
H		-1.68933300	1.41729800	-2.94845800
H		-2.37567300	3.04338400	-2.79525300
H		-0.62129700	2.80031200	-2.66264600
H		1.68934000	-1.41735200	2.94846600
H		0.62131000	-2.80037200	2.66265700
H		2.37568700	-3.04343500	2.79526900
H		-4.83410500	2.59893200	-1.10343300
H		4.83411900	-2.59899400	1.10344900
H		-6.89487500	1.67239700	-0.79188400

H	6.89490300	-1.67243600	0.79190200
H	-11.93731800	-0.61209400	0.06067000
H	-12.63012600	-2.78792700	0.94303800
H	-10.97655300	-4.48220400	1.63901200
H	-8.52173500	-3.98415100	1.44773300
H	11.93726900	0.61227300	-0.06073300
H	12.62996500	2.78812700	-0.94314800
H	10.97630300	4.48231800	-1.63912000
H	8.52151100	3.98415800	-1.44778900
H	-1.28395900	4.77556900	-1.74365200
H	-1.11120600	6.78442700	-0.35943400
H	-1.77385000	4.43428400	3.16318300
H	-1.94873700	2.41363700	1.78225700
H	1.28400300	-4.77563200	1.74367700
H	1.11126500	-6.78449800	0.35946900
H	1.77387900	-4.43436600	-3.16316100
H	1.94875000	-2.41371100	-1.78224500
H	1.13157000	-7.89004200	-1.75239700
H	0.51693100	-6.91005700	-3.09144700
H	2.24980400	-7.17226000	-2.92056000
H	-1.13070800	7.88984000	1.75251800
H	-2.25024300	7.17269100	2.91981000
H	-0.51764100	6.90964300	3.09214700

## IDT-20

0 1			
C	-0.69958400	1.20821200	0.00042100
C	-1.37430900	-0.04042300	0.00053300
C	-0.68210400	-1.25727100	0.00067000
C	0.69957400	-1.20817500	0.00067600
C	1.37429900	0.04046100	0.00056400
C	0.68209400	1.25730800	0.00044500
C	1.68055200	-2.37636400	0.00075500
C	2.99459800	-1.62930600	0.00064000
C	2.78449900	-0.25474500	0.00054800
C	-1.68056200	2.37640200	0.00024600
C	-2.99460800	1.62934400	0.00024700
C	-2.78450900	0.25478300	0.00042800
C	1.52208200	-3.23891600	1.26170800
C	1.52199500	-3.23915200	-1.26002600
C	-1.52197500	3.23893900	-1.26070200
C	-1.52212200	3.23920400	1.26103200
C	4.34550200	-1.95074200	0.00055700
C	5.18289400	-0.82066400	0.00040600
S	4.22811000	0.66259000	0.00040400
C	-4.34551100	1.95078100	0.00008700
C	-5.18290200	0.82070300	0.00014900
S	-4.22812000	-0.66255200	0.00043500
C	6.58805600	-0.98000000	0.00014000
C	-6.58806400	0.98003100	-0.00007900
C	7.65226700	-0.10640000	-0.00006100
C	-7.65226000	0.10641300	-0.00009700
C	9.06679400	-0.46105000	-0.00046300
C	9.83968500	0.80194900	-0.00011000
C	8.94228400	1.88006400	0.00029700
C	7.55981500	1.36577800	0.00029100
C	-9.06679700	0.46103000	-0.00043900
C	-9.83965400	-0.80199000	-0.00020600
C	-8.94222600	-1.88008300	0.00020700
C	-7.55977100	-1.36576100	0.00027200
C	11.21118500	1.06082300	-0.00015400
C	11.63715200	2.38920500	0.00020800
C	10.72988700	3.45095500	0.00059800
C	9.35961700	3.19998800	0.00064500
C	-11.21114800	-1.06089700	-0.00033900
C	-11.63708200	-2.38929000	-0.00005000
C	-10.72979100	-3.45101800	0.00036000
C	-9.35952700	-3.20001600	0.00049200
O	6.54408100	2.04587800	0.00057600
O	-6.54401700	-2.04583400	0.00059200
C	-9.63217300	1.72153000	-0.00093600
C	9.63213000	-1.72156800	-0.00119500
C	11.03706400	-1.95543600	-0.00151000
N	12.17294200	-2.20835300	-0.00178900
C	8.89152800	-2.93798300	-0.00181200
N	8.33485400	-3.96036800	-0.00235700
C	-11.03711600	1.95534700	-0.00123100
N	-12.17300500	2.20821500	-0.00148800
C	-8.89161600	2.93797200	-0.00124700

N	-8.33499200	3.96038400	-0.00152300
H	-1.21595600	-2.20381000	0.00074500
H	1.21594600	2.20384700	0.00035000
H	2.27873200	-4.02928500	1.27762300
H	0.53637900	-3.71393800	1.27797400
H	1.63098400	-2.63742600	2.16821300
H	1.63083600	-2.63783300	-2.16665200
H	2.27864200	-4.02952500	-1.27584600
H	0.53629000	-3.71417500	-1.27613600
H	-2.27862000	4.02931100	-1.27669500
H	-0.53626800	3.71395700	-1.27688400
H	-1.63079600	2.63744000	-2.16721000
H	-0.53642000	3.71423100	1.27722500
H	-2.27877300	4.02957500	1.27677400
H	-1.63104200	2.63789500	2.16765500
H	4.75523000	-2.95558700	0.00056500
H	-4.75524000	2.95562600	-0.00009200
H	6.84317500	-2.03527300	0.00008700
H	-6.84319400	2.03530100	-0.00029100
H	11.94857100	0.26914600	-0.00044600
H	12.70244100	2.59812500	0.00018500
H	11.09730200	4.47236200	0.00086600
H	8.62897200	4.00274100	0.00094600
H	-11.94855300	-0.26923900	-0.00065300
H	-12.70236600	-2.59823600	-0.00014800
H	-11.09718000	-4.47243300	0.00057400
H	-8.62886200	-4.00275200	0.00080700

## CO5IC

0 1			
C	-1.35840000	0.32389100	0.02094700
C	0.95106200	1.01834700	0.05522700
C	-0.39136700	1.35369500	0.08035900
C	0.39156000	-1.35077600	-0.09164400
C	1.35862800	-0.32096100	-0.03243900
C	-0.86461600	2.80782700	0.06272500
O	-2.07749600	2.92938300	0.85733100
C	-3.03114000	2.01776500	0.57671000
C	-2.73099500	0.73615300	0.13273200
C	-4.39597300	2.22356000	0.76974600
C	-5.16447400	1.09786300	0.45675200
S	-4.14475000	-0.22050900	-0.08789200
C	-1.19113600	3.27149300	-1.35864600
C	0.13454600	3.72547500	0.75636300
C	-1.98169700	4.41493200	-1.52312700
C	-2.28335200	4.89070500	-2.79059000
C	-1.80210200	4.24919600	-3.93933700
C	-1.00759900	3.11648200	-3.76703100
C	-0.70716500	2.62901600	-2.49557400
C	1.03411600	4.51048200	0.03686900
C	1.97243800	5.29837800	0.70016100
C	2.03316400	5.33380500	2.09378500
C	1.12764700	4.54013400	2.80759500
C	0.19748100	3.74395900	2.15328800
C	3.02117000	6.21045400	2.80943000
C	-2.14835200	4.76270000	-5.30798000
C	0.86409500	-2.80511100	-0.07159500
O	2.07890500	-2.92822800	-0.86291200
C	3.03217500	-2.01654800	-0.58109900
C	2.73134600	-0.73362400	-0.14138000
C	4.39761900	-2.22440800	-0.76712900
C	5.16580900	-1.09824600	-0.45498700
S	4.14492300	0.22335300	0.07942300
C	-0.13380200	-3.72281700	-0.76700400
C	1.18683600	-3.26756900	1.35106400
C	1.97661800	-4.41100600	1.51849900
C	2.27471400	-4.88601000	2.78719200
C	1.79074900	-4.24350200	3.93410100
C	0.99672100	-3.11078100	3.75883200
C	0.69990900	-2.62414600	2.48631300
C	-1.03446100	-4.50815900	-0.04929400
C	-1.97126900	-5.29633000	-0.71445600
C	-2.02934300	-5.33165400	-2.10816800
C	-1.12272700	-4.53760700	-2.82021500
C	-0.19409900	-3.74119700	-2.16407100
C	-3.01574300	-6.20842300	-2.82587300
C	2.13499000	-4.75416400	5.30429600
C	6.57828100	-1.15254000	-0.57113700

C	-6.57588800	1.14731900	0.58747500
C	7.58903300	-0.25211200	-0.33560500
C	-7.58679000	0.24789500	0.34858900
C	-9.01640800	0.47089000	0.54674000
C	-9.71864200	-0.75962000	0.11959200
C	-8.76718000	-1.70067400	-0.30199400
C	-7.41703300	-1.12240100	-0.17353400
C	-11.07233300	-1.09727500	0.07744400
C	-11.42723700	-2.36474600	-0.38397000
C	-10.46688200	-3.29069400	-0.79803400
C	-9.11428500	-2.96070500	-0.75919000
C	9.02008600	-0.48240900	-0.51408700
C	9.71770900	0.77080200	-0.15004900
C	8.76377800	1.72405300	0.23717100
C	7.41584700	1.13471600	0.13958400
C	11.06948000	1.11816900	-0.13455000
C	11.42022200	2.40680900	0.26758300
C	10.45758800	3.34388900	0.65014500
C	9.10680600	3.00454000	0.63703200
O	6.36496500	1.70030200	0.40213500
C	9.65200600	-1.63460300	-0.93632000
O	-6.36731100	-1.68284200	-0.45124300
C	-9.64259500	1.59498500	1.04607500
C	-0.95086000	-1.01537500	-0.06706500
C	11.06478400	-1.75184400	-1.07702100
N	12.21014400	-1.90682600	-1.21097300
C	8.98153000	-2.84326800	-1.28065100
N	8.48422000	-3.85419600	-1.57292700
C	-11.05433600	1.70696400	1.20060900
N	-12.19865500	1.85625600	1.34912100
C	-8.96573300	2.77312700	1.47355900
N	-8.46285200	3.75789900	1.83693300
H	1.69887300	1.80568900	0.07950300
H	-4.82900400	3.15106600	1.12605000
H	-2.36330100	4.92838100	-0.64573100
H	-2.90242300	5.77873400	-2.89424600
H	-0.61797300	2.59861800	-4.63988900
H	-0.08987100	1.74116900	-2.40078500
H	1.00553600	4.51011500	-1.04835000
H	2.66692800	5.89992500	0.11905300
H	1.15583600	4.54368600	3.89461100
H	-0.49336000	3.13505600	2.72757400
H	3.86030100	6.47764100	2.16193400
H	2.54937700	7.14342100	3.13954400
H	3.41904100	5.71691800	3.70091400
H	-1.98434100	5.84248300	-5.38064700
H	-1.55042200	4.27416500	-6.08131900
H	-3.20427800	4.58213800	-5.53938900
H	4.83144400	-3.15428300	-1.11624700
H	2.36019300	-4.92541500	0.64253000
H	2.89293900	-5.77434100	2.89314500
H	0.60446100	-2.59246300	4.63025200
H	0.08281600	-1.73640400	2.38925000
H	-1.00792200	-4.50794300	1.03597200
H	-2.66663600	-5.89818900	-0.13472400
H	-1.14884600	-4.54109500	-3.90728600
H	0.49766400	-3.13203200	-2.73697900
H	-3.85376300	-6.47967900	-2.17864500
H	-3.41546000	-5.71297800	-3.71549100
H	-2.54193100	-7.13914800	-3.15938300
H	2.00995200	-5.83960200	5.36728100
H	3.17998500	-4.53613300	5.55296500
H	1.50856000	-4.29293300	6.07188400
H	6.88580100	-2.13017900	-0.92888000
H	-6.88225200	2.11992500	0.95972000
H	-11.84904200	-0.41103500	0.38784600
H	-12.47819300	-2.63415700	-0.42047800
H	-10.77960700	-4.26839700	-1.15096300
H	-8.34421200	-3.65764200	-1.07452000
H	11.84776000	0.42424600	-0.42307600
H	12.46964300	2.68418600	0.28197900
H	10.76706500	4.33785200	0.95758500
H	8.33493400	3.71000500	0.92805300
H	-1.69868700	-1.80271000	-0.09109600

## IDT-BOC6

0 1			
C	1.31905400	0.40432100	-0.01575300

C	0.99366000	-0.97305400	-0.00191800
C	-0.32739900	-1.38512800	-0.00803700
C	-1.31851200	-0.39878600	-0.02117500
C	-0.99291500	0.97842400	-0.03583900
C	0.32802300	1.39070000	-0.02826400
C	-2.76023100	-0.48373800	-0.00810300
C	-3.32835000	0.77192500	0.00080800
C	-2.25752700	1.85113100	-0.03456100
C	2.76077000	0.48956700	-0.01580100
C	3.32919800	-0.76580000	-0.02068000
C	2.25884500	-1.84543500	-0.00514200
S	-3.93107900	-1.73326700	-0.04745800
C	-5.23806400	-0.55555100	-0.01485100
C	-4.73059000	0.73721200	-0.00683000
S	3.93140400	1.73957100	-0.04479400
C	5.23853800	0.56192900	-0.02832300
C	4.73143500	-0.73095400	-0.02313800
C	-1.50639700	4.74295200	2.36194300
C	-1.59670800	3.97364000	1.20763300
C	-2.24158400	2.73219700	1.21924500
C	-2.78642600	2.28919500	2.42577600
C	-2.69529800	3.06392000	3.57875300
C	-2.05742700	4.30597800	3.57024700
C	-1.97585000	3.08816500	-3.66388700
C	-1.72655200	2.38392800	-2.48782900
C	-2.43763600	2.66575300	-1.32142500
C	-3.41200500	3.66993300	-1.37376100
C	-3.65813400	4.36805100	-2.54881800
C	-2.94139800	4.09363400	-3.71865300
C	2.82883400	-2.26457900	-2.46137900
C	2.74626500	-3.02596600	-3.62399400
C	2.08530200	-4.25557800	-3.64135100
C	1.50226600	-4.69479000	-2.44884800
C	1.58417300	-3.93936200	-1.28503000
C	2.25169300	-2.70976100	-1.27093600
C	3.39109900	-3.69696500	1.30863100
C	3.62997000	-4.41237900	2.47517700
C	2.92030900	-4.14153900	3.64996100
C	1.96996200	-3.12060200	3.60996600
C	1.72786700	-2.39955800	2.44283300
C	2.43119600	-2.67862300	1.27076100
C	2.02592900	-5.09241300	-4.88806000
C	3.15799600	-4.94067200	4.90016200
C	-1.98822500	5.15706200	4.80680900
C	-3.19113500	4.87197000	-4.97948500
C	6.64582400	0.92503400	0.01955700
C	-6.64487500	-0.91869000	0.04293400
C	7.12104000	2.22780100	-0.28906200
C	8.47386300	2.49932100	-0.25000200
C	9.43467200	1.50932700	0.05132200
C	8.95644400	0.22287500	0.40822800
C	7.59237700	-0.04090300	0.38994200
C	-7.12162000	-2.22284200	-0.25742000
C	-8.47344500	-2.49660600	-0.20208500
C	-9.43271700	-1.50748900	0.10705700
C	-8.95283200	-0.21834500	0.45182100
C	-7.58947600	0.04740100	0.41823900
O	6.17671500	3.14284900	-0.60425800
O	9.87905300	-0.66696000	0.81052300
O	-9.87246800	0.67201000	0.86002700
O	-6.17930000	-3.13730300	-0.57958200
C	6.58411800	4.46288700	-0.90902700
C	9.45629500	-1.96087200	1.20666000
C	-6.58815500	-4.45690800	-0.88432500
C	-9.44835800	1.97026500	1.23966600
C	10.80425800	1.92796600	0.09076200
C	-10.80051600	-1.92944800	0.16821500
C	12.03059200	1.31884800	0.08053200
C	-12.02861100	-1.32379800	0.17623500
C	13.18435600	2.15315500	0.54760500
C	14.31094200	1.22076300	0.75498200
C	13.92924900	-0.06353600	0.33460200
C	12.56286300	0.00558900	-0.22966500
C	-13.17175600	-2.15952200	0.66633900
C	-14.29708600	-1.22938000	0.89012700
C	-13.92643600	0.05429800	0.45815700
C	-12.57013400	-0.01336100	-0.13009800
C	15.56186100	1.48482200	1.28851500
C	16.45421600	0.42324200	1.42031600
C	16.08069000	-0.86252000	1.02190800
C	14.82538300	-1.12291600	0.47151000

C	-15.53742000	-1.49454800	1.44730600
C	-16.42991800	-0.43467800	1.59147200
C	-16.06695000	0.85054900	1.18171600
C	-14.82254100	1.11198600	0.60757300
O	13.17762000	3.35305600	0.75507400
C	12.01444800	-0.92757900	-1.08169600
O	-13.15799800	-3.35857200	0.87844700
C	-12.03991600	0.91723200	-0.99624200
C	10.83687400	-0.67975400	-1.84016200
N	9.90488200	-0.49473900	-2.51147000
C	12.63136800	-2.17719400	-1.37431700
N	13.09533300	-3.21386800	-1.62781300
C	-10.87409000	0.66945900	-1.77269100
N	-9.95247100	0.48368800	-2.45793900
C	-12.66674300	2.16285900	-1.28486600
N	-13.13935800	3.19625000	-1.53576800
H	-0.58836500	-2.43941000	-0.00446800
H	0.58856600	2.44515300	-0.03063600
H	-5.36019100	1.61840900	-0.03159000
H	5.36096300	-1.61232300	-0.04363900
H	-0.99881700	5.70404600	2.32247900
H	-1.16908500	4.34916900	0.28223500
H	-3.28621700	1.32585500	2.46850800
H	-3.12986300	2.69299000	4.50415200
H	-1.40532700	2.84623400	-4.55751500
H	-0.97033500	1.60531800	-2.48587300
H	-3.97937200	3.91426600	-0.47972700
H	-4.42236600	5.14184200	-2.55886800
H	3.34898900	-1.31158000	-2.48491500
H	3.20747200	-2.65423100	-4.53595400
H	0.97644400	-5.64665700	-2.42968300
H	1.13190400	-4.31716000	-0.37224100
H	3.95165900	-3.93896000	0.40973700
H	4.38134000	-5.19883100	2.47355900
H	1.40524500	-2.88107900	4.50798500
H	0.98312700	-1.60989600	2.45139000
H	2.14155500	-4.47951100	-5.78601700
H	2.82659200	-5.84156300	-4.89791700
H	1.07733200	-5.63215000	-4.96195100
H	4.21709000	-5.18670100	5.02159700
H	2.82934700	-4.39713600	5.78997700
H	2.60751600	-5.88857900	4.87267400
H	-2.08959700	4.55377800	5.71298000
H	-1.04176000	5.70265800	4.86339200
H	-2.79229900	5.90254100	4.81771500
H	-4.25891400	5.05924300	-5.12749900
H	-2.69370500	5.84852000	-4.94545700
H	-2.81307800	4.34134100	-5.85725400
H	8.83326800	3.49436300	-0.48578300
H	7.24036500	-1.01579500	0.69813500
H	-8.83353800	-3.49327700	-0.42985000
H	-7.23620000	1.02455400	0.71771100
H	5.67016200	5.01523700	-1.12592400
H	7.09756300	4.92775400	-0.05947300
H	7.23820700	4.48218600	-1.78824100
H	10.36539700	-2.50240800	1.46682700
H	8.79827400	-1.91115700	2.08102000
H	8.94549400	-2.47919000	0.38787000
H	-5.67577100	-5.00730200	-1.11243300
H	-7.09228500	-4.92522600	-0.03105200
H	-7.25115700	-4.47391300	-1.75681000
H	-10.35574500	2.51235000	1.50464100
H	-8.78107300	1.93011300	2.10751600
H	-8.94740000	2.48201800	0.41075900
H	10.91596800	3.00693400	0.22321200
H	-10.90725200	-3.00826700	0.30592400
H	15.82297800	2.49363000	1.59273700
H	17.44216600	0.59070500	1.83775900
H	16.78225200	-1.68238400	1.14188100
H	14.56947000	-2.13300300	0.17699500
H	-15.79038900	-2.50283900	1.76001100
H	-17.40968400	-0.60304600	2.02743800
H	-16.76826700	1.66912200	1.31152600
H	-14.57448200	2.12156100	0.30469500

## ATT-1

0 1			
C	1.29595600	-0.46342200	0.27274300



C	1.03799300	0.92916700	0.28216500
C	-0.26075800	1.40393500	0.26982100
C	-1.29591100	0.46343500	0.27270000
C	-1.03794900	-0.92915700	0.28177300
C	0.26080400	-1.40392200	0.26946400
C	-2.72890700	0.61337400	0.25067100
C	-3.36054200	-0.61440800	0.23090100
C	-2.34102900	-1.74172400	0.27164400
C	2.72895500	-0.61335800	0.25086400
C	3.36059300	0.61442800	0.23151800
C	2.34108000	1.74173500	0.27244300
C	-2.35985300	-2.62405500	-0.98127300
C	-2.56755700	-2.54404800	1.55982100
C	2.36008700	2.62441400	-0.98022700
C	2.56740900	2.54370000	1.56088100
C	1.78945800	3.90058500	-0.95665500
C	1.72552900	4.67518500	-2.10996400
C	2.23042500	4.20821500	-3.32646600
C	2.79435900	2.93022900	-3.34591900
C	2.85817700	2.15020600	-2.19560400
C	1.83777600	2.30808800	2.72598000
C	2.12578100	3.00009600	3.90067500
C	3.14930200	3.94655800	3.95437100
C	3.88429800	4.17381000	2.78549400
C	3.60046700	3.48765500	1.61204700
C	-1.78926500	-3.90024200	-0.95795500
C	-1.72516500	-4.67452900	-2.11147200
C	-2.22984100	-4.20721400	-3.32792400
C	-2.79373800	-2.92920000	-3.34712200
C	-2.85772600	-2.14949500	-2.19660900
C	-1.83807800	-2.30885700	2.72507000
C	-2.12633000	-3.00120200	3.89953900
C	-3.14994700	-3.94754400	3.95281700
C	-3.88475800	-4.17444500	2.78372300
C	-3.60069600	-3.48797800	1.61054700
C	-2.19391600	-5.05995900	-4.56449300
C	-3.44188200	-4.71552200	5.21073700
C	3.44059600	4.71441800	5.21251100
S	3.83875200	-1.91906500	0.24832100
C	5.19530800	-0.80384500	0.22995200
C	4.75822900	0.51575900	0.22413700
S	-3.83870600	1.91907700	0.24837300
C	-5.19526200	0.80386600	0.22953800
C	-4.75817400	-0.51573700	0.22339100
C	2.19466400	5.06134200	-4.56277600
C	-6.54775400	1.27167300	0.20023700
C	6.54780200	-1.27165100	0.20058600
C	-7.06130900	2.55188700	0.45376700
C	-8.47359500	2.58992700	0.32463400
C	-9.07864900	1.37838600	-0.01941200
S	-7.82146200	0.16881500	-0.20066900
C	7.06137500	-2.55184800	0.45414200
C	8.47365000	-2.58989400	0.32490200
C	9.07867500	-1.37837000	-0.01925300
S	7.82147000	-0.16881300	-0.20048900
C	-6.52218800	3.81947200	0.83506800
C	-7.49642200	4.76076300	0.97133900
S	-9.11619400	4.16639700	0.65387300
C	6.52227800	-3.81940800	0.83555700
C	7.49652000	-4.76069400	0.97179900
S	9.11626900	-4.16635000	0.65417500
C	-10.47689500	1.23495700	-0.18343200
C	10.47690900	-1.23495200	-0.18340000
C	-11.28206400	0.17820100	-0.50407700
C	11.28205500	-0.17822200	-0.50418700
C	-10.89895600	-1.19211000	-0.78490200
N	-12.03537000	-1.97942900	-1.05557000
C	-13.22332100	-1.32806200	-1.03012200
S	-13.02828700	0.35822000	-0.62624800
C	10.89892800	1.19206800	-0.78508900
N	12.03531900	1.97935700	-1.05594000
C	13.22327000	1.32798800	-1.03053700
S	13.02826700	-0.35825700	-0.62649300
O	9.77229800	1.66078300	-0.79667200
O	-9.77232500	-1.66082300	-0.79655200
C	-14.49778600	-1.82897800	-1.27269500
C	14.49771500	1.82888400	-1.27325100
C	-11.83228400	-3.39489200	-1.37783000
C	-11.72144000	-3.63888900	-2.87340500
C	11.83221100	3.39478500	-1.37834000
C	11.72121900	3.63861700	-2.87393200

C	-7.36430800	6.17474800	1.34670100
O	-8.30894900	6.93274200	1.43994600
O	-6.09335600	6.51650600	1.56913300
C	-5.88628400	7.88244100	1.94206100
C	7.36443300	-6.17465900	1.34724600
O	8.30907900	-6.93265200	1.44045500
O	6.09349800	-6.51640100	1.56980200
C	5.88645300	-7.88231500	1.94282100
C	-14.81685100	-3.16273100	-1.62834700
N	-15.13958500	-4.24122000	-1.92769300
C	-15.59597200	-0.93477000	-1.17059600
N	-16.48772800	-0.19096100	-1.08356700
C	14.81675500	3.16261700	-1.62900200
N	15.13944700	4.24107900	-1.92849000
C	15.59590900	0.93468400	-1.17117200
N	16.48767500	0.19088900	-1.08413000
H	-0.46955000	2.46939800	0.25269200
H	0.46959800	-2.46938000	0.25205300
H	1.40022700	4.30022000	-0.02448100
H	1.27635900	5.66438900	-2.06193800
H	3.19185400	2.53556400	-4.27799200
H	3.29906200	1.15901500	-2.24913600
H	1.03503400	1.57743900	2.72500000
H	1.53901100	2.79658400	4.79331500
H	4.69255800	4.90129700	2.79469800
H	4.18385200	3.69574000	0.71919500
H	-1.40020500	-4.30014400	-0.02582400
H	-1.27603600	-5.66376100	-2.06364600
H	-3.19106200	-2.53426300	-4.27915300
H	-3.29857200	-1.15827600	-2.24994000
H	-1.03524700	-1.57830500	2.72442900
H	-1.53964600	-2.79803900	4.79231400
H	-4.69303400	-4.90192100	2.79256600
H	-4.18391500	-3.69578900	0.71752300
H	-1.35475300	-5.76067800	-4.54228600
H	-3.11129000	-5.65303200	-4.65943400
H	-2.10739900	-4.44972100	-5.46784000
H	-3.00190100	-5.71892000	5.17025600
H	-3.03170800	-4.21220800	6.09010100
H	-4.51834800	-4.84199300	5.35983600
H	3.03584800	4.20757300	6.09237600
H	4.51672400	4.84690300	5.35861400
H	2.99461000	5.71528100	5.17475600
H	5.44008800	1.35897000	0.23361400
H	-5.44002400	-1.35896000	0.23253800
H	3.11102400	5.65622900	-4.65615000
H	2.11060100	4.45128200	-5.46646800
H	1.35413700	5.76046500	-4.54151500
H	-5.47771600	4.04174100	1.01105900
H	5.47781800	-4.04164900	1.01165600
H	-11.00371200	2.17384200	-0.01419800
H	11.00373800	-2.17382800	-0.01415100
H	-10.90237300	-3.66750500	-0.87545800
H	-12.64062100	-3.97052300	-0.92711200
H	-11.54730500	-4.70330600	-3.05183500
H	-12.63557800	-3.35460500	-3.40016900
H	-10.88211200	-3.07846300	-3.29300500
H	10.90235000	3.66745600	-0.87590900
H	12.64059400	3.97046400	-0.92776200
H	11.54708000	4.70301700	-3.05246300
H	12.63529800	3.35426300	-3.40076000
H	10.88184000	3.07815700	-3.29338500
H	-4.81216300	7.98785300	2.08434100
H	-6.23513400	8.55101100	1.15212600
H	-6.41918800	8.11036800	2.86767700
H	4.81235400	-7.98769200	2.08529200
H	6.23514400	-8.55092600	1.15285000
H	6.41951300	-8.11022300	2.86835200

## DC-IDT2T

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C	1.28809700	0.48474300	0.00952000
C	1.05284800	-0.91126900	0.04064300
C	0.23798700	1.40750600	-0.02671300
C	-1.05283500	0.91128700	-0.04030600
C	-1.28808300	-0.48472500	-0.00919700
C	-0.23797200	-1.40748900	0.02703600
C	-2.36947600	1.70177900	-0.06445200

C	-3.37047400	0.55830300	-0.02570100
C	-2.71890200	-0.65899700	-0.01294900
C	-4.76754000	0.43530100	-0.03772700
C	-5.17881800	-0.89006100	-0.02759400
S	-3.80522400	-1.98439400	-0.01250800
C	2.36948900	-1.70176000	0.06486500
C	3.37048800	-0.55828400	0.02613400
C	2.71891700	0.65901500	0.01331100
C	4.76755300	-0.43528600	0.03830100
C	5.17883500	0.89007300	0.02818800
S	3.80524300	1.98441300	0.01292600
C	2.42253600	-2.59978700	-1.17594600
C	2.58674800	-2.48414300	1.36664200
C	-2.42246200	2.59977000	1.17638800
C	-2.58680000	2.48419900	-1.36619500
C	1.85768600	-3.87862800	-1.14856900
C	1.82310100	-4.66840800	-2.29247500
C	2.35325400	-4.21494400	-3.50348100
C	2.91247100	-2.93522300	-3.52678300
C	2.94671500	-2.13975100	-2.38559300
C	3.62413600	-3.42111100	1.44349200
C	3.89784000	-4.08849800	2.63031800
C	3.14806000	-3.84832500	3.78679500
C	2.12096100	-2.90730800	3.70772800
C	1.84304800	-2.23427500	2.52003800
C	-1.85767100	3.87863400	1.14900500
C	-1.82302600	4.66838000	2.29293800
C	-2.35305800	4.21485300	3.50396900
C	-2.91221800	2.93510500	3.52727600
C	-2.94652300	2.13967000	2.38606500
C	-3.62422400	3.42114300	-1.44297100
C	-3.89799000	4.08856500	-2.62975400
C	-3.14824200	3.84845700	-3.78627500
C	-2.12111100	2.90748000	-3.70727900
C	-1.84313200	2.23440500	-2.51962000
C	2.34834600	-5.08458900	-4.72878300
C	3.42652600	-4.59726700	5.05921000
C	-2.34808600	5.08444800	4.72930800
C	-3.42683200	4.59741900	-5.05864900
C	6.51530700	1.40788500	0.02785600
C	-6.51528700	-1.40787700	-0.02712700
S	-7.88252700	-0.34218900	0.01901600
C	-9.00041200	-1.68971900	-0.00716300
C	-8.28731600	-2.89480000	-0.04855800
C	-6.90657700	-2.74535000	-0.05969700
S	7.88252200	0.34221700	-0.01946400
C	9.00043200	1.68970600	0.00770100
C	8.28736100	2.89476300	0.05019900
C	6.90662100	2.74532300	0.06146400
C	-10.41322600	-1.69931300	0.01255200
C	10.41324500	1.69928800	-0.01220900
C	-11.37374000	-0.71322200	0.05112200
C	11.37373300	0.71320600	-0.05161500
C	-12.81773800	-0.90638800	0.06871300
C	-13.44325600	0.43568800	0.09187000
C	-12.43039300	1.40626400	0.09645900
C	-11.11469700	0.73840800	0.07381600
C	12.81773300	0.90635500	-0.06921500
C	13.44322200	-0.43571600	-0.09337400
C	12.43033800	-1.40626800	-0.09856500
C	11.11465900	-0.73840200	-0.07535300
C	-14.77689500	0.84571100	0.10876100
C	-15.05187700	2.21330100	0.12989900
C	-14.03161300	3.16677600	0.13494900
C	-12.69795000	2.76450500	0.11805900
C	14.77685100	-0.84575700	-0.11062500
C	15.05180300	-2.21333800	-0.13270400
C	14.03151800	-3.16678800	-0.13834000
C	12.69786500	-2.76450000	-0.12110200
O	-10.02792800	1.29818100	0.07310400
O	10.02787900	-1.29815500	-0.07498500
C	13.52172700	2.09535000	-0.06986300
C	-13.52170700	-2.09539700	0.07014400
C	14.94382800	2.16921300	-0.08869900
N	16.10104600	2.29146100	-0.10345400
C	12.92163400	3.38670600	-0.05552300
N	12.48111600	4.46422200	-0.04499900
C	-14.94380900	-2.16927800	0.08883300
N	-16.10102600	-2.29154200	0.10351800
C	-12.92158400	-3.38675000	0.05681900
N	-12.48103800	-4.46426300	0.04713900

H	0.42989100	2.47620800	-0.04201800
H	-0.42987800	-2.47619000	0.04235800
H	-5.46412000	1.26624000	-0.05784200
H	5.46412900	-1.26622500	0.05858600
H	1.44975800	-4.26778500	-0.21995800
H	1.37722200	-5.65897300	-2.24160100
H	3.33021300	-2.55136500	-4.45453900
H	3.38569500	-1.14786900	-2.44170200
H	4.21966900	-3.63813900	0.56084800
H	4.71016800	-4.81089800	2.65974500
H	1.52365900	-2.69279500	4.59076300
H	1.03814100	-1.50637800	2.49931000
H	-1.44983700	4.26784000	0.22037300
H	-1.37719500	5.65896600	2.24205700
H	-3.32986800	2.55120000	4.45505400
H	-3.38545300	1.14776700	2.44217500
H	-4.21972600	3.63812000	-0.56029300
H	-4.71033800	4.81094500	-2.65912500
H	-1.52382600	2.69302700	-4.59034000
H	-1.03819500	1.50653900	-2.49895000
H	1.50134000	-5.77624000	-4.72415100
H	2.29732700	-4.48642600	-5.64282200
H	3.26171100	-5.68865000	-4.78561100
H	4.49925400	-4.75839200	5.20063000
H	3.04353000	-4.05987700	5.93077600
H	2.95009900	-5.58473600	5.04671500
H	-1.50133500	5.77640800	4.72444300
H	-3.26165900	5.68816500	4.78645200
H	-2.29656300	4.48626200	5.64330500
H	-4.49965600	4.75750900	-5.20054800
H	-2.95141300	5.58536700	-5.04569200
H	-3.04289400	4.06060700	-5.93015400
H	-8.79503100	-3.85324500	-0.07065200
H	-6.20746900	-3.57312300	-0.09397100
H	8.79509400	3.85318200	0.07304000
H	6.20752800	3.57307200	0.09664700
H	-10.77996900	-2.72094900	-0.00836600
H	10.78001100	2.72090000	0.00941700
H	-15.59796000	0.14107900	0.10530400
H	-16.08711900	2.53993400	0.14262300
H	-14.28228200	4.22283200	0.15181300
H	-11.88227100	3.48073000	0.12116200
H	15.59793300	-0.14114500	-0.10674000
H	16.08703700	-2.53998500	-0.14570600
H	14.28216300	-4.22283800	-0.15592800
H	11.88217000	-3.48070400	-0.12464000

## BZIC

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C	1.22606400	1.27659200	-0.25496400
C	0.85743700	-0.09873200	-0.20173100
C	-0.52077100	-0.46456000	-0.22948200
C	-1.52322300	0.54130900	-0.09777700
C	-1.14032000	1.90975200	-0.07575100
C	0.21473200	2.27396600	-0.20502600
N	-1.13608700	-1.69835300	-0.37124500
C	-2.49357000	-1.49539100	-0.28842600
C	-2.75404900	-0.13036900	-0.10806100
C	2.62882400	1.30493800	-0.27486200
C	3.08213200	-0.01965000	-0.18992700
N	2.00563400	-0.87479800	-0.13712400
N	-1.87393300	3.02714700	0.00681800
N	-0.96437300	3.98378000	-0.06675800
N	0.29706400	3.61072500	-0.19892500
C	-1.34070700	5.37966200	-0.07679200
C	-0.57884000	-2.92833400	-0.90370900
C	2.14184800	-2.22438900	0.38575400
C	-3.64127700	-2.28294400	-0.39994100
C	-4.79861900	-1.51618100	-0.25626400
S	-4.43720200	0.19622800	-0.03282100
S	3.93107800	2.41529000	-0.30533200
C	5.09801300	1.08948300	-0.17569900
C	4.46958600	-0.15484200	-0.12906400
C	-6.10096100	-2.04893300	-0.42409300
C	6.46743400	1.43280000	-0.25613500
C	-7.36106400	-1.53525100	-0.26456600
C	7.63502200	0.71982300	-0.12527700
C	-8.46530300	-2.16405600	-1.04678000

C	-9.56621800	-1.17501800	-1.05362900
C	-9.21641900	-0.08226400	-0.24112600
C	-7.91528200	-0.37166800	0.39797700
C	-10.76754700	-1.22718300	-1.74086900
C	-11.63563100	-0.14331000	-1.62455800
C	-11.29045800	0.95543200	-0.83385200
C	-10.08759200	0.99963500	-0.12839800
C	8.85185400	1.33042500	-0.74095400
C	9.85249900	0.24715300	-0.83161700
C	9.33583100	-0.91066200	-0.22694800
C	8.01379400	-0.59027900	0.35906600
C	11.10340600	0.27781100	-1.42451100
C	11.85438000	-0.89606000	-1.42783400
C	11.34444400	-2.05910700	-0.84663300
C	10.09010600	-2.08308300	-0.23567500
C	-7.46024400	0.19306100	1.57155600
C	7.39562000	-1.32807500	1.35089900
O	-8.43820400	-3.24263400	-1.61143300
O	8.97034800	2.47700200	-1.13321600
C	-6.42891700	-0.40401800	2.35089300
N	-5.63457700	-0.90420500	3.03791400
C	-8.08409600	1.31604900	2.18532900
N	-8.56368800	2.24072600	2.70354300
C	6.32223300	-0.82447800	2.13411800
N	5.45921800	-0.43848700	2.81272200
C	7.85702200	-2.60670600	1.77610300
N	8.18854400	-3.66060200	2.14126500
H	-2.25024800	5.49237800	0.51096800
H	-0.52851500	5.95632900	0.36300300
H	-1.51883900	5.71521900	-1.10159900
H	-0.34461000	-3.64907700	-0.11622100
H	-1.30843800	-3.37563400	-1.58162500
H	0.31837400	-2.70877900	-1.48147700
H	2.99677100	-2.24799500	1.06459400
H	1.25610600	-2.48781600	0.96233200
H	2.29883400	-2.95933200	-0.40755000
H	-3.67355100	-3.35324100	-0.56634700
H	5.00977000	-1.09194300	-0.10752500
H	-6.10936800	-3.03680900	-0.88896400
H	6.66565700	2.45584600	-0.58472600
H	-11.01071400	-2.09187700	-2.35031600
H	-12.58391100	-0.14726000	-2.15282100
H	-11.97258000	1.79711000	-0.76425300
H	-9.84788200	1.86770500	0.47322900
H	11.47266200	1.19519600	-1.87201200
H	12.83775500	-0.91177000	-1.88714400
H	11.93594100	-2.96918200	-0.86812800
H	9.72596400	-3.00393900	0.20215400

## ITOIC

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C	-1.01900500	-0.94599700	0.03285000
C	-1.30505600	0.44072100	0.05837200
C	-0.28747400	1.39998400	0.08705200
C	1.02046100	0.95046200	0.09744100
C	1.30645300	-0.43618300	0.06873700
C	0.28893200	-1.39547100	0.04182400
C	-2.30655800	-1.78315100	0.01924900
C	2.30815400	1.78742500	0.11336600
C	-2.74181300	0.56631600	0.05863800
C	-3.34671100	-0.67513600	0.05452400
C	-4.74550700	-0.60209400	0.04504000
C	-5.20610500	0.70889400	0.04900800
S	-3.87158300	1.85601700	0.04852500
C	2.74311400	-0.56181000	0.06272900
C	3.34820700	0.67949800	0.07013700
C	4.74706000	0.60615000	0.06813300
C	5.20725400	-0.70491200	0.05322300
S	3.87245200	-1.85168600	0.04689800
C	-2.32352800	-2.67361700	1.26647900
C	-2.50147200	-2.58228700	-1.27567300
C	2.32398100	2.68440500	-1.12922500
C	-1.71827500	-3.93398100	1.24585000
C	-1.65509900	-4.71467200	2.39485600
C	-2.19523900	-4.27014600	3.60470500
C	-2.79387600	-3.00823100	3.62171700
C	-2.85729400	-2.22224100	2.47526600
C	-3.50867100	-3.55247000	-1.34260600

C	-3.76537600	-4.23612000	-2.52390400
C	-3.02749700	-3.98024200	-3.68473200
C	-2.03005800	-3.00719600	-3.61541400
C	-1.76967000	-2.31745500	-2.43324600
C	1.72418600	3.94715500	-1.10011900
C	1.65921200	4.73332000	-2.24533000
C	2.19206900	4.29199000	-3.45952500
C	2.78528600	3.02762700	-3.48491600
C	2.85038100	2.23612600	-2.34244100
C	-2.16026800	-5.13150000	4.83541000
C	-3.28746300	-4.74553500	-4.95136700
C	2.15476400	5.15879100	-4.68630800
C	3.29615400	4.72228900	5.09911000
C	3.51539600	3.54571100	1.48486500
C	3.77358600	4.22286000	2.66951700
C	3.03403400	3.96401000	3.82869000
C	2.03324900	2.99488300	3.75397700
C	1.77126400	2.31171200	2.56824800
C	2.50488000	2.57927300	1.41248400
C	-9.07447000	1.26805100	0.05572100
C	-8.44032000	2.52585600	0.06962700
C	-7.03654400	2.45277300	0.07909100
C	-6.56906800	1.14243400	0.04874800
S	-7.87253600	-0.00630500	0.04447300
C	-10.47665900	1.19533500	-0.01271000
C	-11.37140000	0.14542100	-0.03770400
C	-11.02569100	-1.27804500	0.11044100
C	-12.29932300	-2.02400500	0.15018600
C	-13.36705100	-1.12422100	0.01386600
C	-12.81797800	0.24323900	-0.14113700
O	-9.90766800	-1.76624200	0.20140700
C	-13.58126000	1.37070800	-0.38153200
C	-12.48678700	-3.38674100	0.30366200
C	-13.79448500	-3.86772600	0.32621700
C	-14.86830600	-2.98498200	0.19658600
C	-14.67373800	-1.61212100	0.03802500
C	9.07485800	-1.26823800	0.00518600
C	8.43963400	-2.52506200	0.04252700
C	7.03623900	-2.45000700	0.07103300
C	6.56983600	-1.13942900	0.03593000
S	7.87427900	0.00753400	-0.00108200
O	6.19894400	-3.51873600	0.10923800
C	10.47559700	-1.19808900	-0.08973900
C	11.37084200	-0.14969000	-0.14385300
C	11.03023700	1.27573800	-0.00270300
C	12.30575000	2.01962400	0.00668200
C	13.36914500	1.11663200	-0.14191600
C	12.81479500	-0.25087500	-0.27566200
O	9.91488600	1.76684800	0.10389600
C	13.57082500	-1.38122400	-0.52528500
C	12.49861300	3.38331300	0.14434700
C	13.80738800	3.86186600	0.13784000
C	14.87698900	2.97587400	-0.00394900
C	14.67694000	1.60204600	-0.14655800
O	-9.15632400	3.66348600	0.11423700
O	-6.19976100	3.52239900	0.09531400
O	9.15522500	-3.66266300	0.09043500
C	-8.92280600	4.59447900	-0.95274800
C	-6.24418200	4.28564400	1.30788500
C	6.25074500	-4.26213800	1.33404700
C	8.90299200	-4.60911200	-0.95839800
C	-13.04567400	2.67129500	-0.60444100
N	-12.66496700	3.75349600	-0.80277300
C	-15.00264500	1.35535400	-0.46198600
N	-16.16334800	1.40111400	-0.53586800
C	14.99025600	-1.36915200	-0.63514000
N	16.14908300	-1.41752300	-0.73293600
C	13.02803300	-2.68158400	-0.73151200
N	12.64126300	-3.76374700	-0.91796600
H	-0.51739500	2.46129100	0.09852200
H	0.51900200	-2.45672300	0.02877900
H	-5.41128200	-1.45821800	0.03393500
H	5.41323600	1.46195200	0.07941700
H	-1.30134400	-4.31632000	0.31839500
H	-1.17873400	-5.69122100	2.34887000
H	-3.22023700	-2.63144200	4.54848500
H	-3.32754300	-1.24450300	2.52564200
H	-4.09391900	-3.78215700	-0.45627300
H	-4.55483300	-4.98375800	-2.54558200
H	-1.44270000	-2.77999900	-4.50196000
H	-0.98816500	-1.56432200	-2.42015700

H	1.31262700	4.32688700	-0.16920800
H	1.18677800	5.71145000	-2.19295300
H	3.20556900	2.65301900	-4.41531900
H	3.31563100	1.25637700	-2.39972200
H	-3.05604100	-5.76057800	4.90036700
H	-1.29422500	-5.79920600	4.83125300
H	-2.12202400	-4.52638500	5.74551100
H	-4.35627600	-4.93086100	-5.09315600
H	-2.91479900	-4.20706000	-5.82671900
H	-2.79006900	-5.72246700	-4.93019000
H	3.05158200	5.78636700	-4.75154400
H	2.11220000	4.55765600	-5.59883200
H	1.29001100	5.82810100	-4.67635100
H	4.36619600	4.89612700	5.24626600
H	2.80913500	5.70444500	5.07906200
H	2.91416600	4.18469800	5.97097600
H	4.10199700	3.77776200	0.60004500
H	4.56557000	4.96768700	2.69521400
H	1.44441300	2.76560200	4.63904100
H	0.98691100	1.56161800	2.55079900
H	-10.89591900	2.19769500	-0.03977000
H	-11.63076300	-4.04679100	0.40343500
H	-15.53408400	-0.96275700	-0.05742700
H	10.89330200	-2.20122200	-0.11311000
H	11.64584300	4.04594300	0.25438700
H	15.53415600	0.95009800	-0.25214700
H	-9.56492600	5.44921300	-0.74458200
H	-7.87555500	4.90400800	-0.98518600
H	-9.20778900	4.14485100	-1.90825300
H	-7.24607600	4.69030800	1.47800300
H	-5.94672100	3.66736300	2.16058500
H	-5.53283900	5.10133700	1.17848700
H	7.25347900	-4.66520500	1.50327700
H	5.96002300	-3.62945900	2.17835100
H	5.53757600	-5.07893600	1.22298600
H	9.54716600	-5.46169100	-0.74786200
H	7.85498000	-4.91732700	-0.96922700
H	9.17328100	-4.17453600	-1.92509300
H	13.99966900	4.92490800	0.24448300
H	15.89208000	3.36078900	-0.00374700
H	-15.88244700	-3.37174300	0.21915800
H	-13.98263300	-4.93010600	0.44601200

## IDTOT2F

0 1			
C	0.34590700	-1.34791500	-0.20664600
C	1.33369100	-0.33509300	-0.20143700
C	0.99818300	1.02219400	-0.19412400
C	-0.34594200	1.34800800	-0.20669500
C	-1.33372400	0.33518500	-0.20138900
C	-0.99821700	-1.02210100	-0.19402700
C	-0.97437600	2.74981800	-0.19768100
C	-2.45066700	2.37854800	-0.16259600
C	-2.60777200	1.00966600	-0.19100300
C	0.97433900	-2.74972700	-0.19761200
C	2.45062700	-2.37845500	-0.16266700
C	2.60774100	-1.00957600	-0.19112200
C	0.69608800	-3.53384900	-1.48844400
C	0.49255400	-3.47149800	1.06634500
C	-0.49248600	3.47166400	1.06619700
C	-0.69623000	3.53388200	-1.48856700
C	1.00795300	-4.89735200	-1.55788600
C	0.82310300	-5.61311100	-2.73301600
C	0.32435800	-4.99963100	-3.88753600
C	0.02640200	-3.63905700	-3.81779700
C	0.20762500	-2.91657100	-2.64024600
C	1.10673800	-3.23666800	2.29958900
C	0.61586100	-3.81585200	3.46513300
C	-0.50998900	-4.64358700	3.44514500
C	-1.13183900	-4.86014400	2.21323800
C	-0.64222300	-4.28633400	1.04382500
C	0.64223600	4.28659800	1.04350100
C	1.13196400	4.86046800	2.21281900
C	0.51028600	4.64389000	3.44483000
C	-0.61549000	3.81609000	3.46498800
C	-1.10648700	3.23682900	2.29951200
C	-1.00829200	4.89735900	-1.55805800
C	-0.82352000	5.61310600	-2.73318300

C	-0.32467200	4.99964800	-3.88769600
C	-0.02644100	3.63916000	-3.81788200
C	-0.20759900	2.91666200	-2.64030300
C	0.10219400	-5.78755600	-5.14739900
C	-1.02021400	-5.29406500	4.69961100
C	1.02071700	5.29446300	4.69916300
C	-0.10309000	5.78754700	-5.14768000
C	-3.68571900	3.06155500	-0.16536000
C	-4.77787300	2.18849400	-0.20654100
S	-4.25020600	0.51988300	-0.22840600
C	3.68566600	-3.06148200	-0.16546900
C	4.77782800	-2.18843800	-0.20671300
S	4.25017900	-0.51981400	-0.22859600
C	-6.16595600	2.53449700	-0.27089300
S	-7.40663100	1.36648600	0.04435900
C	-8.67376800	2.52013600	-0.28324000
C	-8.11109000	3.75284600	-0.62149700
C	-6.71958100	3.77305700	-0.59920500
C	6.16590500	-2.53446300	-0.27112500
S	7.40661400	-1.36650100	0.04416900
C	8.67371500	-2.52016400	-0.28353800
C	8.11099800	-3.75283600	-0.62186100
C	6.71948800	-3.77301500	-0.59953000
C	-10.05639100	2.24457900	-0.36459800
C	-10.82904600	1.14322600	-0.08671600
C	10.05634300	-2.24463100	-0.36490900
C	10.82903200	-1.14332700	-0.08693600
C	-12.12419400	1.01582500	-0.81029600
C	-12.51374300	-0.40765400	-0.68719500
C	-11.59519100	-1.07171300	0.14077400
C	-10.62974300	-0.07952400	0.65918300
C	12.12416900	-1.01588900	-0.81053200
C	12.51377600	0.40755800	-0.68727300
C	11.59526900	1.07155500	0.14079500
C	10.62979500	0.07934300	0.65911400
C	-13.58557800	-1.05418000	-1.28170900
C	-13.71628400	-2.41050100	-1.04095100
C	-12.79962000	-3.08638600	-0.22768700
C	-11.73754000	-2.43750400	0.38156800
C	13.58562000	1.05411100	-1.28174100
C	13.71638500	2.41039900	-1.04083000
C	12.79976700	3.08622500	-0.22746600
C	11.73767600	2.43731400	0.38174200
O	3.81458100	-4.41157400	-0.15690100
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C	-4.08724900	4.98099700	1.12934200
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O	-12.71369000	1.88517700	-1.42550900
C	-9.87768200	-0.22989000	1.80764900
O	12.71361000	-1.88519000	-1.42586900
C	9.87776600	0.22959900	1.80761500
F	14.71191400	3.10841000	-1.57923500
F	12.97241400	4.39260600	-0.04704400
F	-14.71180000	-3.10848800	-1.57941200
F	-12.97221400	-4.39279400	-0.04741100
C	-9.31064200	0.88110800	2.49271500
N	-8.88906700	1.77606300	3.10492300
C	-9.74602500	-1.47191700	2.48987400
N	-9.61023400	-2.47943000	3.05594500
C	9.31069700	-0.88145600	2.49256200
N	8.88910400	-1.77648400	3.10465100
C	9.74616800	1.47154700	2.48999600
N	9.61040800	2.47899000	3.05619800
H	1.76306700	1.79313200	-0.17602100
H	-1.76309800	-1.79304000	-0.17584900
H	1.40551900	-5.40118600	-0.68335600
H	1.07369200	-6.67119200	-2.75549900
H	-0.35716000	-3.12943000	-4.69845700
H	-0.03650500	-1.85922500	-2.62835000
H	1.97447500	-2.58457000	2.35448300
H	1.11598100	-3.61556900	4.40970400
H	-2.01662300	-5.49052700	2.16462800
H	-1.14749200	-4.48228100	0.10284000
H	1.14735600	4.48255700	0.10243800
H	2.01669700	5.49091500	2.16407300
H	-1.11547600	3.61581300	4.40963000
H	-1.97417000	2.58467100	2.35454600
H	-1.40591800	5.40116100	-0.68353800
H	-1.07422800	6.67116000	-2.75568100
H	0.35731900	3.12959700	-4.69849000
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H	0.94249600	-6.45828100	-5.35153600
H	-0.79570000	-6.41161800	-5.06870300
H	-0.02758400	-5.13078300	-6.01143800
H	-0.56792000	-6.28280200	4.84181500
H	-0.78169100	-4.69698000	5.58404200
H	-2.10402700	-5.43528900	4.66363900
H	0.57149900	6.28490300	4.83924000
H	0.77890700	4.69940900	5.58405800
H	2.10504900	5.43211000	4.66463800
H	-0.94652300	6.45340200	-5.35495100
H	0.79103700	6.41671200	-5.06697700
H	0.03275300	5.13064300	-6.01067800
H	-8.72646000	4.60535000	-0.88811400
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H	8.72633800	-4.60533700	-0.88855500
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H	-10.62106600	3.03287700	-0.86642700
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H	-14.29509300	-0.52757000	-1.91077200
H	-11.06154800	-3.01368400	1.00090600
H	14.29510000	0.52754700	-1.91088200
H	11.06172200	3.01345000	1.00115900
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H	-4.19475400	6.05402000	0.96741600
H	-5.01550800	4.57932600	1.54841600
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C	1.04242900	0.92467800	0.06497000
C	1.29508900	-0.46823900	0.02762600
C	0.25503700	-1.40276400	-0.00751900
C	-2.34894200	-1.72785500	-0.03456400
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C	-2.72743900	0.63099600	0.02555800
C	-3.36224700	-0.59559600	0.01217800
C	-4.75868000	-0.48827800	0.00811300
C	-5.18697000	0.83370800	0.02639400
S	-3.82479100	1.94795300	0.03138100
C	2.72817100	-0.62821100	0.02543600
C	3.36308600	0.59827700	0.04178500
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C	5.18759600	-0.83125500	0.03027400
S	3.82533600	-1.94521200	0.01188800
C	-2.38631100	-2.63014100	1.20365400
C	-2.56310400	-2.50914900	-1.33741600
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C	3.11643200	3.86840200	3.81829300
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C	-11.36761200	0.43420700	-0.01443900
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C	-12.35558500	-1.71180300	0.11106100
C	-13.39791500	-0.77838500	0.01362600
C	-12.81303300	0.57585900	-0.09402300
O	-9.95770100	-1.52577800	0.15502300
C	-13.54769800	1.73384200	-0.27181500
C	-12.56697000	-3.07367500	0.21662100
C	-13.89056200	-3.49288000	0.22574300
C	-14.95606400	-2.60170300	0.13495600
C	-14.71833200	-1.23432700	0.02652000
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C	8.37213200	-2.73261800	0.05538100
C	6.97135200	-2.62174400	0.06947200
C	6.53878700	-1.29948800	0.02285600
S	7.87190100	-0.18626100	-0.01360900
O	6.10675200	-3.66833100	0.10772500
C	10.44216000	-1.45986200	-0.05718100
C	11.36730100	-0.43705700	-0.11370000
C	11.06126600	0.99762600	-0.02315200
C	12.35809800	1.70980400	-0.03154800
C	13.39815500	0.77467300	-0.13642400
C	12.81110100	-0.58057900	-0.21595400
O	9.96130000	1.52554200	0.05736300
C	13.54272700	-1.74112400	-0.38976400
C	12.57184800	3.07282100	0.05250100
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C	14.95883000	2.59860700	-0.06827700
O	14.71869000	1.23006400	-0.15443800
C	-9.05869500	3.88714400	0.16064900
O	-6.10652100	3.67014900	0.11347500
O	9.05903700	-3.88641400	0.11985500
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N	-12.57545300	4.11059300	-0.58740300
C	-14.96979600	1.75758300	-0.33207200
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C	12.97403500	-3.03922000	-0.52776100
N	12.56655300	-4.12245000	-0.65435200
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H	0.45937800	-2.46911300	-0.02775200
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H	5.44642900	1.32991200	0.06766400
H	-1.40360800	-4.28673300	0.23819100
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H	-3.27860100	-2.59956000	4.48695900
H	-3.35586300	-1.19067400	2.47804400
H	-4.18288800	-3.67999700	-0.52933000
H	-4.67029500	-4.85133100	-2.62962300
H	-1.50901500	-2.70020200	-4.56564400
H	-1.02699000	-1.51505300	-2.47258100
H	1.40549300	4.29006700	-0.18222300
H	1.31401100	5.68897700	-2.19781700
H	3.28486600	2.60701600	-4.43063600
H	3.35976100	1.19597600	-2.42343600
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H	2.23371000	4.53847100	-5.60709800
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H	4.46457300	4.77148200	5.23956200
H	2.91859800	5.60264300	5.08160900
H	3.00421400	4.07524900	5.96239100
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H	4.66801100	4.84918100	2.69218900
H	1.50337200	2.69582600	4.62019700
H	1.02380800	1.51446600	2.52410900

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H	10.83270600	-2.47399800	-0.05998100
H	11.75175600	3.77813100	0.13133400
H	15.56190100	0.55619900	-0.22991300
H	-9.43299200	5.69367700	-0.66927000
H	-7.75653900	5.11656600	-0.92621200
H	-9.10836300	4.39978200	-1.85420300
H	-7.11030900	4.84904300	1.51846400
H	-5.83601300	3.78096400	2.17867700
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H	7.11669300	-4.82997400	1.52235900
H	5.84453200	-3.75445000	2.17524800
H	5.39319400	-5.20060100	1.22809400
H	9.41928200	-5.70099000	-0.69805500
H	7.73910100	-5.12571500	-0.93363600
H	9.07602500	-4.41882400	-1.89031800
H	15.97144500	2.98685400	-0.07736800
H	-15.96846200	-2.99033200	0.15010500
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C	-3.37141200	0.54153700	-0.01850400
C	-4.76571100	0.41155600	-0.01479800
C	-5.17246300	-0.91736200	-0.03539500
S	-3.79242500	-2.00945800	-0.04233700
C	2.71735100	0.67124800	-0.02259000
C	3.37200300	-0.54503200	-0.03910500
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S	3.79261400	2.00594600	-0.00852000
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C	-9.01311700	-1.63761000	-0.07496000
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C	-10.41621100	-1.62726100	-0.02227800
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C	-13.40603900	0.56151000	0.01057600
C	-12.79880200	-0.78621300	0.09992300
O	-9.98177200	1.36651000	-0.14092200
C	-13.51828000	-1.95526700	0.26292600
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C	9.01308500	1.63761100	-0.01529100
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C	6.92662500	2.73370800	-0.07008900
C	6.51589700	1.40433900	-0.02037500
S	7.86691000	0.31292700	0.01797200
O	6.04484300	3.76572800	-0.111105000
C	10.41540800	1.62892000	0.05428700
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C	12.38324200	-1.50794600	0.04137100
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C	12.62317400	-2.87001600	-0.03380700
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C	14.97939200	-2.34180600	0.08200700
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F	14.26524600	-4.56707500	-0.08129400
F	16.23077000	-2.79443500	0.09560500
O	-8.99457900	-4.03203800	-0.17590100
O	-6.04531600	-3.76794900	-0.13235200
O	8.99409000	4.03117000	-0.12585700
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C	8.71006900	4.98584500	0.90741200
C	-12.93415600	-3.24563600	0.40913300
N	-12.51239200	-4.32260700	0.54109400
C	-14.93989200	-1.99589600	0.32384400
N	-16.09969300	-2.07789100	0.37714900
C	14.93483600	2.00517000	0.44616000
N	16.09382800	2.08899600	0.51265000
C	12.92748400	3.25395500	0.49613200
N	12.50359200	4.33183700	0.61302400
H	-0.41936100	-2.47938500	-0.08300200
H	0.41992200	2.47566000	0.02935600
H	-5.46599200	1.23956800	0.00276100
H	5.46684300	-1.24256700	-0.06537400
H	-1.46281600	4.25978700	-0.23916300
H	-1.38708200	5.66057200	-2.25410000
H	-3.32073000	2.55665800	-4.48900000
H	-3.37971300	1.14395800	-2.48220900
H	-4.23668700	3.61758900	0.52358200
H	-4.74399500	4.77985100	2.62428200
H	-1.56151900	2.66513400	4.56562000
H	-1.05916200	1.48924000	2.47213100
H	1.46393300	-4.26358600	0.18159000
H	1.38942100	-5.66488100	2.19618800
H	3.32522800	-2.56184400	4.43044900
H	3.38270400	-1.14844500	2.42438300
H	-3.26256800	5.69485600	-4.80557100
H	-1.50294900	5.78989600	-4.73633200
H	-2.28941600	4.50093300	-5.66438800
H	-4.54855400	4.71450000	5.16780500
H	-3.09175800	4.02250100	5.90194300
H	-3.00407500	5.55124800	5.02397500
H	3.26490100	-5.70275900	4.74487400
H	2.29723500	-4.50597100	5.60603100
H	1.50477500	-5.79235800	4.67960900
H	4.54591500	-4.70494200	-5.23383700
H	3.00880200	-5.55350200	-5.08217200
H	3.08046500	-4.02452100	-5.96143100
H	4.23653700	-3.62085600	-0.58419200
H	4.74225100	-4.78099000	-2.68640900
H	1.55807000	-2.66466300	-4.62315000
H	1.05721500	-1.49095300	-2.52773900
H	-10.79112100	-2.64728100	-0.02283400
H	-11.80848700	3.59160000	-0.24240400

H	-15.58517800	0.31959400	0.07823100
H	10.78918000	2.64935600	0.05337900
H	11.81540900	-3.59020400	-0.10712800
H	15.58484900	-0.31155300	0.23008100
H	-9.33441000	-5.85150700	0.64040400
H	-7.66783800	-5.24691000	0.89782200
H	-9.02941500	-4.56137900	1.83484600
H	-7.02946800	-4.95681500	-1.54295700
H	-5.77472500	-3.86300300	-2.19835700
H	-5.30076900	-5.29439500	-1.23990100
H	7.03163500	4.93749300	-1.53380900
H	5.77702600	3.83674000	-2.17847500
H	5.30254900	5.27966800	-1.23773500
H	9.32235900	5.85720300	0.67972000
H	7.65166000	5.25572500	0.91672600
H	8.99825900	4.57779000	1.88048300

## IEICO

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C	1.12281500	0.82504000	-0.01410400
C	1.24604300	-0.58443800	0.05565600
C	0.12416100	-1.42033700	0.06661800
C	-1.12278400	-0.82499800	0.01454600
C	-1.24601600	0.58448100	-0.05519400
C	-0.12413300	1.42038000	-0.06616600
C	2.49855800	1.50841100	0.00598600
C	-2.49852100	-1.50837700	-0.00560400
C	2.65629600	-0.87355500	0.11048400
C	3.40229900	0.28943400	0.09818000
C	4.78126500	0.05518200	0.14345100
C	5.08663800	-1.30158800	0.19578100
S	3.62651500	-2.28441200	0.18319200
C	-2.65627200	0.87359200	-0.11001900
C	-3.40226600	-0.28939900	-0.09775000
C	-4.78123900	-0.05515900	-0.14302000
C	-5.08662100	1.30160500	-0.19531700
S	-3.62651100	2.28444600	-0.18266600
C	2.57415800	2.41511900	1.23979200
C	2.83006400	2.25744300	-1.29051800
C	-2.57408700	-2.41501300	-1.23945800
C	2.08611000	3.72475200	1.18459200
C	2.07190300	4.52983600	2.31780700
C	2.54776200	4.06201300	3.54614400
C	3.03072600	2.75281300	3.59708200
C	3.04345900	1.94149700	2.46625300
C	3.93417800	3.11778900	-1.32641000
C	4.30942600	3.75065900	-2.50417500
C	3.59838700	3.55126800	-3.69256300
C	2.50452000	2.68612500	-3.65415000
C	2.12480100	2.04757800	-2.47537800
C	-2.08608600	-3.72463900	-1.18433800
C	-2.07184600	-4.52964600	-2.31764000
C	-2.54763000	-4.06172800	-3.54593900
C	-3.03057100	-2.75248600	-3.59679800
C	-3.04332900	-1.94127600	-2.46592700
C	2.56665100	4.94706400	4.76029200
C	3.98866300	4.26428700	-4.95634500
C	-2.56656400	-4.94655700	-4.76024700
C	-3.98911400	-4.26437200	4.95652100
C	-3.93421900	-3.11780700	1.32666700
C	-4.30949400	-3.75076100	2.50434600
C	-3.59846400	-3.55146700	3.69278700
C	-2.50456200	-2.68640900	3.65444600
C	-2.12479700	-2.04775700	2.47571300
C	-2.83005700	-2.25747600	1.29085700
C	8.85938700	-2.30609300	0.27817100
C	8.10241500	-3.47651900	0.34373600
C	6.72416400	-3.24558200	0.34337600
C	6.38754300	-1.88632900	0.24483100
S	7.81671400	-0.91492400	0.17378800
C	10.26527800	-2.29134700	0.14548500
C	11.20776300	-1.29252500	0.09036400
C	12.48910400	-1.59973500	-0.60660600
C	13.10747200	-0.28944300	-0.91116400
C	12.32763400	0.73418600	-0.34578000
C	11.22924300	0.11326500	0.42656500
O	12.90995900	-2.70153300	-0.91179100
C	10.54169800	0.72169700	1.45976300

C	14.25054800	-0.02427900	-1.64623800
C	14.61204500	1.30846600	-1.83689200
C	13.83471700	2.33415000	-1.29479700
C	12.69265300	2.06484300	-0.53902300
C	-8.85937500	2.30605300	-0.27809600
C	-8.10242800	3.47650700	-0.34334500
C	-6.72416300	3.24559800	-0.34279300
C	-6.38753100	1.88633900	-0.24445000
S	-7.81669900	0.91489400	-0.17382200
C	-10.26529300	2.29126500	-0.14561800
C	-11.20778400	1.29243300	-0.09079000
C	-12.48924300	1.59953600	0.60602100
C	-13.10761900	0.28919400	0.91034600
C	-12.32767200	-0.73435000	0.34496100
C	-11.22919200	-0.11332500	-0.42716100
O	-12.91019000	2.70129200	0.91123100
C	-10.54149600	-0.72160600	-1.46034300
C	-14.25079800	0.02391700	1.64522000
C	-14.61229200	-1.30885600	1.83566200
C	-13.83486600	-2.33446100	1.29355300
C	-12.69269700	-2.06504000	0.53798300
C	9.81842900	-0.02387900	2.43204300
N	9.27017000	-0.61078500	3.27399400
C	10.63098800	2.11405300	1.74020000
N	10.66924300	3.25080000	1.98656200
C	-10.63070900	-2.11393100	-1.74095400
N	-10.66892100	-3.25064800	-1.98746000
C	-9.81814100	0.02413000	-2.43243800
N	-9.26980900	0.61117800	-3.27424200
H	0.23213100	-2.49995900	0.11265000
H	-0.23210400	2.50000100	-0.11220400
H	5.54252100	0.82765400	0.14182200
H	-5.54248200	-0.82764300	-0.14140100
H	1.72304100	4.12535600	0.24222000
H	1.68612800	5.54403700	2.24510300
H	3.40590200	2.35753500	4.53811600
H	3.42360400	0.92718300	2.54390300
H	4.50172000	3.30171000	-0.41817700
H	5.17118000	4.41411200	-2.50090900
H	1.93454000	2.50482100	-4.56231200
H	1.27024800	1.37830600	-2.48621600
H	-1.72306200	-4.12533300	-0.24198700
H	-1.68610200	-5.54386100	-2.24500300
H	-3.40568400	-2.35711700	-4.53782300
H	-3.42343500	-0.92694300	-2.54350600
H	3.50182800	5.51679200	4.81683700
H	1.74663100	5.67040100	4.74001100
H	2.48584700	4.36314700	5.68131000
H	5.07597400	4.30830500	-5.07017000
H	3.57262800	3.77032200	-5.83834300
H	3.62259500	5.29779400	-4.95440700
H	-3.50437800	-5.51157700	-4.82024800
H	-2.47964900	-4.36292200	-5.68090800
H	-1.75019200	-5.67389900	-4.73717300
H	-5.07632900	-4.30143200	5.07395000
H	-3.62999400	-5.30028900	4.95133500
H	-3.56693000	-3.77480900	5.83803400
H	-4.50172400	-3.30166300	0.41839700
H	-5.17124100	-4.41422700	2.50098800
H	-1.93455500	-2.50525600	4.56261800
H	-1.27018200	-1.37856500	2.48661700
H	8.56467500	-4.45477400	0.39231200
H	10.68743700	-3.27261000	-0.08019700
H	14.83627200	-0.84003500	-2.05828800
H	12.11043900	2.88334700	-0.13401600
H	-8.56469300	4.45476300	-0.39182300
H	-10.68750200	3.27249500	0.08011900
H	-14.83659800	0.83961500	2.05727800
H	-12.11041500	-2.88348100	0.13294700
O	5.73921900	-4.15623500	0.41264900
O	-5.73923400	4.15630200	-0.41170500
C	6.12352200	-5.52061800	0.49817300
C	-6.12359400	5.52065100	-0.49748600
H	5.19761900	-6.09185100	0.55012900
H	6.69161100	-5.82374500	-0.38802500
H	6.71790600	-5.70336300	1.39988800
H	-6.69201900	5.82382300	0.38848200
H	-5.19770900	6.09194200	-0.54914700
H	-6.71767300	5.70327500	-1.39942700
H	14.12301500	3.36726600	-1.46268700
H	15.49904700	1.55409000	-2.41249100

H	-14.12317300	-3.36760300	1.46127100
H	-15.49937200	-1.55457000	2.41110300

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C	1.41940100	-0.31831100	-0.11217900
C	0.61461900	0.82423800	-0.16332200
C	-0.75625200	0.64455900	-0.14023700
C	-1.30891400	-0.65697400	-0.05986600
C	-0.50415900	-1.79971200	-0.01214400
C	0.86677700	-1.62001600	-0.03430100
C	-1.85258600	1.72012200	-0.16544000
C	-3.09089000	0.84322500	-0.07211600
C	-2.73989600	-0.49154100	-0.03245100
C	1.96338600	-2.69559800	-0.00595700
C	3.20269200	-1.81789700	-0.07796100
C	2.85043000	-0.48269500	-0.12603500
C	-4.47817300	1.05029800	-0.05832500
C	-5.18331300	-0.14476400	0.00559800
S	-4.10340600	-1.52721700	0.03960000
C	4.58833800	-2.02200500	-0.07910600
C	5.29499200	-0.82629500	-0.13341100
S	4.21243300	0.55434200	-0.16560400
C	1.78860400	-3.59998200	-1.23155600
C	2.01020800	-3.48652300	1.30725400
C	-1.66486000	2.63787000	1.04788700
C	-1.91371300	2.49848200	-1.48586500
C	0.92155400	-4.69634600	-1.18268800
C	0.68793200	-5.47241200	-2.31208100
C	1.31266600	-5.18797600	-3.52992700
C	2.17496000	-4.09054900	-3.57433000
C	2.40941000	-3.30820800	-2.44738600
C	2.78458700	-4.64992500	1.38520400
C	2.91456200	-5.34251600	2.58217600
C	2.27741600	-4.90268300	3.74720600
C	1.51373900	-3.73758100	3.66638000
C	1.38114200	-3.03850900	2.46898000
C	-0.79388600	3.73003500	0.97779500
C	-0.54855300	4.51997300	2.09484300
C	-1.16579400	4.25453800	3.32083700
C	-2.03246400	3.16176500	3.38625500
C	-2.27819400	2.36503400	2.27173300
C	-2.69465700	3.65741000	-1.56713100
C	-2.83771200	4.33909600	-2.76867000
C	-2.20690100	3.89302400	-3.93491300
C	-1.43576000	2.73327700	-3.85028100
C	-1.29049500	2.04449800	-2.64823700
C	1.08513100	-6.04986500	-4.73943000
C	2.39352100	-5.67327700	5.03175400
C	-2.33841000	4.65224000	-5.22471600
C	-0.92613800	5.13222200	4.51654000
C	-6.60269100	-0.31581300	0.05550700
C	6.71322300	-0.64785700	-0.15346700
S	-7.37271600	-1.80841900	-0.35637100
C	-8.98661200	-1.20990100	-0.06375100
C	-8.91070300	0.13138600	0.35691900
C	-7.57703100	0.61351700	0.41269900
S	7.78040900	-1.96225800	0.20825700
C	9.23105000	-1.01022900	0.01614400
C	8.87665600	0.30385800	-0.33992900
C	7.47175100	0.48958500	-0.42525600
C	9.59148200	1.47103300	-0.73494100
C	8.74630300	2.49113400	-1.06309800
S	7.05267500	2.09648800	-0.93413700
C	-9.83974900	1.09030100	0.85477300
C	-9.21755300	2.24497000	1.23285400
S	-7.48582500	2.23272700	1.02763200
C	10.47391100	-1.66366500	0.13252000
C	-10.05560900	-2.12077700	-0.17587900
C	11.75550200	-1.19365100	0.31296300
C	-11.41869800	-1.95274300	-0.27214500
C	12.87274500	-2.09444900	-0.09405900
C	14.09345900	-1.25994400	-0.08811800
C	13.77345600	0.02163600	0.39046700
C	12.34584900	0.03671800	0.78607100
C	-12.27174400	-3.11394600	0.11507600
C	-13.65055600	-2.59083800	0.22144800
C	-13.66425800	-1.24304400	-0.17509800

C	-12.30428500	-0.86905100	-0.62845000
C	15.37362600	-1.60084600	-0.49045800
C	16.36223700	-0.62014600	-0.42792500
C	16.05290300	0.66219700	0.02984400
C	14.76497600	0.99902500	0.44971900
C	-14.79170700	-3.24710200	0.65052000
C	-15.98237500	-2.52422500	0.70093700
C	-16.00552100	-1.17954300	0.32525800
C	-14.85696300	-0.52447600	-0.12226200
O	12.78295600	-3.26816200	-0.40761700
C	11.77033200	0.95872600	1.64144700
C	-12.00742800	0.21283100	-1.43736800
O	-11.89464000	-4.25058900	0.33819000
C	9.08484200	3.85567800	-1.50543800
O	8.24978300	4.69292600	-1.77814700
O	10.40233600	4.04551400	-1.56613100
C	10.81123300	5.35271600	-1.98337300
C	-9.82082400	3.47173800	1.78327800
O	-9.17391800	4.45194600	2.08888800
O	-11.14384500	3.36496200	1.90060000
C	-11.80513800	4.52204300	2.42384400
C	10.51148300	0.74286100	2.26672800
N	9.50698900	0.57355600	2.82907800
C	12.43759000	2.13651900	2.08157300
N	12.94596100	3.11628300	2.45029700
C	-10.77210100	0.33235500	-2.13155500
N	-9.79046300	0.43259900	-2.74817000
C	-12.95132000	1.22847700	-1.75921100
N	-13.69148500	2.08440800	-2.03098300
H	1.05300500	1.81634300	-0.21543000
H	-0.94239400	-2.79193200	0.04058000
H	-4.95943800	2.01865100	-0.13154100
H	5.07359300	-2.99154700	-0.05376400
H	0.43101600	-4.95425000	-0.24831200
H	0.00772200	-6.31820700	-2.24482300
H	2.67354500	-3.84022300	-4.50775100
H	3.08272700	-2.45922400	-2.52070300
H	3.28530400	-5.02355500	0.49612200
H	3.52291600	-6.24342700	2.61267300
H	1.01170700	-3.36479700	4.55596300
H	0.78283200	-2.13307700	2.44751600
H	-0.30979300	3.97380300	0.03625000
H	0.13449200	5.36198000	2.01123800
H	-2.52626000	2.92701500	4.32621900
H	-2.95524300	1.52057200	2.36125700
H	-3.19008500	4.03621000	-0.67726100
H	-3.45158700	5.23609800	-2.80178700
H	-0.93751400	2.35664200	-4.74038800
H	-0.68619000	1.14311800	-2.62377500
H	0.07539500	-6.46985900	-4.74595800
H	1.22698700	-5.48471100	-5.66467400
H	1.78733900	-6.89180400	-4.76029200
H	3.39046100	-6.10838800	5.14728300
H	2.19561600	-5.03681500	5.89829100
H	1.67403400	-6.50018800	5.06078200
H	-3.34686300	5.05804200	-5.34740400
H	-1.64296300	5.49938300	-5.25527100
H	-2.11854500	4.01644500	-6.08639700
H	0.08875800	5.53972100	4.51537500
H	-1.61786000	5.98298900	4.52462000
H	-1.07387500	4.58344900	5.45066700
H	10.66660800	1.56694400	-0.78838800
H	-10.90724400	0.94939000	0.94719300
H	10.45244500	-2.74429900	-0.02603300
H	-9.78114700	-3.17481100	-0.09152200
H	15.58524800	-2.60506600	-0.84417200
H	17.37659300	-0.84932800	-0.73917500
H	16.83084200	1.41879500	0.06204500
H	14.56089500	2.00395100	0.79757600
H	-14.74469900	-4.29280100	0.93804400
H	-16.89638300	-3.00410600	1.03653800
H	-16.93819100	-0.62663000	0.38028500
H	-14.91104400	0.51949200	-0.40460800
H	11.89950000	5.33598700	-1.97355100
H	10.43894400	5.56511800	-2.98776500
H	10.43310200	6.10766400	-1.29105200
H	-12.86245800	4.26550600	2.45545800
H	-11.43494100	4.75168700	3.42522300
H	-11.63898600	5.38191400	1.77162400



# IEICO4F

0	1			
C		1.14813200	0.78878200	0.03514800
C		1.22623900	-0.62576000	0.04596300
C		0.07870800	-1.42535900	0.00672100
C		-1.14799000	-0.78892300	-0.03517900
C		-1.22609800	0.62562000	-0.04598500
C		-0.07856600	1.42521700	-0.00675600
C		2.54364300	1.42697900	0.10146500
C		-2.54350300	-1.42712100	-0.10147900
C		2.62557700	-0.96162300	0.10916500
C		3.40728700	0.17731000	0.15961700
C		4.77681400	-0.10179100	0.21573700
C		5.03966200	-1.46890200	0.21138500
S		3.55044300	-2.40405400	0.13238400
C		-2.62543500	0.96148100	-0.10916500
C		-3.40714900	-0.17745300	-0.15959800
C		-4.77668100	0.10164900	-0.21553500
C		-5.03953500	1.46876200	-0.21107000
S		-3.55030300	2.40391100	-0.13215800
C		2.62863800	2.28485800	1.36900900
C		2.91966800	2.21129000	-1.16175800
C		-2.62851000	-2.28498900	-1.36902800
C		2.19609500	3.61478600	1.35308500
C		2.19070000	4.37771000	2.51525000
C		2.62013600	3.84550700	3.73441900
C		3.04670000	2.51584800	3.74603800
C		3.05046600	1.74674500	2.58612400
C		4.05833900	3.02576700	-1.15288200
C		4.47348200	3.68697900	-2.30148200
C		3.76931700	3.56294300	-3.50396600
C		2.63989600	2.74372500	-3.51009100
C		2.22021300	2.07697400	-2.36100700
C		-2.19591600	-3.61491000	-1.35312600
C		-2.19053300	-4.37782400	-2.51528600
C		-2.62002300	-3.84562100	-3.73444900
C		-3.04663200	-2.51598700	-3.74604500
C		-3.05039500	-1.74688700	-2.58611800
C		2.64902700	4.68402300	4.98097500
C		4.20240200	4.30701600	-4.73545300
C		-2.64888400	-4.68416700	-4.98098500
C		-4.20226200	-4.30721000	4.73541200
C		-4.05813900	-3.02599200	1.15286500
C		-4.47323700	-3.68723700	2.30144600
C		-3.76908000	-3.56315300	3.50394800
C		-2.63972400	-2.74387300	3.51007900
C		-2.22007000	-2.07708400	2.36098800
C		-2.91950200	-2.21144100	1.16174700
C		8.77716900	-2.59458700	0.30049000
C		7.98284900	-3.74268400	0.28515900
C		6.61353500	-3.46850900	0.27784100
C		6.32060200	-2.09480300	0.25254600
S		7.77986600	-1.16664100	0.26228000
C		10.18338000	-2.61517500	0.19161800
C		11.15490100	-1.64117900	0.22192500
C		12.43482400	-1.93059900	-0.48015800
C		13.09878500	-0.61957700	-0.66272200
C		12.34358200	0.37622900	-0.02410900
C		11.20958600	-0.26960200	0.67193700
O		12.83170300	-3.01245600	-0.87378300
C		10.51620600	0.27995300	1.73389300
C		14.26570300	-0.34206100	-1.35618600
C		14.66485100	0.98177800	-1.41500900
C		13.91403200	1.98527700	-0.79327100
C		12.75589900	1.70638000	-0.08455200
C		-8.77703200	2.59451900	-0.29988200
C		-7.98268200	3.74259600	-0.28382900
C		-6.61338200	3.46840200	-0.27661600
C		-6.32046800	2.09467200	-0.25210100
S		-7.77973800	1.16653300	-0.26255400
C		-10.18323200	2.61514100	-0.19102900
C		-11.15487600	1.64126700	-0.22171600
C		-12.43474300	1.93060900	0.48049200
C		-13.09892500	0.61962100	0.66251600
C		-12.34388400	-0.37605000	0.02351000
O		-11.20975600	0.26987800	-0.67223900
C		-12.83145000	3.01236300	0.87457700
C		-10.51638100	-0.27940000	-1.73434500
C		-14.26594900	0.34205500	1.35578500

C	-14.66537800	-0.98172400	1.41399800
C	-13.91472900	-1.98510200	0.79185000
C	-12.75649300	-1.70614300	0.08333200
C	9.74713700	-0.51424500	2.62915800
N	9.16062000	-1.14766800	3.40926100
C	10.64043900	1.64444100	2.11716700
N	10.71234600	2.76019200	2.44017600
C	-10.64066300	-1.64377400	-2.11802200
N	-10.71256400	-2.75943600	-2.44134100
C	-9.74725900	0.51501400	-2.62936600
N	-9.16068300	1.14860800	-3.40928500
H	0.15152900	-2.50886800	0.00727100
H	-0.15138200	2.50872700	-0.00730300
H	5.56109000	0.64599200	0.25929700
H	-5.56095700	-0.64614000	-0.25900300
H	1.86997000	4.06416300	0.41924000
H	1.84902200	5.40929200	2.47286200
H	3.38417600	2.07090400	4.67911800
H	3.38567100	0.71479000	2.63330500
H	4.62224700	3.15132900	-0.23246000
H	5.36202200	4.31296800	-2.26357500
H	2.07358700	2.62086200	-4.43028500
H	1.33883700	1.44502600	-2.40720200
H	-1.86974600	-4.06427700	-0.41929300
H	-1.84881900	-5.40939500	-2.47291700
H	-3.38415200	-2.07105000	-4.67911200
H	-3.38564000	-0.71494400	-2.63328500
H	3.60231200	5.21787400	5.07358300
H	1.85512900	5.43618800	4.97459500
H	2.53202500	4.06994100	5.87815400
H	5.29275200	4.35336600	-4.81110400
H	3.81637600	3.83570900	-5.64321100
H	3.83537800	5.34014200	-4.72046500
H	-3.60141300	-5.21953300	-5.07260700
H	-2.53374600	-4.06990300	-5.87827500
H	-1.85380500	-5.43509900	-4.97541600
H	-5.29262700	-4.35009000	4.81305000
H	-3.83869900	-5.34152500	4.71855000
H	-3.81304100	-3.83817200	5.64297100
H	-4.62202400	-3.15159100	0.23243500
H	-5.36172600	-4.31329900	2.26352500
H	-2.07341800	-2.62098700	4.43027100
H	-1.33872200	-1.44509800	2.40719200
H	8.41325800	-4.73644000	0.28392400
H	10.58108900	-3.59097000	-0.09384200
H	14.84650300	-1.12240900	-1.83600900
H	12.21808500	2.52541600	0.37634100
H	-8.41307700	4.73635700	-0.28199900
H	-10.58085500	3.59084700	0.09485100
H	-14.84659900	1.12233100	1.83590500
H	-12.21883000	-2.52509100	-0.37789400
O	5.59988400	-4.34896900	0.27929000
O	-5.59971700	4.34884700	-0.27752300
C	5.93946000	-5.72814400	0.28824700
C	-5.93928100	5.72803300	-0.28529200
H	4.99513600	-6.27076800	0.29350600
H	6.51115700	-5.99622600	-0.60686800
H	6.51373200	-5.98300900	1.18547200
H	-6.51085800	5.99537200	0.61012200
H	-4.99495300	6.27065000	-0.29023400
H	-6.51367300	5.98364900	-1.18222700
F	-15.76890300	-1.33556600	2.06658400
F	-14.34390400	-3.23988300	0.89638900
F	15.76826100	1.33554900	-2.06783200
F	14.34292400	3.24010200	-0.89840000

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C	-2.97911700	1.22305300	-0.06167500
C	-2.75304500	-0.18196400	-0.02218400
C	-1.46748200	-0.68176000	-0.01335000
C	-0.40370000	0.22923300	-0.06462200
C	-0.65258300	1.63054400	-0.12014600
C	-1.94348300	2.15181000	-0.10911600
C	1.02204400	0.06899900	-0.07175900
C	1.57538400	1.37976800	-0.13096600
N	0.55077800	2.30062900	-0.17493800
C	1.85735400	-1.05576200	-0.03262800
C	3.22135100	-0.85421100	-0.05675400

C	3.75353000	0.46579500	-0.10032200
C	2.95013000	1.60153800	-0.13517900
C	0.71315500	3.73399300	-0.20400800
C	4.33571200	-1.91115700	-0.01409100
C	5.55966800	-1.00911400	-0.01748300
C	5.18622000	0.32531300	-0.08453200
C	6.94225000	-1.17777800	0.01619400
C	7.63779000	0.03529900	-0.04699800
S	6.52121100	1.39016200	-0.12475000
C	-4.40612900	1.40661100	-0.01951600
C	-5.06760900	0.18580500	0.05915300
C	-4.07269700	-0.96480800	0.04028700
S	-5.47662900	2.72943200	-0.04151900
C	-6.87106600	1.64336700	0.05682700
C	-6.45372000	0.30760200	0.10089600
C	4.19319100	-2.73201100	1.27275000
C	4.38975600	-2.79295600	-1.26904600
C	-4.09112600	-1.80581100	1.32144100
C	-4.34504000	-1.80671700	-1.21390200
C	-5.41944900	-2.70573600	-1.21848000
C	-5.74120000	-3.42918500	-2.35861400
C	-5.00481300	-3.28599700	-3.54040900
C	-3.94008200	-2.38540500	-3.53316800
C	-3.61380900	-1.65548800	-2.39109100
C	-3.56014600	-3.09904800	1.32699000
C	-3.49005600	-3.83773900	2.50341200
C	-3.95018300	-3.31676000	3.71552400
C	-4.47522600	-2.02216400	3.70601200
C	-4.54415800	-1.27809600	2.53246700
C	3.36955300	-3.86204100	1.30515000
C	3.16570600	-4.56361200	2.48815200
C	3.77792100	-4.16865400	3.68112800
C	4.59527600	-3.03684900	3.64505700
C	4.79938100	-2.32929400	2.46422000
C	5.20509000	-3.93156300	-1.28050200
C	5.33496800	-4.70617900	-2.42547200
C	4.65770300	-4.37625700	-3.60497600
C	3.85368500	-3.23657300	-3.59125900
C	3.72055800	-2.45568400	-2.44483600
C	-5.34344000	-4.09085700	-4.76326700
C	-3.90870600	-4.13025800	4.97822700
C	4.78161300	-5.23377900	-4.83252900
C	3.58471700	-4.95084300	4.94939500
C	-8.13609400	2.27607000	0.08435300
C	9.04113300	0.13335000	0.10668900
C	9.93902600	1.17033900	0.08302000
C	-9.42865600	1.79457300	0.11517000
C	-10.62739100	2.62871400	0.13879800
C	-11.79809100	1.73755700	-0.01406100
C	-11.34721600	0.41144900	-0.05215300
C	-9.87402000	0.38178400	0.04633400
C	11.21845100	0.98254000	0.82719200
C	11.76312100	2.34209400	1.04177700
C	10.94950400	3.27847600	0.38066900
C	9.90486700	2.54613500	-0.36631500
C	12.87119500	2.72140200	1.78096400
C	13.16084000	4.08147700	1.87511100
C	12.34867800	5.02180100	1.23675200
C	11.24251300	4.63731900	0.47819800
C	-13.16699400	1.99355100	-0.10932300
C	-14.03785300	0.91140400	-0.23604900
C	-13.57243600	-0.40518100	-0.26500200
C	-12.20741200	-0.66675900	-0.17238100
C	9.22241100	3.03287000	-1.46322200
C	-10.71300100	3.99661300	0.31677600
O	-9.19936700	-0.63697500	0.05486200
O	11.68416900	-0.06934000	1.22695400
C	-11.94353900	4.71404500	0.31674300
N	-12.91491300	5.35489100	0.32465500
C	-9.60294500	4.85778800	0.55123900
N	-8.73640300	5.60839800	0.75364900
C	8.55842000	2.17597200	-2.38529700
N	8.05785100	1.49716300	-3.18666500
C	9.26027000	4.39959200	-1.85959000
N	9.25674300	5.51163500	-2.20193900
H	-1.28078700	-1.75056500	0.03817300
H	-2.13925200	3.21859000	-0.12498100
H	1.43800000	-2.05626900	0.01897800
H	3.37792400	2.59823300	-0.15704500
H	1.62147700	3.98785500	-0.75344100
H	-0.12928700	4.18675800	-0.72966300

H	0.77459100	4.15707400	0.80425900
H	7.46146400	-2.12703900	0.08935000
H	-7.17429200	-0.49729700	0.15930500
H	-6.00719100	-2.84672200	-0.31547000
H	-6.58163300	-4.11885400	-2.33176400
H	-3.35070200	-2.24761400	-4.43658700
H	-2.77995400	-0.96158700	-2.42553200
H	-3.20599300	-3.53993400	0.39952200
H	-3.07181300	-4.84127100	2.47704200
H	-4.83770600	-1.58571300	4.63377100
H	-4.95398600	-0.27273700	2.56462500
H	2.88906700	-4.20489300	0.39318100
H	2.51926300	-5.43816800	2.48287900
H	5.08247900	-2.70006900	4.55710000
H	5.43761300	-1.45059200	2.47585600
H	5.73749300	-4.22109500	-0.37850000
H	5.97510600	-5.58514400	-2.40379600
H	3.31934400	-2.94870900	-4.49349900
H	3.08870700	-1.57374000	-2.47383000
H	-6.42238400	-4.10202300	-4.94628700
H	-4.85088300	-3.69106400	-5.65336100
H	-5.02595900	-5.13394400	-4.64948900
H	-4.83662500	-4.69946900	5.10996700
H	-3.08548200	-4.84990700	4.96267400
H	-3.79081100	-3.49368600	5.85960500
H	5.82083100	-5.52699100	-5.01033300
H	4.19991600	-6.15721300	-4.72886700
H	4.41775100	-4.71250600	-5.72164500
H	2.58369500	-5.38863900	4.99979900
H	4.30348200	-5.77626800	5.01604400
H	3.72824400	-4.32174500	5.83207100
H	-8.05402000	3.35864400	0.06233400
H	9.49994500	-0.80201200	0.43386200
H	13.48488300	1.97106000	2.26946400
H	14.01865600	4.41589100	2.45009700
H	12.58105800	6.07806100	1.33081300
H	10.63070400	5.39142400	-0.00136300
H	-13.56959000	2.99751500	-0.09333800
H	-15.10369900	1.10209000	-0.31406300
H	-14.27914100	-1.22342500	-0.36209300
H	-11.81315000	-1.67786200	-0.19417100

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C	-1.15301600	0.88298000	-0.06132100
C	-1.36819000	-0.51610300	-0.03340900
C	-0.30748400	-1.42707000	-0.01338200
C	0.97615700	-0.91387100	-0.03054100
C	1.19139400	0.48531000	-0.05119800
C	0.13066800	1.39636600	-0.06265600
C	2.30344200	-1.68473200	-0.00302300
C	3.28283000	-0.52551200	-0.00272500
C	2.61898100	0.68461500	-0.04587000
C	-2.48063600	1.65424000	-0.06055600
C	-3.45983900	0.49540200	-0.02130600
C	-2.79573800	-0.71529800	-0.02140400
C	-4.85340200	0.30954200	-0.02129200
C	-5.22074500	-1.05234800	-0.00991300
S	-3.82682400	-2.10417800	-0.01514000
S	-6.24257900	1.31435700	-0.01762700
C	-7.31854600	-0.09318700	0.00563100
C	-6.59407000	-1.28619800	0.00394400
C	4.67625500	-0.34028100	-0.01461500
C	5.04450000	1.02077100	-0.05533100
S	3.65076200	2.07227800	-0.09404600
S	6.06482600	-1.34552700	0.01717400
C	7.14172300	0.06082800	-0.02010400
C	6.41814900	1.25370100	-0.05945100
C	-2.72932600	2.44330400	-1.35496300
C	-2.53005400	2.53439900	1.19414200
C	2.35044900	-2.52649500	1.27789000
C	2.55430500	-2.51333600	-1.27203800
C	-8.70460300	0.19983800	0.00376000
C	8.52730900	-0.23365300	-0.02861800
C	-9.83313100	-0.58987200	0.05287900

C	9.65651400	0.55619000	-0.01407500
C	11.02870800	0.05154700	-0.03254100
C	11.93305600	1.20313100	0.17513900
C	11.16097000	2.37080300	0.24129700
C	9.73053400	2.03237400	0.10766000
C	-11.20653100	-0.08749500	0.03873300
C	-12.10781700	-1.23877500	0.26229600
C	-11.33292600	-2.40347100	0.34356100
C	-9.90380800	-2.06378800	0.20136600
C	13.32053800	1.29782200	0.29645200
C	13.88670400	2.55974300	0.47590300
C	13.10302300	3.71471900	0.53198100
C	11.71815400	3.62656300	0.41390600
C	-13.49494600	-1.33563600	0.38682400
C	-14.05751500	-2.59637900	0.58475500
C	-13.27075300	-3.74837700	0.65660800
C	-11.88634600	-3.65812600	0.53528600
C	-2.05086000	2.13759800	-2.53609200
C	-2.33449900	2.79396900	-3.73700800
C	-3.33316500	3.77060300	-3.74342400
C	-4.02236300	4.08177600	-2.57601900
C	-3.72477300	3.42522300	-1.38625600
C	-3.08207200	2.06576400	2.38576700
C	-3.04286100	2.85684400	3.53257300
C	-2.45229600	4.11320600	3.50222200
C	-1.88960400	4.60441900	2.31870800
C	-1.93902400	3.80315700	1.17824600
C	1.76461500	-3.79659700	1.30122400
C	1.72935200	-4.52686900	2.48351200
C	2.27854600	-4.00474700	3.65121400
C	2.87233300	-2.74143400	3.65137200
C	2.89412100	-2.01503600	2.45635000
C	3.55936000	-3.48458500	-1.26975700
C	3.89303700	-4.20263200	-2.42116500
C	3.18657600	-3.93681200	-3.59633500
C	2.18358000	-2.97292400	-3.61398800
C	1.86800000	-2.25941300	-2.46177800
C	-1.56126200	2.47209200	-4.98538300
C	-1.25661600	5.96737600	2.27970000
C	3.49940500	-2.17853800	4.89614400
C	4.99952600	-5.21934600	-2.38848500
O	8.82019700	2.84758800	0.11468300
O	-8.99202500	-2.87724800	0.21978000
C	11.45810400	-1.24314200	-0.24897700
C	-11.64090000	1.20513800	-0.18022300
C	-13.01393900	1.58526100	-0.16822300
N	-14.11663400	1.95679300	-0.16906500
C	-10.79192700	2.31241300	-0.46786100
N	-10.14992700	3.25223400	-0.71185000
C	12.83002900	-1.62719300	-0.24140600
N	13.93196000	-2.00094000	-0.24502400
C	10.60314000	-2.34666600	-0.53358000
N	9.95471300	-3.28234500	-0.77653000
H	-0.48710700	-2.49733900	0.01830100
H	0.31035100	2.46705100	-0.06860500
H	-7.08852800	-2.24856100	0.01448300
H	6.91343100	2.21531200	-0.08779800
H	-8.89596000	1.26821200	-0.03325900
H	8.71786400	-1.30281500	-0.03682300
H	13.96441400	0.42911800	0.26096900
H	14.96475300	2.64153600	0.57410200
H	13.57829400	4.68088600	0.66986900
H	11.08035300	4.50392300	0.45509000
H	-14.14152000	-0.46956500	0.33938700
H	-15.13526400	-2.67957000	0.68508800
H	-13.74324800	-4.71371700	0.80907700
H	-11.24596900	-4.53297700	0.58820800
H	-1.28032200	1.37157600	-2.52930000
H	-3.57145300	4.28902700	-4.66880100
H	-4.79915100	4.84086000	-2.59009200
H	-4.25769000	3.68908300	-0.47740500
H	-3.54079600	1.08247300	2.42522400
H	-3.47984800	2.48514200	4.45500200
H	-2.42893700	4.72400500	4.40141800
H	-1.52134400	4.18549300	0.25015800
H	1.34833400	-4.21944700	0.39178700
H	1.27095200	-5.51167300	2.49356700
H	2.24859300	-4.58372400	4.57079100
H	3.34380200	-1.02520200	2.45328800
H	4.08629700	-3.70599000	-0.34450100
H	3.42300200	-4.49101300	-4.50111800

H	1.63806000	-2.77642900	-4.53265100
H	1.08362200	-1.51005000	-2.49040700
H	-1.17095900	1.45105000	-4.96272800
H	-2.18313700	2.58145500	-5.87822800
H	-0.70493400	3.14703300	-5.10113800
H	-1.98951600	6.74939400	2.50600400
H	-0.45654600	6.05320500	3.02257700
H	-0.82961100	6.18261000	1.29710100
H	3.06188800	-2.61788300	5.79652200
H	4.57589000	-2.38509700	4.92000400
H	3.37654600	-1.09309700	4.94990600
H	5.98044200	-4.73013700	-2.40259400
H	4.95662900	-5.82764400	-1.48008000
H	4.95216700	-5.88885800	-3.25111100

## IT-DM

0	1		
C	1.01917300	0.95060700	0.05453300
C	1.30308400	-0.43625700	0.05599100
C	0.28871600	-1.39876800	0.05125000
C	-1.01906900	-0.95024900	0.05702400
C	-1.30299400	0.43660700	0.05395300
C	-0.28861900	1.39909900	0.04668700
C	-2.30707400	-1.78638500	0.04337700
C	-3.34232600	-0.67642700	0.03070000
C	-2.73892600	0.56507500	0.05062000
C	2.30722100	1.78666700	0.03883000
C	3.34245000	0.67665200	0.03026200
C	2.73901000	-0.56476300	0.05383900
C	-2.32296300	-2.64188500	-1.22801900
C	-2.50492500	-2.61459500	1.32067100
C	-1.66651300	-3.87727900	-1.25484600
C	-1.60430200	-4.62615400	-2.42348500
C	-2.19744900	-4.17505200	-3.60696800
C	-2.84792500	-2.94057900	-3.57580900
C	-2.91030200	-2.18447700	-2.40829100
C	-3.43948900	-3.65527500	1.34141800
C	-3.69944800	-4.35859100	2.51216500
C	-3.03644100	-4.05280500	3.70387100
C	-2.10945500	-3.00848100	3.67967200
C	-1.84753600	-2.29924100	2.51134000
C	2.50446200	2.61906900	1.31348600
C	2.32375100	2.63811400	-1.23528000
C	1.84663800	2.30752000	2.50492900
C	2.10807500	3.02055300	3.67104400
C	3.03500300	4.06501200	3.69220500
C	3.69839800	4.36700800	2.49976300
C	3.43889500	3.65989900	1.33118900
C	2.91248300	2.17750500	-2.41357600
C	2.85055700	2.92997200	-3.58350800
C	2.19918200	4.16381100	-3.61908800
C	1.60472300	4.61819800	-2.43748200
C	1.66649400	3.87301000	-1.26650600
C	3.29204700	4.85370200	4.94482600
C	2.16068500	4.99065700	-4.87294600
C	-3.29400400	-4.83750700	4.95888800
C	-2.15877400	-5.00584200	-4.85820700
C	-4.74371600	-0.56001900	0.03808000
C	-5.17850200	0.78112100	0.05500200
S	-3.83856200	1.90052400	0.07530100
C	4.74383500	0.56022400	0.03889300
C	5.17856500	-0.78086500	0.06047100
S	3.83858500	-1.90015300	0.08359300
S	-6.08221100	-1.63213100	0.01561100
C	-7.22675800	-0.27946000	0.02507100
C	-6.56241200	0.94662300	0.04903700
S	6.08238400	1.63222000	0.01377900
C	7.22686700	0.27955200	0.02824500
C	6.56247800	-0.94642300	0.05591500
C	-8.59812400	-0.64163300	0.01444900
C	8.59827900	0.64155800	0.01743600
C	-9.76432800	0.09035900	0.00144700
C	9.76434800	-0.09066600	0.00629800
C	-11.11310300	-0.48024300	-0.01340900
C	-12.07030000	0.64027000	-0.09671000
C	-11.35623400	1.84267500	-0.10050300
C	-9.91103600	1.56799300	-0.03330000

C	11.11317300	0.47975800	-0.00939000
C	12.07008600	-0.64071200	-0.09612500
C	11.35593700	-1.84307700	-0.09859900
C	9.91089600	-1.56833300	-0.02803900
C	13.46256100	-0.68895800	-0.16699400
C	14.11593600	-1.92277200	-0.23705000
C	13.37654900	-3.12999300	-0.23421900
C	11.98398100	-3.07364700	-0.16388700
C	-13.46296800	0.68851500	-0.16376000
C	-14.11657600	1.92233000	-0.23157700
C	-13.37722700	3.12957300	-0.23047800
C	-11.98448200	3.07324400	-0.16382100
O	-9.03813000	2.42397900	-0.01669900
O	9.03799800	-2.42427500	-0.00918100
C	-11.48001400	-1.81109600	0.05378300
C	11.48028800	1.81036900	0.06113200
C	14.07818200	-4.45243800	-0.30690700
C	-14.07909200	4.45201100	-0.30101900
C	15.61382600	-1.95957300	-0.31600100
C	-15.61468900	1.95909400	-0.30622700
C	12.83418400	2.25276500	0.03468100
N	13.91793200	2.67640000	0.01698700
C	10.57610600	2.90428500	0.18090700
N	9.88879700	3.83848000	0.28213900
C	-12.83391600	-2.25355100	0.02843700
N	-13.91762200	-2.67732500	0.01145100
C	-10.57562900	-2.90546400	0.16774200
N	-9.88818100	-3.84008900	0.26396800
H	0.52159900	-2.45912900	0.04085400
H	-0.52152700	2.45941200	0.03284000
H	-1.20929800	-4.26569500	-0.34906900
H	-1.08713200	-5.58271500	-2.41533300
H	-3.31673300	-2.56024600	-4.48009800
H	-3.41933800	-1.22517500	-2.42352200
H	-3.96106600	-3.93111500	0.42915400
H	-4.43244000	-5.16152500	2.49773300
H	-1.58093900	-2.74196300	4.59189200
H	-1.12292000	-1.49107100	2.53296400
H	1.12207100	1.49937200	2.52888700
H	1.57924900	2.75696100	4.58393300
H	4.43134200	5.16993900	2.48301800
H	3.96073900	3.93283800	0.41820600
H	3.42226100	1.21855000	-2.42542000
H	3.32047500	2.54721000	-4.48619400
H	1.08688600	5.57442300	-2.43272500
H	1.20830300	4.26392200	-0.36230000
H	3.10892400	4.25261700	5.83967100
H	4.32225100	5.21857100	4.98168800
H	2.63460500	5.72956900	4.99967900
H	2.30373100	4.37261600	-5.76326400
H	1.20880300	5.52032000	-4.97266100
H	2.95369000	5.74776800	-4.86817300
H	-4.32500500	-5.19993200	4.99777200
H	-2.63853800	-5.71474500	5.01540900
H	-3.10861700	-4.23443200	5.85191700
H	-1.20931200	-5.54069100	-4.95299600
H	-2.95574300	-5.75879100	-4.85399100
H	-2.29556500	-4.38975600	-5.75087200
H	-7.10516700	1.88252500	0.05973600
H	7.10519100	-1.88230800	0.06996400
H	-8.73413500	-1.71887700	0.00973900
H	8.73447700	1.71877200	0.01011200
H	14.06487200	0.21053800	-0.17234700
H	11.38878300	-3.98262000	-0.16075800
H	-14.06529300	-0.21097300	-0.16760900
H	-11.38929700	3.98222900	-0.16196600
H	14.68170100	-4.53337400	-1.21812000
H	14.76388300	-4.58597300	0.53756000
H	13.36427400	-5.27850100	-0.29825400
H	-14.68481700	4.53319700	-1.21074500
H	-14.76274900	4.58524900	0.54514800
H	-13.36520600	5.27810900	-0.29385500
H	16.03579500	-0.95273300	-0.30862700
H	16.04268800	-2.51424700	0.52629900
H	15.95127800	-2.46303600	-1.22910700
H	-16.03657400	0.95222400	-0.29821600
H	-16.04116400	2.51325900	0.53762200
H	-15.95478800	2.46306100	-1.21806800

# IT-M

0	1		
C	1.03402400	0.93419700	0.01519600
C	1.29600100	-0.45703500	0.01790900
C	0.26643500	-1.40322700	0.01368100
C	-1.03394400	-0.93379700	0.01884400
C	-1.29593300	0.45743100	0.01475000
C	-0.26636100	1.40359100	0.00681500
C	-2.33482600	-1.74961600	0.00570500
C	-3.35236000	-0.62352600	-0.00601900
C	-2.72962500	0.60859900	0.01239400
C	2.33493700	1.74993100	-0.00086100
C	3.35246700	0.62378800	-0.00662500
C	2.72968800	-0.60822000	0.01731500
C	-2.36398000	-2.60426200	-1.26611200
C	-2.54522200	-2.57531100	1.28263000
C	-1.72561100	-3.84908700	-1.29328700
C	-1.67408100	-4.59837600	-2.46212300
C	-2.26050600	-4.13827900	-3.64553200
C	-2.89322800	-2.89465300	-3.61390600
C	-2.94470500	-2.13801900	-2.44614600
C	-3.49463700	-3.60241100	1.30248600
C	-3.76500200	-4.30254300	2.47286100
C	-3.09813900	-4.00685800	3.66489500
C	-2.15642000	-2.97568300	3.64163000
C	-1.88392600	-2.26977100	2.47376800
C	2.54443800	2.58153900	1.27238700
C	2.36500400	2.59881800	-1.27649300
C	1.88251300	2.28139500	2.46453800
C	2.15430700	2.99269000	3.62930100
C	3.09590700	4.02404800	3.64835100
C	3.76334700	4.31438800	2.45531500
C	3.49367100	3.60888200	1.28802300
C	2.94758700	2.12783800	-2.45371900
C	2.89683800	2.87923700	-3.62490400
C	2.26304000	4.12212600	-3.66285900
C	1.67485200	4.58702300	-2.48219300
C	1.72568000	3.84300600	-1.30997900
C	3.36390800	4.81143500	4.89948500
C	2.23638100	4.94720800	-4.91817200
C	-3.36680300	-4.78853400	4.91946600
C	-2.23325500	-4.96903900	-4.89707800
C	-4.75144800	-0.48525400	0.00542000
C	-5.16539400	0.86280600	0.02332000
S	-3.80795800	1.96130900	0.03933500
C	4.75154900	0.48552600	0.00653100
C	5.16542500	-0.86244200	0.03139200
S	3.80795000	-1.96081400	0.05180100
S	-6.10573700	-1.53683000	-0.01083500
C	-7.22962100	-0.16688500	0.00347700
C	-6.54629000	1.04946000	0.02302800
S	6.10590200	1.53695700	-0.01405800
C	7.22970800	0.16704200	0.00766300
C	6.54631100	-1.04915200	0.03293800
C	-8.60529300	-0.50912900	0.00139600
C	8.60542900	0.50908100	0.00497900
C	-9.76193200	0.23918300	0.00258500
C	9.76188400	-0.23950600	0.00887200
C	-11.11848400	-0.31205400	0.00020700
C	-12.06182600	0.82237400	-0.03916700
C	-11.33169400	2.01678900	-0.04118500
C	-9.88713300	1.71736700	-0.01283900
C	11.11851500	0.31148400	0.00504900
C	12.06156400	-0.82295900	-0.03977300
C	11.33128400	-2.01729400	-0.03973700
C	9.88685500	-1.71772400	-0.00607900
C	13.45653900	-0.89337300	-0.07950200
C	14.05942300	-2.14689600	-0.11437400
C	13.32476200	-3.34402300	-0.10835100
C	11.93016300	-3.26402800	-0.07274900
C	-13.45697400	0.89269700	-0.07280000
C	-14.06013200	2.14617300	-0.10413800
C	-13.32556500	3.34337400	-0.10060100
C	-11.93083300	3.26348800	-0.07094800
O	-9.00309900	2.56140700	-0.00734400
O	9.00276700	-2.56167500	0.00276100
C	-11.50425700	-1.63860300	0.03921000
C	11.50453900	1.63778200	0.04918700
C	14.02968200	-4.66764100	-0.12396300



C	-14.03071300	4.66691100	-0.11244900
C	12.86579800	2.05766800	0.03942700
N	13.95712900	2.46161300	0.03348800
C	10.61527400	2.74810100	0.11867400
N	9.94003500	3.69459800	0.17795100
C	-12.86548700	-2.05863500	0.03167500
N	-13.95674400	-2.46280500	0.02733400
C	-10.61476600	-2.74929900	0.09915800
N	-9.93938800	-3.69617700	0.15026000
H	0.48203200	-2.46718100	0.00454500
H	-0.48198500	2.46747900	-0.00753500
H	-1.27430000	-4.24438800	-0.38754900
H	-1.17078800	-5.56230600	-2.45423000
H	-3.35654600	-2.50735900	-4.51806500
H	-3.43975900	-1.17140700	-2.46125200
H	-4.01974200	-3.87039600	0.38989000
H	-4.50925700	-5.09502400	2.45779300
H	-1.62456300	-2.71715700	4.55420300
H	-1.14782900	-1.47204400	2.49606600
H	1.14648600	1.48370100	2.49009500
H	1.62199200	2.73830700	4.54276800
H	4.50751500	5.10688300	2.43702900
H	4.01915000	3.87278000	0.37445700
H	3.44352500	1.16161800	-2.46392900
H	3.36160600	2.48835500	-4.52677300
H	1.17074300	5.55055500	-2.47917400
H	1.27304700	4.24197300	-0.40651500
H	3.17982400	4.21223200	5.79541300
H	4.39691500	5.16863000	4.93203600
H	2.71311000	5.69210700	4.95647100
H	2.37107400	4.32571600	-5.80737700
H	1.29194700	5.48981400	-5.01905800
H	3.03977100	5.69329100	-4.91443300
H	-4.39937900	-5.14692400	4.95236700
H	-2.71490300	-5.66804200	4.98158000
H	-3.18469700	-4.18477200	5.81273700
H	-1.28970700	-5.51391500	-4.99389400
H	-3.03810400	-5.71353800	-4.89137900
H	-2.36524100	-4.35130000	-5.78930100
H	-7.07391700	1.99391100	0.03572100
H	7.07387800	-1.99355900	0.05058400
H	-8.75670000	-1.58432900	-0.00528300
H	8.75709200	1.58422100	-0.00582400
H	14.08038500	-0.00946400	-0.08806400
H	15.14438300	-2.20066800	-0.14893600
H	11.31356400	-4.15856500	-0.07219300
H	-14.08078900	0.00875200	-0.07902300
H	-15.14524200	2.19985300	-0.13379700
H	-11.31433400	4.15809100	-0.07240700
H	14.48700900	-4.87257300	0.85074200
H	13.34050200	-5.48485600	-0.34769500
H	14.83370800	-4.67911900	-0.86569200
H	-14.83639400	4.67948100	-0.85237100
H	-14.48593600	4.87015900	0.86359200
H	-13.34217100	5.48460100	-0.33639700

## ITCPTC

0 1			
C	-1.27988400	-0.50047900	0.06082800
C	-1.06424400	0.89894800	0.06401300
C	-0.21939300	-1.41201700	0.05738300
C	1.06425600	-0.89893000	0.06414400
C	1.27989600	0.50049900	0.06073400
C	0.21940500	1.41203700	0.05715200
C	2.39103700	-1.67133700	0.04688900
C	3.37053600	-0.51232700	0.02368400
C	2.70740400	0.69904600	0.04811700
C	4.76359300	-0.32761100	0.01857200
C	5.13266400	1.03438900	0.02981600
S	3.73956300	2.08718800	0.06110400
S	6.15080200	-1.33422000	-0.01530400
C	7.22892600	0.07242200	-0.01817800
C	6.50551000	1.26672100	0.01000800
C	-2.39102400	1.67135300	0.04665500
C	-3.37052500	0.51233600	0.02361900
C	-2.70739100	-0.69903100	0.04824100

C	-4.76358300	0.32761700	0.01857500
C	-5.13265000	-1.03438300	0.03006100
S	-3.73954400	-2.08717500	0.06149500
S	-6.15079400	1.33421200	-0.01547700
C	-7.22891600	-0.07243200	-0.01810400
C	-6.50549500	-1.26672100	0.01028900
C	-2.63689500	2.48134800	1.32748100
C	-2.44014700	2.53227200	-1.22017200
C	2.63690600	-2.48115300	1.32783300
C	2.44016500	-2.53245300	-1.21979800
C	-3.62709600	3.46918900	1.34965200
C	-3.92692900	4.15364700	2.52213400
C	-3.25037400	3.88063900	3.71409000
C	-2.26826800	2.88786300	3.68866000
C	-1.96576700	2.19799900	2.51862800
C	-1.85602700	3.80326000	-1.23171000
C	-1.82058600	4.56083800	-2.39613800
C	-2.36972200	4.08270200	-3.58988100
C	-2.94788600	2.81212000	-3.57382000
C	-2.98287400	2.04747800	-2.41104900
C	3.62705000	-3.46906300	1.35010500
C	3.92688400	-4.15336900	2.52266400
C	3.25038800	-3.88014100	3.71461700
C	2.26835500	-2.88731200	3.68908200
C	1.96584800	-2.19759000	2.51895500
C	1.85580000	-3.80335900	-1.23118300
C	1.82034300	-4.56112300	-2.39545800
C	2.36973000	-4.08329100	-3.58923800
C	2.94816900	-2.81286300	-3.57332000
C	2.98314900	-2.04799400	-2.41066600
C	-3.55058400	4.64687000	4.97101500
C	-2.36280800	4.92077900	-4.83677200
C	3.55064100	-4.64624700	4.97160800
C	2.36260400	-4.92165700	-4.83593400
C	8.61298700	-0.22250700	-0.04668700
C	-8.61297700	0.22249000	-0.04659300
C	9.74872100	0.56053200	-0.05514900
C	-9.74872400	-0.56053400	-0.05497500
C	11.11077600	0.02294800	-0.08892500
C	12.02308300	1.16721100	-0.07429800
C	11.26469800	2.37193400	-0.03762600
C	9.82899000	2.05089700	-0.02612500
C	-11.11076900	-0.02291900	-0.08875500
C	-12.02309900	-1.16716500	-0.07433300
C	-11.26474100	-2.37190500	-0.03767200
C	-9.82902700	-2.05089900	-0.02598900
C	13.37504500	1.39705500	-0.08685000
S	13.69148200	3.08834600	-0.05316400
C	12.02123400	3.50401900	-0.02240700
C	-13.37506400	-1.39698500	-0.08705600
S	-13.69153400	-3.08827400	-0.05354400
C	-12.02129700	-3.50397900	-0.02262600
O	8.91312200	2.85821000	0.00204100
O	-8.91318100	-2.85823100	0.00227000
C	-11.54514500	1.28858300	-0.13016600
C	11.54517400	-1.28853900	-0.13055000
C	-10.70652300	2.43652000	-0.15213200
N	-10.05868300	3.40369300	-0.17170900
C	-12.93446900	1.59510200	-0.15701900
N	-14.06838600	1.85616600	-0.17908200
C	10.70656200	-2.43647400	-0.15285900
N	10.05872100	-3.40364100	-0.17273900
C	12.93450400	-1.59503400	-0.15732700
N	14.06843600	-1.85603800	-0.17936200
H	-0.39923200	-2.48266600	0.04444700
H	0.39923700	2.48268600	0.04400200
H	7.00198700	2.22810700	0.01450100
H	-7.00196100	-2.22811200	0.01493900
H	-4.16151500	3.71955300	0.43738700
H	-4.70213900	4.91587600	2.50877500
H	-1.72779700	2.64741800	4.60110200
H	-1.19798200	1.43070400	2.53932100
H	-1.43492000	4.21203000	-0.31753200
H	-1.35970900	5.54554200	-2.37610600
H	-3.38055500	2.40997900	-4.48665900
H	-3.43407300	1.05980500	-2.43845500
H	4.16141600	-3.71958400	0.43785100
H	4.70204400	-4.91565200	2.50938200
H	1.72793400	-2.64670400	4.60151000
H	1.19811200	-1.43024400	2.53957200
H	1.43452500	-4.21189100	-0.31697400

H	1.35926900	-5.54573500	-2.37530300
H	3.38107900	-2.41100200	-4.48616400
H	3.43456100	-1.06042300	-2.43819900
H	-2.91832200	5.53949900	5.04695800
H	-4.59094600	4.98256600	4.99455700
H	-3.36547500	4.04065400	5.86206000
H	-1.46855400	5.54810400	-4.89104600
H	-2.40111400	4.29970900	-5.73572700
H	-3.23100200	5.58985600	-4.86411700
H	2.92011700	-5.54019800	5.04643500
H	4.59165200	-4.97986900	4.99624900
H	3.36326900	-4.04074800	5.86266000
H	1.46461000	-5.54334400	-4.89366700
H	2.40843000	-4.30111000	-5.73487700
H	3.22657300	-5.59631400	-4.85952500
H	8.80264600	-1.29216400	-0.06614000
H	-8.80263200	1.29214700	-0.06613900
H	14.20052000	0.70044600	-0.11285700
H	11.70687500	4.53838900	0.00429100
H	-14.20052500	-0.70036100	-0.11310400
H	-11.70695900	-4.53835600	0.00402800

## C8-ITIC

0 1			
C	1.21429500	-0.64597900	0.02263400
C	1.16182100	0.77114500	0.02265200
C	-0.05461700	1.42901800	0.02268200
C	-1.21429600	0.64595900	0.02243200
C	-1.16182200	-0.77116500	0.02274000
C	0.05461600	-1.42903900	0.02297500
C	2.61116600	-1.00273500	0.02094600
C	3.40434100	0.12918700	0.01997700
C	2.55970000	1.38078800	0.02136100
C	-2.61116700	1.00271500	0.02060000
C	-3.40434200	-0.12920800	0.01981400
C	-2.55970200	-1.38080900	0.02148600
S	-3.48938600	2.49659900	0.01717500
C	-4.98576700	1.59625100	0.01404600
C	-4.76928900	0.20434600	0.01603200
C	-6.33071500	1.94467300	0.00857000
C	-7.17772200	0.82706000	0.00667600
S	-6.25199400	-0.67803700	0.01298800
S	3.48938500	-2.49662000	0.01782600
C	4.98576600	-1.59627400	0.01456700
C	4.76928800	-0.20436800	0.01629400
C	6.33071400	-1.94469700	0.00917300
C	7.17772100	-0.82708500	0.00708700
S	6.25199400	0.67801300	0.01311400
C	2.80157800	2.22181400	-1.24116200
C	2.80457000	2.22122000	1.28369700
C	-2.80149700	-2.22207800	-1.24089200
C	-2.80465300	-2.22099800	1.28396700
C	8.57950600	-1.01466400	-0.00386300
C	-8.57950700	1.01464200	-0.00431400
C	9.65913600	-0.16029700	-0.00868500
C	-9.65914600	0.16028400	-0.00900300
C	11.06650500	-0.54077000	-0.02396700
C	11.86256000	0.70756200	-0.00544100
C	10.98540800	1.80210300	0.01327000
C	9.59376600	1.31350000	0.00993200
C	-11.06650600	0.54078200	-0.02434700
C	-11.86258700	-0.70753200	-0.00568700
C	-10.98545500	-1.80208700	0.01318800
C	-9.59380300	-1.31351100	0.00982000
C	13.23857200	0.94088400	-0.00520800
C	13.68928700	2.26096600	0.01393600
C	12.80206800	3.33934200	0.03209600
C	11.42738100	3.11393700	0.03183200
C	-13.23860300	-0.94083100	-0.00546200
C	-13.68934100	-2.26090300	0.01383800
C	-12.80214200	-3.33929300	0.03216100
C	-11.42745100	-3.11391100	0.03190600
O	8.59099500	2.01234300	0.02222300
C	11.60851400	-1.81133100	-0.05551500
O	-8.59104700	-2.01237200	0.02223000
C	-11.60847000	1.81135800	-0.05603300
C	13.00880300	-2.07109900	-0.06586300
N	14.13984300	-2.34479800	-0.07525200

C	10.84523100	-3.01321800	-0.08418100
N	10.26878400	-4.02431500	-0.10920100
C	-13.00874700	2.07118700	-0.06641900
N	-14.13977300	2.34494200	-0.07584500
C	-10.84513100	3.01320600	-0.08480200
N	-10.26861300	4.02426100	-0.10990200
H	-0.11212100	2.51427700	0.02228800
H	0.11211900	-2.51429800	0.02280500
H	-6.71734200	2.95743500	0.00467000
H	6.71734100	-2.95746100	0.00545700
H	2.13524200	3.08964700	-1.25445100
H	3.83252200	2.58895200	-1.26455400
H	2.62341900	1.63450900	-2.14586200
H	2.62853300	1.63351100	2.18855200
H	3.83561300	2.58825500	1.30476000
H	2.13830800	3.08907800	1.29895700
H	-2.13515200	-3.08990700	-1.25397500
H	-3.83243500	-2.58923100	-1.26427700
H	-2.62328800	-1.63494500	-2.14569300
H	-2.62866500	-1.63311700	2.18872000
H	-3.83570200	-2.58801700	1.30503700
H	-2.13840000	-3.08885900	1.29943300
H	8.81556700	-2.07421500	-0.00922500
H	-8.81556300	2.07419400	-0.00985500
H	13.96113700	0.13575800	-0.01870800
H	14.75829100	2.44993200	0.01464800
H	13.18838700	4.35364200	0.04645700
H	10.71193900	3.93014600	0.04569000
H	-13.96115500	-0.13569600	-0.01908600
H	-14.75834900	-2.44985000	0.01454300
H	-13.18848000	-4.35358400	0.04664000
H	-10.71202300	-3.93013000	0.04588800

## CI-TIC

0 1			
C	-0.09044500	-1.42532800	0.04642500
C	1.14148100	-0.76424300	0.01254700
C	1.23357000	0.64784000	-0.03683400
C	0.09044900	1.42531700	-0.04676900
C	-1.14147800	0.76423100	-0.01289700
C	-1.23356700	-0.64785200	0.03648800
C	-2.49222200	1.26583900	-0.02546400
C	-3.40324400	0.22762300	-0.00645800
C	-2.69592800	-1.11467900	0.05301900
C	2.49222500	-1.26584900	0.02512800
C	3.40324600	-0.22763200	0.00613400
C	2.69592900	1.11466900	-0.05335300
C	-2.94688900	-1.98442800	-1.18384200
C	-3.09393100	-1.80945600	1.36259800
C	2.94688900	1.98444300	1.18348600
C	3.09393100	1.80942600	-1.36295000
C	-2.66051200	-3.35333200	-1.15707600
C	-2.80859500	-4.13473500	-2.29690200
C	-3.25098300	-3.58277000	-3.50292600
C	-3.53045400	-2.21506800	-3.52548000
C	-3.38060900	-1.42729500	-2.38788800
C	-2.35982900	-1.64381000	2.53829100
C	-2.79137800	-2.21166900	3.73364800
C	-3.96863900	-2.95959900	3.80030000
C	-4.70550400	-3.11452800	2.62263800
C	-4.27780000	-2.55256200	1.42553400
C	2.66052400	3.35334300	1.15669700
C	2.80861300	4.13476800	2.29651600
C	3.25099600	3.58282300	3.50254400
C	3.53044900	2.21511200	3.52512400
C	3.38059800	1.42732400	2.38755100
C	4.27780800	2.55249000	-1.42591500
C	4.70549800	3.11445600	-2.62304000
C	3.96860200	2.95956200	-3.80066800
C	2.79131600	2.21164300	-3.73399100
C	2.35979100	1.64379400	-2.53863700
S	-3.19808200	2.84544800	-0.05481500
C	-4.78372400	2.11544800	-0.04744100
C	-4.72526200	0.70799000	-0.01484100
C	-6.07989900	2.61371800	-0.07174800
C	-7.04586500	1.59722500	-0.05991700
S	-6.29637400	-0.00143400	-0.01446600

S	3.19808700	-2.84545900	0.05453900
C	4.78372900	-2.11545300	0.04722300
C	4.72526500	-0.70799600	0.01457900
C	6.07990300	-2.61372000	0.07160200
C	7.04587000	-1.59722700	0.05978900
S	6.29637800	0.00143200	0.01424500
C	-8.41660500	1.94382700	-0.08060500
C	8.41660800	-1.94382800	0.08058100
C	-9.58747300	1.21879600	-0.07494500
C	9.58747800	-1.21880000	0.07500100
C	-10.94198700	1.75848000	-0.09871800
C	-11.87551100	0.61107000	-0.07338700
C	-11.13149300	-0.57565900	-0.03992900
C	-9.68950100	-0.25100800	-0.04027500
C	10.94199100	-1.75848000	0.09895600
C	11.87551300	-0.61106100	0.07403400
C	11.13149800	0.57566600	0.04046300
C	9.68950800	0.25100700	0.04041200
C	-13.26935600	0.53242100	-0.07797000
C	-13.87255800	-0.72225200	-0.04943600
C	-13.10013800	-1.88537200	-0.01700200
C	-11.70922300	-1.83114600	-0.01163500
C	13.26935600	-0.53240300	0.07907900
C	13.87255900	0.72227700	0.05085200
C	13.10014200	1.88539400	0.01826500
C	11.70922900	1.83116000	0.01245800
O	-8.77846200	-1.06352900	-0.01637500
O	8.77847100	1.06352500	0.01631500
C	11.33642500	-3.08168400	0.13956800
C	-11.33641000	3.08167900	-0.13959100
C	-4.41569300	-3.59789100	5.08478300
C	-3.44677000	-4.43808900	-4.72244100
C	3.44682400	4.43813800	4.72205600
C	4.41554600	3.59788300	-5.08517500
Cl	-13.89384600	-3.42637100	0.01733200
Cl	13.89384900	3.42640100	-0.01569000
C	12.69930800	-3.49433800	0.15906600
N	13.79510200	-3.88550000	0.17641500
C	10.44120700	-4.18876000	0.16881500
N	9.75129900	-5.12595000	0.19452700
C	-12.69928900	3.49435600	-0.15888000
N	-13.79507400	3.88555000	-0.17603800
C	-10.44117400	4.18872600	-0.16938300
N	-9.75124300	5.12588600	-0.19555900
H	-0.14457000	-2.50931900	0.07781100
H	0.14457500	2.50930800	-0.07814700
H	-2.33121800	-3.81835600	-0.23213300
H	-2.57904600	-5.19646800	-2.24714500
H	-3.87341200	-1.75463000	-4.44887300
H	-3.60189400	-0.36540300	-2.44408500
H	-1.44170700	-1.06449300	2.52849600
H	-2.19817500	-2.06731800	4.63348300
H	-5.63107600	-3.68481600	2.64033500
H	-4.86827100	-2.70610000	0.52661900
H	2.33123600	3.81835700	0.23174800
H	2.57907400	5.19650200	2.24674000
H	3.87339600	1.75468900	4.44853000
H	3.60186600	0.36543100	2.44376400
H	4.86831200	2.70601600	-0.52701900
H	5.63108200	3.68472300	-2.64075300
H	2.19809300	2.06730100	-4.63381500
H	1.44165500	1.06449900	-2.52881300
H	-6.35010400	3.66332400	-0.09693600
H	6.35010800	-3.66332500	0.09683200
H	-8.52978400	3.02312200	-0.10646000
H	8.52978200	-3.02312200	0.10649000
H	-13.90015000	1.41108700	-0.10253000
H	-14.95410200	-0.80054600	-0.05233400
H	-11.09786800	-2.72657900	0.01344400
H	13.90014600	-1.41106800	0.10377800
H	14.95410100	0.80057800	0.05411500
H	11.09787500	2.72659100	-0.01272900
H	-4.06436500	-4.63444200	5.15135300
H	-4.02298400	-3.06361700	5.95406400
H	-5.50652500	-3.62047800	5.16032900
H	-2.72672700	-5.26069600	-4.75351200
H	-4.44891200	-4.88285200	-4.73259600
H	-3.34015200	-3.85436000	-5.64079700
H	2.72750900	5.26139800	4.75258900
H	3.33913900	3.85462700	5.64042900
H	4.44937000	4.88197800	4.73275700

H	5.50639000	3.62250500	-5.15981100
H	4.02459300	3.06230900	-5.95445400
H	4.06225400	4.63370400	-5.15272600

## Br-ITIC

0 1			
C	-0.15391100	-1.41930700	0.05902700
C	1.10631100	-0.81437900	0.01680100
C	1.26123500	0.59173900	-0.04482200
C	0.15391900	1.41929300	-0.05961200
C	-1.10630400	0.81436500	-0.01737700
C	-1.26122700	-0.59175300	0.04423500
C	-2.43335200	1.37569700	-0.03132300
C	-3.38965400	0.37936800	-0.00155700
C	-2.74289500	-0.99257300	0.06765700
C	2.43335900	-1.37570800	0.03079400
C	3.38966300	-0.37938000	0.00103100
C	2.74290100	0.99255800	-0.06823800
C	-3.03558600	-1.86116700	-1.16069500
C	-3.16834100	-1.65741300	1.38418900
C	3.03558800	1.86121000	1.16007200
C	3.16834800	1.65734400	-1.38479900
C	-2.80518100	-3.24039000	-1.12298100
C	-2.99118200	-4.02515000	-2.25483300
C	-3.41737400	-3.46615800	-3.46353600
C	-3.64110900	-2.08850000	-3.49700700
C	-3.45310400	-1.29740000	-2.36729400
C	-2.42618400	-1.51154200	2.55744600
C	-2.87933700	-2.04933200	3.75868700
C	-4.08656200	-2.74698400	3.83370900
C	-4.83111800	-2.88193700	2.65840700
C	-4.38228600	-2.34949100	1.45553700
C	2.80523700	3.24044800	1.12227200
C	2.99124100	4.02526300	2.25407600
C	3.41738000	3.46631900	3.46283100
C	3.64105600	2.08866300	3.49638700
C	3.45304900	1.29750000	2.36670800
C	4.38232100	2.34936100	-1.45618700
C	4.83114800	2.88177400	-2.65907700
C	4.08655200	2.74684900	-3.83435300
C	2.87929300	2.04925200	-3.75929100
C	2.42614900	1.51149600	-2.55803500
S	-3.06839600	2.98480300	-0.07333400
C	-4.68499500	2.32630300	-0.05649200
C	-4.68902100	0.91806700	-0.01160800
C	-5.95790700	2.88158100	-0.08289600
C	-6.96803900	1.90902200	-0.06111100
S	-6.28978900	0.27902400	-0.00279900
S	3.06839800	-2.98481400	0.07289200
C	4.68500000	-2.32631500	0.05609600
C	4.68902900	-0.91808100	0.01114500
C	5.95790800	-2.88159300	0.08264100
C	6.96804300	-1.90903700	0.06088900
S	6.28979800	-0.27904100	0.00242900
C	-8.32243300	2.31492800	-0.08296600
C	8.32243600	-2.31494200	0.08286300
C	-9.52346700	1.64086000	-0.07284100
C	9.52347000	-1.64087400	0.07283400
C	-10.85364300	2.23782600	-0.10062900
C	-11.83533700	1.13114500	-0.08146000
C	-11.14247300	-0.08616000	-0.04294400
C	-9.68816000	0.17672300	-0.03514400
C	10.85364300	-2.23783800	0.10082000
C	11.83533400	-1.13114600	0.08219600
C	11.14247400	0.08615800	0.04358900
C	9.68816600	-0.17673300	0.03529300
C	-13.23131100	1.11224200	-0.09512700
C	-13.88701500	-0.11613500	-0.07033400
C	-13.16551100	-1.31052300	-0.03245200
C	-11.77421600	-1.31560200	-0.01790700
C	13.23130200	-1.11223500	0.09641500
C	13.88700600	0.11615000	0.07203900
C	13.16550700	1.31053700	0.03402100
C	11.77421800	1.31560800	0.01894500
O	-8.81264400	-0.67369500	-0.00422200
O	8.81265500	0.67368200	0.00416800
C	11.19139800	-3.57677700	0.13745800
C	-11.19139300	3.57675600	-0.13764700

C	-4.55811300	-3.35394200	5.12459500
C	-3.65471200	-4.32366600	-4.67409800
C	3.65467700	4.32393100	4.67332700
C	4.55806700	3.35378400	-5.12526300
Br	-14.10021300	-2.94573000	-0.00050700
Br	14.10021200	2.94575300	0.00264200
C	12.53531300	-4.04725300	0.16263700
N	13.61322700	-4.48508100	0.18448700
C	10.24971400	-4.64485900	0.15471900
N	9.52035400	-5.55191200	0.17030700
C	-12.53530900	4.04724200	-0.16257400
N	-13.61321400	4.48510400	-0.18423100
C	-10.24969900	4.64481700	-0.15564300
N	-9.52034100	5.55186100	-0.17182000
H	-0.25643400	-2.49936000	0.10029500
H	0.25644200	2.49934700	-0.10087100
H	-2.49009000	-3.71002500	-0.19542000
H	-2.80490600	-5.09489400	-2.19669600
H	-3.97015600	-1.62259200	-4.42271500
H	-3.63148600	-0.22795200	-2.43184100
H	-1.48455900	-0.97139700	2.54131900
H	-2.27936200	-1.92108500	4.65648400
H	-5.77976800	-3.41271700	2.68262600
H	-4.98011800	-2.48636800	0.55876600
H	2.49019200	3.71004000	0.19467300
H	2.80501100	5.09501300	2.19586900
H	3.97006400	1.62279800	4.42212900
H	3.63138800	0.22804900	2.43132400
H	4.98018600	2.48622200	-0.55943500
H	5.77982400	3.41250400	-2.68332800
H	2.27928800	1.92102000	-4.65707000
H	1.48450100	0.97139100	-2.54187700
H	-6.18078100	3.94196500	-0.11661900
H	6.18077700	-3.94197600	0.11643500
H	-8.38902700	3.39792200	-0.11614100
H	8.38902600	-3.39793400	0.11609700
H	-13.82425800	2.01676000	-0.12435600
H	-14.97074500	-0.14701800	-0.08055900
H	-11.20187200	-2.23618300	0.01152700
H	13.82424400	-2.01675300	0.12577400
H	14.97073200	0.14704100	0.08270400
H	11.20187900	2.23619000	-0.01058600
H	-4.25583900	-4.40539700	5.19776800
H	-4.13729600	-2.83230700	5.98835700
H	-5.64851700	-3.32443100	5.20414600
H	-2.96296400	-5.17021600	-4.70629900
H	-4.67114800	-4.73480800	-4.67005900
H	-3.53857600	-3.75086800	-5.59812700
H	2.96143100	5.16922200	4.70660800
H	3.54071500	3.75068800	5.59734400
H	4.67034300	4.73695300	4.66811300
H	5.64850700	3.32492400	-5.20452700
H	4.13779100	2.83168200	-5.98900900
H	4.25515200	4.40503100	-5.19877600

## NFBDT

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C	3.69136000	2.62593800	-1.21461300
C	-3.69369400	-2.62568700	1.21956300
C	2.76329900	3.69670500	1.37381700
C	2.50854500	4.34716300	2.57955900
C	2.98524100	3.84458500	3.79008800
C	3.72398600	2.65649300	3.75318400
C	3.97992700	2.00424100	2.55473700
C	2.95605400	2.28231300	-2.34726200
C	2.99401000	3.07919400	-3.49101000
C	3.76596600	4.23854900	-3.54252000
C	4.50720800	4.57701000	-2.40338900
C	4.47231700	3.78844100	-1.26261400
C	-2.96359100	-2.27866600	2.35507100
C	-3.00401900	-3.07377600	3.49938800
C	-3.77235200	-4.23621600	3.54878200
C	-4.50930500	-4.57691900	2.40812900
C	-4.47221900	-3.78936100	1.26617900
C	2.73333300	4.55534300	5.08946200

C	3.80080200	5.10650200	-4.76833300
C	-3.79693900	-5.10856600	4.77166400
C	-2.72743500	-4.55922000	-5.08110900
C	-3.97288800	-2.00184000	-2.55036800
C	-3.71278000	-2.65288700	-3.74923100
C	-2.97645000	-3.84178100	-3.78493100
C	-2.50389300	-4.34637900	-2.57289000
C	-2.76217100	-3.69735600	-1.36780700
C	-3.50650400	-2.51701500	-1.33692900
C	8.63447400	0.27186000	0.03669400
C	9.68573800	-0.61900100	0.01948800
C	11.10527700	-0.29113400	0.04592700
C	11.85514400	-1.56819100	0.01016100
C	10.93782400	-2.62841800	-0.03440600
C	9.56580000	-2.08701200	-0.02994000
C	11.69418600	0.95779700	0.09726100
O	8.53664500	-2.74673700	-0.06157300
C	13.22127200	-1.85305600	0.01486300
C	13.62212900	-3.18884100	-0.02526400
C	12.69528200	-4.23237500	-0.06936900
C	11.32995200	-3.95529200	-0.07430400
C	-8.63502200	-0.27221300	-0.04122400
C	-9.68644200	0.61849900	-0.02573700
C	-11.10588700	0.29043300	-0.05482500
C	-11.85600200	1.56737400	-0.02022500
C	-10.93892100	2.62772400	0.02620500
C	-9.56681300	2.08651700	0.02415500
C	-11.69455800	-0.95855900	-0.10739100
O	-8.53782000	2.74639600	0.05781900
C	-13.22216100	1.85203600	-0.02733000
C	-13.62328700	3.18775400	0.01235200
C	-12.69667400	4.23141500	0.05833100
C	-11.33131300	3.95453200	0.06566300
C	-2.75875400	-0.56749300	0.01704700
C	-3.42171600	0.64057100	0.02996000
S	-2.38607100	2.02625300	0.03348800
C	-3.73420200	-1.74056000	-0.02946000
C	-5.05290400	-0.97008500	-0.03260700
C	-4.83001300	0.40662800	0.01376300
C	2.75807900	0.56769600	-0.01043400
C	3.42097800	-0.64040600	-0.02409900
S	2.38533300	-2.02606900	-0.02606400
C	3.73371900	1.74068600	0.03422200
C	5.05239400	0.97013100	0.03509500
C	4.82929700	-0.40657500	-0.01051400
C	-6.40519400	-1.27278100	-0.04943600
C	-7.22974700	-0.13206300	-0.02094200
S	-6.25851900	1.34158700	0.03628500
C	6.40476800	1.27267500	0.04911200
C	7.22914600	0.13186800	0.01916300
S	6.25765500	-1.34168800	-0.03581700
C	-0.33542900	-1.39221600	-0.00631800
C	-1.34261200	-0.41616300	0.00405700
C	-0.98091400	0.96895900	0.01625500
C	0.33472300	1.39240600	0.01489800
C	-13.10343700	-1.16511700	-0.13129700
N	-14.24412600	-1.39457200	-0.15297200
C	-10.97513700	-2.18692200	-0.14516500
N	-10.43429000	-3.21726600	-0.17813300
C	13.10312600	1.16423200	0.11845600
N	14.24386300	1.39364600	0.13791400
C	10.97494400	2.18622500	0.13626700
N	10.43419400	3.21658600	0.17025400
H	2.38811900	4.12693500	0.44999300
H	1.92845000	5.26670800	2.57336300
H	4.10736800	2.23581900	4.67979200
H	4.55626100	1.08321300	2.56298300
H	2.34703800	1.38379800	-2.34909400
H	2.40823500	2.78745500	-4.35920700
H	5.12184000	5.47403600	-2.41144000
H	5.04967600	4.08743500	-0.39194100
H	-2.35825400	-1.37765100	2.35845000
H	-2.42388900	-2.77827800	4.37016000
H	-5.12334500	-5.47431200	2.41582500
H	-5.04751500	-4.08968600	0.39459600
H	1.99708900	5.35440800	4.97181300
H	2.36721300	3.86472200	5.85574300
H	3.65431300	5.00591200	5.47665500
H	3.25389000	4.64957600	-5.59674800
H	3.35249400	6.08666900	-4.57102100
H	4.82934900	5.28540300	-5.09836300



H	-3.17841500	-6.00237100	4.62921700
H	-3.41437400	-4.57891900	5.64781800
H	-4.81150200	-5.45183900	4.99552700
H	-2.54814800	-3.85489600	-5.89866500
H	-1.86481300	-5.22685700	-5.00905400
H	-3.59294400	-5.16980900	-5.36415000
H	-4.54677300	-1.07928500	-2.55986000
H	-4.09028200	-2.22950100	-4.67694100
H	-1.92385600	-5.26604600	-2.56584000
H	-2.38936700	-4.12808400	-0.44326300
H	8.90475900	1.32279500	0.07147500
H	13.97323000	-1.07589300	0.04821400
H	14.68329900	-3.41790700	-0.02203100
H	13.04342400	-5.26009600	-0.09978100
H	10.58406000	-4.74318500	-0.10806900
H	-8.90510000	-1.32317200	-0.07680300
H	-13.97394100	1.07476500	-0.06218900
H	-14.68448300	3.41666400	0.00726500
H	-13.04502200	5.25907900	0.08832900
H	-10.58559700	4.74252700	0.10092700
H	-6.82695200	-2.27132800	-0.08309900
H	6.82671500	2.27117400	0.08170200
H	-0.59198600	-2.44543100	-0.01776400
H	0.59128100	2.44561700	0.02615400

## ITIC2

0 1			
C	-0.71237300	-1.11293100	0.29763900
C	-1.43693400	0.10297800	0.06921700
C	-0.67933400	1.27738700	-0.14396200
C	0.70874900	1.14431600	-0.13904100
C	1.43360700	-0.07245200	0.08551300
C	0.67582900	-1.24543600	0.30591800
S	1.75559500	2.51729500	-0.44650200
C	3.12554500	1.49779500	-0.23944200
C	2.84892300	0.17457300	0.04537300
S	-1.76001700	-2.48456200	0.60883800
C	-3.12941900	-1.46717500	0.38981700
C	-2.85196500	-0.14538700	0.10057600
C	4.53342700	1.71222700	-0.26580800
C	5.17475800	0.50693100	-0.00569400
C	4.15547100	-0.60010600	0.28715400
S	5.61397000	2.99754300	-0.54989900
C	6.98764500	1.91287600	-0.35442100
C	6.56118000	0.61230000	-0.06658400
C	-4.53781200	-1.67734200	0.42910100
C	-5.17799100	-0.47906800	0.13552600
C	-4.15752200	0.63159600	-0.13792600
S	-5.61910700	-2.95451100	0.74482100
C	-6.99253200	-1.88689100	0.47130300
C	-6.56508200	-0.59407000	0.15202500
C	4.35253500	-0.96714800	1.76627700
C	4.35026300	-1.74464700	-0.72003700
C	-4.35365800	1.75210400	0.89842500
C	-4.34572500	1.03364500	-1.60787900
C	5.51346900	-1.63692900	2.17690100
C	5.75620400	-1.89962200	3.51846400
C	4.85921500	-1.49347100	4.51225500
C	3.71636700	-0.80625100	4.10448500
C	3.46675300	-0.54576300	2.75832800
C	4.54616100	-3.07371500	-0.35808800
C	4.78010500	-4.04801400	-1.32862400
C	4.81012800	-3.73415500	-2.68535300
C	4.58841300	-2.39905500	-3.04565000
C	4.36866900	-1.42479600	-2.08414800
C	-4.34547700	1.40364300	2.25626500
C	-4.56435800	2.35310100	3.24235100
C	-4.81132600	3.69269900	2.91454500
C	-4.80786200	4.03530500	1.56480900
C	-4.57413500	3.08564300	0.56949400
C	-3.45126000	0.63818000	-2.60232500
C	-3.69035700	0.93166600	-3.94350700
C	-4.83148500	1.62573700	-4.34365900
C	-5.73793200	2.00513000	-3.34805800
C	-5.50558700	1.70902100	-2.01195500
C	5.11701500	-1.79981400	5.96008700
C	5.07832800	-4.77983300	-3.73042100
C	-5.06543100	4.71387900	3.98717800

C	-5.08202400	1.96152900	-5.78608100
C	1.22496100	-2.60300000	0.49477700
C	-1.22991500	2.63731300	-0.31179500
C	-1.65196600	3.27485200	-1.44837500
C	-1.95056500	4.64948700	-1.24021900
C	-1.74454800	5.06699500	0.04744100
S	-1.18099100	3.75548700	1.02251200
C	1.64575800	-3.21831200	1.64425400
C	1.93581400	-4.59868700	1.46520500
C	1.72495800	-5.04199000	0.18677300
S	1.16808900	-3.74834900	-0.81526500
C	8.28343500	2.47984500	-0.37653000
C	-8.28707500	-2.39816200	0.72532300
C	9.54101900	1.92765900	-0.36410700
C	-9.54422800	-1.88451300	0.51983800
C	10.65522300	2.80050600	0.10907600
C	11.78399000	1.89326400	0.40866800
C	11.43243300	0.58186500	0.04693400
C	10.09384500	0.60827400	-0.58423500
C	-10.64934700	-2.45084600	1.34700400
C	-11.76983300	-1.49150800	1.24034000
C	-11.42329200	-0.47233800	0.33702600
C	-10.09857000	-0.78626600	-0.24272400
C	13.00916800	2.19975700	0.97671700
C	13.90342500	1.15581900	1.20627100
C	13.55827000	-0.15447500	0.86758000
C	12.32958000	-0.45897000	0.28040000
C	-12.98479800	-1.50826000	1.90446900
C	-13.87331800	-0.46073200	1.66951500
C	-13.53302000	0.56718400	0.78710600
C	-12.31486700	0.57394200	0.10652300
O	10.61943200	4.00802400	0.26359500
C	9.59439400	-0.37046400	-1.42132900
O	-10.61248100	-3.46963200	2.01335900
C	-9.61176000	-0.27782700	-1.43124200
C	-8.53115200	-0.88228400	-2.13016900
N	-7.67777500	-1.38329000	-2.74185600
C	-10.22668500	0.79792200	-2.13213700
N	-10.68845700	1.68729300	-2.72370500
C	8.48833500	-0.14321000	-2.28527200
N	7.61372100	0.03064000	-3.03254800
C	10.22285000	-1.63492700	-1.60480600
N	10.70004700	-2.68354100	-1.76793100
H	7.25715700	-0.19404500	0.12652400
H	-7.25994800	0.22083500	-0.00598600
H	6.23983400	-1.96527200	1.43974500
H	6.66566300	-2.42510800	3.80009200
H	3.00427100	-0.46174500	4.85053900
H	2.56787400	-0.00106200	2.48859500
H	4.50453100	-3.36965600	0.68341800
H	4.94001900	-5.07661000	-1.01391900
H	4.60153100	-2.11686300	-4.09559200
H	4.21881200	-0.39456600	-2.39700500
H	-4.16732300	0.37010600	2.54364500
H	-4.55135900	2.05004300	4.28677800
H	-4.98796700	5.06784100	1.27485400
H	-4.55283600	3.40417900	-0.46579600
H	-2.55403000	0.08761500	-2.33923900
H	-2.97232900	0.60553500	-4.69204400
H	-6.64882100	2.53105400	-3.62421500
H	-6.24162200	2.01417600	-1.27433600
H	4.90126600	-2.85098900	6.18432700
H	6.16408100	-1.62326100	6.22456800
H	4.49161200	-1.18784700	6.61509700
H	5.10594300	-5.78205800	-3.29466000
H	4.30920700	-4.76934500	-4.50965500
H	6.03967500	-4.60484600	-4.22642300
H	-4.22557500	4.76984200	4.68808700
H	-5.21644300	5.70965800	3.56240600
H	-5.95523600	4.46079400	4.57411300
H	-4.91986200	3.02880800	-5.97660400
H	-4.41557000	1.40193200	-6.44726600
H	-6.11407800	1.73694600	-6.07248700
H	-1.73827100	2.77346300	-2.40479800
H	-2.30381700	5.31425800	-2.02141500
H	1.73572900	-2.69680100	2.58962100
H	2.28653100	-5.24916000	2.25948100
H	8.31940500	3.56707500	-0.27921900
H	-8.31943600	-3.33436100	1.28694200
H	13.25034100	3.22660500	1.23317700
H	14.87144100	1.35736300	1.65422200

H	14.26079700	-0.95850000	1.06399300
H	12.09338600	-1.48638600	0.03294800
H	-13.22258500	-2.31845000	2.58660100
H	-14.83332800	-0.43782700	2.17565200
H	-14.23124900	1.38226600	0.62365900
H	-12.08208000	1.38779200	-0.56894100
C	1.93482300	-6.41259300	-0.36602200
H	1.01384600	-6.82698600	-0.78870600
H	2.69137400	-6.41527900	-1.15786000
H	2.27357700	-7.08218600	0.42837600
C	-1.96360400	6.42442100	0.62839700
H	-1.04579300	6.83602800	1.06065500
H	-2.30553100	7.10804800	-0.15254500
H	-2.72130500	6.40606700	1.41897800

## BT-IC

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C	0.99805100	0.92359200	0.31390600
C	1.34959200	-0.46249200	0.29175800
C	3.51025200	-2.52554200	-1.24874300
C	3.86592100	-2.65468200	1.31964600
C	-3.63111000	2.55357300	-1.22835700
C	2.89339600	-3.77539800	-1.29726000
C	2.64265000	-4.40026300	-2.51640600
C	2.98753800	-3.79949500	-3.72766200
C	3.58933800	-2.53804200	-3.67565200
C	3.84738800	-1.91463500	-2.46169600
C	3.37424600	-2.21812000	2.55070500
C	3.57078100	-2.96749300	3.70829600
C	4.26681100	-4.17690200	3.67981900
C	4.77525900	-4.60169300	2.44791500
C	4.58538300	-3.85535900	1.29117100
C	-2.64352300	2.28112800	-2.17308700
C	-2.59686200	2.97335600	-3.38242600
C	-3.53069700	3.96038600	-3.69263100
C	-4.52512500	4.22998700	-2.74508000
C	-4.57712500	3.53989500	-1.54238900
C	2.74375400	-4.48856900	-5.04022100
C	4.45196500	-5.00311700	4.92074200
C	-3.47352600	4.71830000	-4.98847700
C	-3.74025700	4.92671900	5.03895500
C	-3.91033500	2.01317900	2.59596500
C	-3.90152400	2.74560500	3.77455900
C	-3.71717000	4.13442000	3.76265300
C	-3.52708500	4.74878400	2.52609500
C	-3.52533600	4.01487400	1.33980200
C	-3.72552100	2.63713900	1.35544700
C	8.63475500	-0.22737200	-0.21057100
C	9.67342400	0.67856700	-0.23883800
C	11.09368700	0.37062400	-0.33647900
C	11.82761900	1.65729900	-0.32834000
C	10.89954000	2.70468900	-0.23140800
C	9.53659900	2.14406900	-0.17236500
C	11.69676500	-0.87008900	-0.42264600
O	8.50114800	2.78937600	-0.08453300
C	13.18797800	1.96050700	-0.39617600
C	13.57304900	3.30131600	-0.36456200
C	12.63576200	4.33186500	-0.26792600
C	11.27580000	4.03636700	-0.19993500
C	-8.63789100	0.21658900	-0.12146900
C	-9.67318500	-0.69135100	-0.18230000
C	-11.09623500	-0.38541100	-0.23707800
C	-11.82540700	-1.67423600	-0.27196900
C	-10.89182300	-2.72098900	-0.24796500
C	-9.52974600	-2.15784200	-0.19322100
C	-11.70470600	0.85538100	-0.26000100
O	-8.49033900	-2.80185500	-0.16028900
C	-13.18606100	-1.97976400	-0.32102600
C	-13.56595700	-3.32218400	-0.34464300
C	-12.62324200	-4.35208900	-0.32108600
C	-11.26298700	-4.05428400	-0.27196400
C	-2.76512700	0.60628300	0.18125500
C	-3.42019600	-0.60616800	0.11259900
S	-2.39814800	-1.99626500	0.16123200
C	-3.75943400	1.76979700	0.08572800
C	-5.07043800	0.97699300	0.03038200
C	-4.82684400	-0.39448200	0.02062900
C	2.76963600	-0.61906300	0.20632100

C	3.42204100	0.59736000	0.17294400
S	2.39261000	1.98275100	0.23198300
C	3.76869700	-1.77500500	0.07029500
C	5.07064200	-0.97841600	-0.00629300
C	4.82947700	0.39122700	0.06315700
C	-6.42877900	1.25435000	-0.01317500
C	-7.23169900	0.09930400	-0.06751700
S	-6.23494100	-1.35733900	-0.05835700
C	6.42333000	-1.26186200	-0.10523000
C	7.23092800	-0.10869500	-0.11637500
S	6.24182900	1.35007700	0.00633900
C	-0.30978100	1.38794100	0.36235100
C	-1.34861000	0.43987100	0.29812900
C	-0.99875500	-0.94750400	0.29101400
C	0.31043000	-1.41289800	0.33381300
O	0.58793000	-2.74387100	0.32680200
O	-0.57375000	2.72270100	0.40033800
C	0.29279400	-3.45050700	1.53526700
C	-0.36670300	3.32135900	1.68604200
C	-13.11543100	1.04094400	-0.31452700
N	-14.25823500	1.25671400	-0.35834300
C	-11.00764100	2.09668000	-0.23578100
N	-10.48920400	3.13891300	-0.21852100
C	13.10535000	-1.05743000	-0.51395500
N	14.24618000	-1.27457600	-0.59051800
C	10.99595100	-2.10947200	-0.43109900
N	10.47461800	-3.15035100	-0.44215100
H	2.59735000	-4.26886400	-0.37950600
H	2.16281800	-5.37610700	-2.52146500
H	3.86301200	-2.03593200	-4.60053800
H	4.31707500	-0.93468400	-2.46050400
H	2.83713700	-1.27617900	2.61492700
H	3.17538700	-2.59933000	4.65197900
H	5.33603500	-5.53169300	2.39271200
H	5.00354700	-4.21457300	0.35534100
H	-1.89873400	1.51702400	-1.98065000
H	-1.81379100	2.73431700	-4.09774200
H	-5.27464300	4.98931400	-2.95485100
H	-5.36335800	3.78310600	-0.83410800
H	1.94691000	-5.23263000	-4.95890400
H	2.46735700	-3.77360400	-5.82061600
H	3.64526300	-5.00969100	-5.38375600
H	4.31734900	-4.40234100	5.82396700
H	3.72492900	-5.82285000	4.95923800
H	5.44796700	-5.45440800	4.95416900
H	-2.74783100	4.27756900	-5.67654000
H	-4.44929300	4.73151400	-5.48451300
H	-3.18415200	5.76217400	-4.82209700
H	-3.14441400	4.44316300	5.81932500
H	-3.35117600	5.93699000	4.88885400
H	-4.76170700	5.01883000	5.42579900
H	-4.06212100	0.93717900	2.63873700
H	-4.04488600	2.23224500	4.72245100
H	-3.36898400	5.82375600	2.48226600
H	-3.35065600	4.52836200	0.40111900
H	8.91719400	-1.27400500	-0.26913500
H	13.94782400	1.19408000	-0.47169100
H	14.62969200	3.54472500	-0.41657500
H	12.97135900	5.36390600	-0.24591400
H	10.52299800	4.81468700	-0.12413800
H	-8.92594500	1.26326000	-0.11051900
H	-13.94996300	-1.21389400	-0.34042700
H	-14.62277800	-3.56745000	-0.38235800
H	-12.95486200	-5.38545700	-0.34105600
H	-10.50608700	-4.83206200	-0.25248600
H	-6.87581700	2.24187800	-0.00004800
H	6.85548500	-2.25468600	-0.16850900
H	0.58755800	-4.48491100	1.35557500
H	0.87337500	-3.04746600	2.36906400
H	-0.77437600	-3.41809600	1.77510100
H	-0.56535700	4.38499400	1.56044400
H	-1.06346700	2.90606200	2.42019400
H	0.66350200	3.18005400	2.02830100

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C		-1.10190800	0.82196700	-0.01870000
C		-1.26465700	-0.58313800	0.04229100
C		-0.16265400	-1.41790900	0.05839200
C		1.10194200	-0.82209100	0.01787000
C		1.26469000	0.58301300	-0.04312500
C		0.16268700	1.41778500	-0.05923000
C		2.42598500	-1.39125700	0.03217200
C		3.38756500	-0.40080300	0.00187600
C		2.74925500	0.97497100	-0.06393300
C		-2.42594900	1.39113900	-0.03294400
C		-3.38753100	0.40068800	-0.00260300
C		-2.74922500	-0.97509100	0.06312900
C		3.04668600	1.83690400	1.16795400
C		3.18148500	1.64110800	-1.37726400
C		-3.04668900	-1.83694800	-1.16880700
C		-3.18141600	-1.64130900	1.37642700
C		2.82230700	3.21736800	1.13661200
C		3.01320900	3.99652900	2.27148300
C		3.43855500	3.43059000	3.47732200
C		3.65631300	2.05187400	3.50455400
C		3.46339400	1.26636500	2.37167400
C		4.39665500	2.33133900	-1.44357000
C		4.85154900	2.86359500	-2.64452000
C		4.11183200	2.73000600	-3.82283400
C		2.90309800	2.03403200	-3.75291600
C		2.44406500	1.49678300	-2.55387500
C		-2.82226700	-3.21741600	-1.13755800
C		-3.01320900	-3.99651300	-2.27245800
C		-3.43863800	-3.43051200	-3.47824800
C		-3.65643700	-2.05180800	-3.50538500
C		-3.46347800	-1.26635500	-2.37246400
C		-2.44399700	-1.49702400	2.55302400
C		-2.90300100	-2.03437600	3.75205100
C		-4.11168800	-2.73039600	3.82194200
C		-4.85142200	-2.86395000	2.64361200
C		-4.39657000	-2.33160500	1.44270600
S		3.05780200	-3.00172100	0.07297000
C		4.67711500	-2.35505600	0.05388800
C		4.68218500	-0.94904200	0.00906400
C		5.95215900	-2.92772800	0.07908400
C		6.95364700	-1.96278100	0.05473500
S		6.29295700	-0.33251800	-0.00396900
S		-3.05776000	3.00160300	-0.07365300
C		-4.67707200	2.35495000	-0.05446100
C		-4.68214900	0.94893500	-0.00967700
C		-5.95211400	2.92763300	-0.07951300
C		-6.95360800	1.96269500	-0.05508500
S		-6.29293100	0.33242400	0.00350300
C		8.34612800	-2.22657200	0.07283500
C		-8.34608600	2.22651400	-0.07299700
C		9.35870700	-1.30268800	0.04964200
C		-9.35869000	1.30266100	-0.04969100
C		10.70404500	-1.73301400	0.07860800
C		-10.70401500	1.73304400	-0.07840600
C		11.81763800	-0.92082400	0.06234200
C		-11.81764500	0.92091000	-0.06189600
C		13.21549700	-1.31647000	0.09327500
C		14.02830500	-0.08067800	0.05416400
C		13.16855400	1.02421900	0.00226500
C		11.76469000	0.56009100	0.00523300
C		-13.21549000	1.31663300	-0.09247600
C		-14.02835900	0.08089900	-0.05279300
C		-13.16865600	-1.02404200	-0.00105000
C		-11.76476400	-0.56000100	-0.00463900
O		10.78115100	1.28238400	-0.03309100
C		13.73786000	-2.59419700	0.14992100
O		-10.78125300	-1.28234800	0.03338900
C		-13.73779200	2.59437500	-0.14935000
C		15.40923200	0.12428300	0.06234500
C		15.86557600	1.43117700	0.01710100
C		14.99270500	2.52351400	-0.03466700
C		13.62289600	2.33222700	-0.04273700
C		-15.40930200	-0.12397700	-0.06034400
C		-15.86571000	-1.43083300	-0.01465300
C		-14.99288500	-2.52321600	0.03693900
C		-13.62306100	-2.33201400	0.04438400
F		15.51555100	3.74525200	-0.07530200

F	17.17290100	1.67825700	0.02253400
F	-17.17305200	-1.67783200	-0.01946600
F	-15.51579000	-3.74491400	0.07802900
C	-4.58864400	-3.33729100	5.11086100
C	-3.68099300	-4.28177400	-4.69223300
C	4.58870500	3.33682300	-5.11182000
C	3.68090600	4.28190800	4.69126700
C	15.13418400	-2.87058000	0.17244600
N	16.26537900	-3.14341300	0.19241000
C	12.94800200	-3.77773600	0.19232500
N	12.34501300	-4.77257900	0.22908800
C	-15.13410600	2.87083900	-0.17148300
N	-16.26528700	3.14375300	-0.19112300
C	-12.94787300	3.77784900	-0.19244200
N	-12.34484400	4.77264700	-0.22974100
H	-0.27249700	-2.49729600	0.09934000
H	0.27253200	2.49717300	-0.10015600
H	2.50778500	3.69228200	0.21154500
H	2.83139700	5.06730500	2.21815300
H	3.98427300	1.58054400	4.42791500
H	3.63685400	0.19582600	2.43142000
H	4.98990300	2.46840300	-0.54368800
H	5.80068100	3.39375900	-2.66468700
H	2.30675500	1.90691400	-4.65331300
H	1.50152000	0.95812800	-2.54118500
H	-2.50768200	-3.69236900	-0.21253200
H	-2.83136800	-5.06728800	-2.21920500
H	-3.98446500	-1.58042700	-4.42869500
H	-3.63698900	-0.19582100	-2.43214300
H	-1.50147000	-0.95834000	2.54036100
H	-2.30665100	-1.90728800	4.65244600
H	-5.80052400	-3.39417200	2.66376000
H	-4.98981100	-2.46864400	0.54281500
H	6.16472100	-3.98990800	0.11342800
H	-6.16467000	3.98981600	-0.11379600
H	8.61149400	-3.28307700	0.11100400
H	-8.61143000	3.28302700	-0.11109300
H	9.15225900	-0.23755700	0.01064400
H	-9.15227400	0.23752000	-0.01076600
H	10.84921500	-2.80895700	0.11827900
H	-10.84914400	2.80899400	-0.11803300
H	16.14039000	-0.67255000	0.10144900
H	12.93904800	3.17325000	-0.08235300
H	-16.14042800	0.67289500	-0.09927500
H	-12.93924800	-3.17307100	0.08386400
H	-4.26612500	-4.38180300	5.19618000
H	-4.18983200	-2.80116300	5.97624300
H	-5.68030600	-3.32901000	5.17574300
H	-2.98983700	-5.12853900	-4.73128000
H	-4.69758800	-4.69250900	-4.68661600
H	-3.56786000	-3.70438800	-5.61376400
H	5.68046500	3.33195600	-5.17514000
H	4.19282000	2.79836200	-5.97710800
H	4.26290400	4.38017100	-5.19893200
H	4.69746300	4.69274000	4.68556900
H	2.98967400	5.12860900	4.73033800
H	3.56789500	3.70454100	5.61282500

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C	-1.36152200	0.19424400	0.01205300
C	-0.53702800	1.32326200	0.00388700
C	0.83040200	1.11756200	-0.01093100
C	1.36152700	-0.19424300	-0.01206000
C	0.53703200	-1.32326000	-0.00389500
C	-1.94533100	-2.17433500	0.00887400
C	1.94533600	2.17433700	-0.00887500
C	-2.79737600	0.05781700	0.01577100
C	-3.16652600	-1.27160700	-0.00011700
C	2.79738000	-0.05781600	-0.01578000
C	3.16653100	1.27160800	0.00010900
C	-1.97922100	-3.01612500	1.29172400
C	-1.81386600	-3.02182300	-1.26138400
C	1.97922300	3.01614100	-1.29171500
C	-1.39481100	-2.56807600	2.47776200
C	-1.51320100	-3.30368400	3.65331000
C	-2.21839800	-4.50832300	3.68926500

C	-2.81080700	-4.94813100	2.50207300
C	-2.69463100	-4.21813700	1.32475400
C	-2.46918000	-2.66764000	-2.44189500
C	-2.27781300	-3.39756800	-3.61143300
C	-1.42582900	-4.50308900	-3.64561000
C	-0.76554200	-4.84964900	-2.46285100
C	-0.95570700	-4.12621200	-1.29142600
C	2.69461900	4.21816100	-1.32472700
C	2.81079000	4.94817100	-2.50203800
C	2.21839100	4.50837000	-3.68923600
C	1.51320800	3.30372100	-3.65329900
C	1.39482400	2.56809800	-2.47776100
C	-2.31668000	-5.31780200	4.95114800
C	-1.24540700	-5.30977600	-4.90014500
C	2.31665600	5.31786700	-4.95111000
C	1.24536000	5.30972200	4.90017200
C	0.95570900	4.12620100	1.29144400
C	0.76553800	4.84962300	2.46287200
C	1.42582300	4.50304800	3.64563500
C	2.27781000	3.39753500	3.61144700
C	2.46918400	2.66761900	2.44189800
C	1.81387200	3.02181100	1.26139300
C	-10.50735800	-0.62817900	-0.03583600
C	-11.46730600	0.35830600	-0.03636900
C	-11.20930400	1.81013900	-0.01021600
C	-12.52472100	2.47775000	-0.01784800
C	-13.53728500	1.50713900	-0.04754000
C	-12.91189100	0.16514300	-0.06118100
O	-10.12246100	2.36913300	0.01400000
C	-13.61516200	-1.02348000	-0.09415500
C	-12.79260600	3.83606600	0.00013700
C	-14.12626500	4.23821200	-0.01202300
C	-15.14622900	3.28473900	-0.04144400
C	-14.87100000	1.91723200	-0.05954100
C	10.50736300	0.62817700	0.03582700
C	11.46730900	-0.35830900	0.03636500
C	11.20930600	-1.81014200	0.01020200
C	12.52472300	-2.47775400	0.01781800
C	13.53728800	-1.50714400	0.04751200
O	12.91189400	-0.16514800	0.06117600
C	10.12246200	-2.36913400	-0.01401000
C	13.61516700	1.02347400	0.09417700
C	12.79260600	-3.83607000	-0.00018300
C	14.12626500	-4.23821700	0.01196000
C	15.14623000	-3.28474500	0.04138000
C	14.87100300	-1.91723800	0.05949400
C	4.56616800	1.41419500	-0.00855500
C	5.23177900	0.17793000	-0.02189300
S	4.12652200	-1.16449600	-0.03841100
S	5.65977200	2.76968800	0.01551400
C	7.01867200	1.67055300	0.01354900
C	6.63083600	0.31979400	-0.00965100
C	-4.56616300	-1.41419400	0.00854800
C	-5.23177500	-0.17792900	0.02188600
S	-4.12651800	1.16449700	0.03840100
S	-5.65976700	-2.76968800	-0.01552600
C	-7.01866800	-1.67055300	-0.01356000
C	-6.63083200	-0.31979400	0.00964200
C	8.39812800	1.83968500	0.02743100
C	9.09342000	0.62281500	0.01763600
S	7.98130300	-0.75009800	-0.01324600
C	-8.39812300	-1.83968500	-0.02744300
C	-9.09341600	-0.62281600	-0.01764600
S	-7.98129900	0.75009700	0.01324000
C	-13.01405000	-2.31438500	-0.11147900
N	-12.57139100	-3.39093200	-0.12712900
C	-15.03729000	-1.09749100	-0.11619700
N	-16.19439400	-1.21967000	-0.13525600
C	13.01405500	2.31437900	0.11153800
N	12.57139800	3.39092600	0.12721900
C	15.03729400	1.09748300	0.11621400
N	16.19439900	1.21966200	0.13527000
H	-0.95685200	2.32459600	0.01074300
H	0.95685600	-2.32459500	-0.01075200
H	-0.84141400	-1.63415300	2.48978900
H	-1.04602700	-2.93066600	4.56156900
H	-3.37284500	-5.87899500	2.49679500
H	-3.15437400	-4.59838500	0.41671200
H	-3.13373300	-1.80859700	-2.45502600
H	-2.80323400	-3.09902700	-4.51541100
H	-0.09167100	-5.70311200	-2.45695700

H	-0.43890300	-4.43307200	-0.38654800
H	3.15435400	4.59840200	-0.41667900
H	3.37281800	5.87904100	-2.49674700
H	1.04604300	2.93070800	-4.56156400
H	0.84143800	1.63416800	-2.48980000
H	-2.17114700	-4.69458700	5.83748400
H	-3.28981000	-5.81024000	5.03452300
H	-1.55274100	-6.10398100	4.97404100
H	-1.94803600	-6.15100900	-4.93060900
H	-1.42327500	-4.70432100	-5.79301500
H	-0.23676200	-5.72758400	-4.96454300
H	1.55255200	6.10388200	-4.97409800
H	3.28969200	5.81051000	-5.03436800
H	2.17136000	4.69462000	-5.83746100
H	0.23640700	5.72672600	4.96500900
H	1.42413700	4.70450600	5.79302000
H	1.94731200	6.15153600	4.93020200
H	0.43891000	4.43307100	0.38656700
H	0.09166500	5.70308500	2.45698600
H	2.80323100	3.09898800	4.51542200
H	3.13374100	1.80857900	2.45502300
H	-10.87607900	-1.64902000	-0.05380100
H	-11.97725900	4.55228400	0.02296000
H	-15.69188100	1.21275200	-0.08207900
H	10.87608400	1.64901900	0.05378800
H	11.97725800	-4.55228700	-0.02300500
H	15.69188400	-1.21275900	0.08203000
H	8.91314500	2.79349000	0.04603400
H	-8.91314000	-2.79349100	-0.04604800
H	-14.37727000	5.29421100	0.00131900
H	-16.18145200	3.61147100	-0.05053200
H	16.18145300	-3.61147800	0.05045300
H	14.37726900	-5.29421600	-0.00139500

## INIC2

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C	-0.80430100	-1.13674800	0.01003100
C	-1.36541100	0.16263300	0.01128100
C	-0.56746200	1.31073100	0.00411000
C	0.80430300	1.13674700	-0.00998500
C	1.36541200	-0.16263300	-0.01123700
C	0.56746300	-1.31073100	-0.00406600
C	-1.89459900	-2.21893300	0.00693900
C	1.89460100	2.21893300	-0.00688800
C	-2.79761400	-0.00695000	0.01369900
C	-3.13631400	-1.34463000	-0.00353800
C	2.79761600	0.00694900	-0.01366200
C	3.13631600	1.34462900	0.00357400
C	-1.91114300	-3.06126500	1.28980300
C	-1.74193100	-3.06392100	-1.26265100
C	1.91113800	3.06128100	-1.28974100
C	-1.33507300	-2.60298100	2.47596300
C	-1.43899300	-3.34180200	3.65096400
C	-2.12093700	-4.55973800	3.68617400
C	-2.70501600	-5.00999600	2.49874000
C	-2.60309600	-4.27697200	1.32205700
C	-2.40258900	-2.72520600	-2.44472500
C	-2.19230600	-3.45135300	-3.61340400
C	-1.31537400	-4.53727000	-3.64512100
C	-0.65013000	-4.86832900	-2.46069200
C	-0.85927900	-4.14885000	-1.29007500
C	2.60310100	4.27698100	-1.32198800
C	2.70501300	5.01002000	-2.49866400
C	2.12091500	4.55978100	-3.68609600
C	1.43896300	3.34184800	-3.65089300
C	1.33505200	2.60301500	-2.47590100
C	-2.20344100	-5.37198100	4.94740700
C	-1.11354700	-5.34011700	-4.89885400
C	2.20339900	5.37204000	-4.94732000
C	1.11353100	5.34005100	4.89894500
C	0.85925800	4.14881200	1.29016700
C	0.65011100	4.86827300	2.46079000
C	1.31538700	4.53721700	3.64520800
C	2.19234700	3.45132900	3.61346200
C	2.40262900	2.72519600	2.44477000
C	1.74194000	3.06390300	1.26271500
C	-10.48864300	-0.86244700	-0.03794100
C	-11.46971100	0.10401500	-0.03560200



C	-11.24234900	1.56176800	-0.00936300
C	-12.56933200	2.20019700	-0.01458700
C	-13.56178600	1.20937100	-0.04287200
C	-12.90783700	-0.12090000	-0.05753800
O	-10.16739100	2.14341200	0.01273700
C	-13.58994100	-1.32125200	-0.08845300
C	-12.86953400	3.55343400	0.00429300
C	-14.20606100	3.93486700	-0.00537500
C	-15.18325400	2.94338300	-0.03357700
C	-14.90385300	1.58126400	-0.05276500
C	10.48864600	0.86244700	0.03789300
C	11.46971400	-0.10401400	0.03555000
C	11.24235400	-1.56176800	0.00931200
C	12.56933700	-2.20019500	0.01450700
C	13.56179100	-1.20936800	0.04277700
C	12.90784000	0.12090200	0.05746700
O	10.16739600	-2.14341300	-0.01277000
C	13.58994300	1.32125500	0.08839200
C	12.86954100	-3.55343100	-0.00438600
C	14.20606800	-3.93486300	0.00525200
C	15.18326000	-2.94337800	0.03343700
C	14.90385800	-1.58125900	0.05263900
C	4.53235500	1.51878800	-0.00376300
C	5.22551600	0.29745400	-0.01785800
S	4.15097800	-1.06918500	-0.03664500
S	5.59576000	2.89813700	0.02224300
C	6.97875400	1.82913100	0.01961800
C	6.62072800	0.46989300	-0.00491500
C	-4.53235300	-1.51878900	0.00378900
C	-5.22551400	-0.29745500	0.01787800
S	-4.15097700	1.06918400	0.03667800
S	-5.59575800	-2.89813800	-0.02223400
C	-6.97875200	-1.82913200	-0.01962700
C	-6.62072600	-0.46989400	0.00491500
C	8.35386700	2.02810700	0.03319700
C	9.07585500	0.82627600	0.02182800
S	7.99384300	-0.57069300	-0.00953100
C	-8.35386500	-2.02810800	-0.03322500
C	-9.07585300	-0.82627700	-0.02186000
S	-7.99384100	0.57069300	0.00951800
C	-12.96475600	-2.60067800	-0.10507000
N	-12.50045000	-3.66794500	-0.11976700
C	-15.01062500	-1.41802800	-0.10836000
N	-16.16628800	-1.55276800	-0.12566700
C	12.96475600	2.60067900	0.10504600
N	12.50045100	3.66794600	0.11977000
C	15.01062700	1.41803200	0.10827700
N	16.16629000	1.55277600	0.12556300
H	-1.01042300	2.30217100	0.01128200
H	1.01042400	-2.30217200	-0.01124000
H	-0.79980500	-1.65856600	2.48880300
H	-0.97879900	-2.96068500	4.55942000
H	-3.24892800	-5.95155300	2.49282100
H	-3.05549700	-4.66541100	0.41378900
H	-3.08629000	-1.88133900	-2.45986500
H	-2.72235000	-3.16531500	-4.51872200
H	0.04276700	-5.70639400	-2.45285000
H	-0.33804700	-4.44374700	-0.38375300
H	3.05551900	4.66540500	-0.41372200
H	3.24893300	5.95157100	-2.49274100
H	0.97875600	2.96074500	-4.55934900
H	0.79977900	1.65860300	-2.48874600
H	-2.06858100	-4.74704100	5.83420200
H	-3.16736200	-5.88215800	5.03105900
H	-1.42530900	-6.14414800	4.96889900
H	-1.79649300	-6.19736300	-4.93058900
H	-1.30316100	-4.73929900	-5.79242700
H	-0.09539500	-5.73459700	-4.96062500
H	1.42511500	6.14405200	-4.96889800
H	3.16722900	5.88240600	-5.03086800
H	2.06875500	4.74707400	-5.83413000
H	0.09507200	5.73366800	4.96119300
H	1.30411800	4.73951000	5.79249500
H	1.79574500	6.19789700	4.93020600
H	0.33800200	4.44370400	0.38385600
H	-0.04280800	5.70632000	2.45296800
H	2.72241900	3.16529800	4.51876700
H	3.08635400	1.88134900	2.45989100
H	-10.83597800	-1.89084000	-0.05639400
H	-15.72809100	0.88103100	-0.07397800
H	10.83597900	1.89084100	0.05633500

H	15.72809600	-0.88102600	0.07383800
H	8.84801000	2.99282900	0.05213800
H	-8.84800700	-2.99283000	-0.05217500
H	-14.50744400	4.97641300	0.00827300
H	14.50745200	-4.97640900	-0.00840800
H	12.07214900	-4.28911600	-0.02614800
H	-12.07214200	4.28911700	0.02606800
F	16.46447100	-3.31902000	0.04256500
F	-16.46446300	3.31902600	-0.04273500

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C	-0.80582800	-1.13570900	0.01013600
C	-1.36512700	0.16445100	0.01031500
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C	0.80583000	1.13570800	-0.01012100
C	1.36512900	-0.16445200	-0.01030100
C	0.56570600	-1.31152200	-0.00299300
C	-1.89760700	-2.21641500	0.00679900
C	1.89761000	2.21641400	-0.00677900
C	-2.79753800	-0.00308500	0.01209600
C	-3.13810700	-1.34038800	-0.00440400
C	2.79754000	0.00308300	-0.01208600
C	3.13810900	1.34038600	0.00441200
C	-1.91574600	-3.05863800	1.28969100
C	-1.74545600	-3.06170700	-1.26267300
C	1.91574300	3.05865200	-1.28966100
C	-1.33986800	-2.60084800	2.47613000
C	-1.44501800	-3.33957200	3.65107500
C	-2.12804900	-4.55690700	3.68593500
C	-2.71198100	-5.00663100	2.49822900
C	-2.60883000	-4.27370500	1.32159200
C	-2.40549400	-2.72254900	-2.44496200
C	-2.19544600	-3.44897400	-3.61351600
C	-1.31936600	-4.53558100	-3.64488400
C	-0.65477000	-4.86711800	-2.46022100
C	-0.86370100	-4.14738500	-1.28973100
C	2.60882100	4.27372200	-1.32155000
C	2.71196600	5.00666300	-2.49817900
C	2.12803000	4.55695100	-3.68588700
C	1.44500600	3.33961000	-3.65104000
C	1.33986400	2.60087300	-2.47610500
C	-2.21177600	-5.36913500	4.94709600
C	-1.11767800	-5.33861200	-4.89852500
C	2.21173800	5.36919600	-4.94703900
C	1.11765700	5.33856400	4.89857100
C	0.86369600	4.14736300	1.28977700
C	0.65476600	4.86708200	2.46027000
C	1.31937500	4.53554000	3.64493000
C	2.19546800	3.44895000	3.61354500
C	2.40551600	2.72253400	2.44498000
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C	-10.48900300	-0.84807600	-0.03968700
C	-11.47362500	0.11569000	-0.03900900
C	-11.24189200	1.57264700	-0.01637000
C	-12.57287400	2.20735400	-0.02379100
C	-13.56926100	1.21637300	-0.04902000
C	-12.90969300	-0.11165400	-0.06016200
O	-10.16245400	2.14319500	0.00466500
C	-13.58691400	-1.31581800	-0.08778600
C	-12.91726700	3.54782600	-0.00969500
C	-14.25396000	3.92738400	-0.01996300
C	-15.23477200	2.93980000	-0.04455700
C	-14.91352600	1.58078100	-0.05943500
C	10.48900600	0.84807400	0.03964900
C	11.47362800	-0.11569100	0.03898200
C	11.24189600	-1.57264900	0.01635000
C	12.57287800	-2.20735500	0.02375700
C	13.56926500	-1.21637300	0.04897400
C	12.90969600	0.11165400	0.06012700
O	10.16245800	-2.14319700	-0.00467400
C	13.58691600	1.31581800	0.08776400
C	12.91727200	-3.54782700	0.00965800
C	14.25396600	-3.92738400	0.01990800
C	15.23477700	-2.93979900	0.04448700
C	14.91353100	-1.58077900	0.05936900
C	4.53434000	1.51241600	-0.00274800
C	5.22561500	0.28993700	-0.01571600

S	4.14910900	-1.07514100	-0.03379700
S	5.59982200	2.89027700	0.02214900
C	6.98124200	1.81902600	0.02058300
C	6.62101500	0.46007100	-0.00269000
C	-4.53433800	-1.51241800	0.00275000
C	-5.22561300	-0.28993900	0.01571800
S	-4.14910700	1.07513900	0.03380800
S	-5.59982000	-2.89027900	-0.02216500
C	-6.98124000	-1.81902800	-0.02060600
C	-6.62101300	-0.46007300	0.00267800
C	8.35634200	2.01558500	0.03393500
C	9.07665900	0.81213300	0.02385900
S	7.99199300	-0.58288100	-0.00599200
C	-8.35634000	-2.01558700	-0.03397200
C	-9.07665700	-0.81213500	-0.02389000
S	-7.99199100	0.58287800	0.00597900
C	-12.95495100	-2.59193600	-0.10056400
N	-12.48684600	-3.65769400	-0.11205600
C	-15.00644400	-1.42704300	-0.10785800
N	-16.15971700	-1.58155400	-0.12530200
C	12.95495200	2.59193500	0.10056800
N	12.48684800	3.65769300	0.11209000
C	15.00644600	1.42704400	0.10782700
N	16.15971900	1.58155700	0.12526300
H	-1.00742600	2.30350900	0.00934000
H	1.00742800	-2.30351100	-0.00932900
H	-0.80372800	-1.65693300	2.48922500
H	-0.98488200	-2.95888400	4.55973800
H	-3.25669400	-5.94772400	2.49204500
H	-3.06107200	-4.66174500	0.41307200
H	-3.08844500	-1.87808200	-2.46042000
H	-2.72494900	-3.16254100	-4.51902700
H	0.03751200	-5.70568300	-2.45211000
H	-0.34291600	-4.44260700	-0.38325900
H	3.06106800	4.66175200	-0.41302700
H	3.25667600	5.94775700	-2.49198600
H	0.98487000	2.95893000	-4.55970600
H	0.80373100	1.65695400	-2.48920800
H	-2.07693200	-4.74431400	5.83397800
H	-3.17609800	-5.87864600	5.03023400
H	-1.43417500	-6.14182600	4.96895300
H	-1.80109200	-6.19548400	-4.93040000
H	-1.30671000	-4.73771900	-5.79217400
H	-0.09972700	-5.73365400	-4.95999900
H	1.43397400	6.14172000	-4.96899000
H	3.17596200	5.87890900	-5.03006400
H	2.07712800	4.74434600	-5.83393700
H	0.09940100	5.73275400	4.96051400
H	1.30764800	4.73794900	5.79220000
H	1.80034700	6.19603000	4.92997500
H	0.34290300	4.44258700	0.38331000
H	-0.03752600	5.70564000	2.45217000
H	2.72498400	3.16251800	4.51904800
H	3.08847900	1.87807600	2.46042800
H	-10.83517700	-1.87676400	-0.05639600
H	-15.71017600	0.85007600	-0.07832500
H	10.83517900	1.87676300	0.05634300
H	15.71018000	-0.85007400	0.07824500
H	8.85216300	2.97948600	0.05182200
H	-8.85216100	-2.97948800	-0.05186800
H	-14.51005000	4.98117300	-0.00870200
H	-16.27889700	3.23543100	-0.05235700
H	16.27890200	-3.23542900	0.05227200
H	14.51005600	-4.98117200	0.00864600
F	-11.97171000	4.48422000	0.01358900
F	11.97171500	-4.48422100	-0.01361000

## INIC3

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C	-0.77392400	1.15767800	-0.01365300
C	-1.36927000	-0.12636300	-0.00791200
C	-0.60196800	-1.29513600	0.00247800
C	0.77391700	-1.15776100	0.01295200
C	1.36925700	0.12628300	0.00722600
C	0.60195900	1.29505500	-0.00317200
C	-1.83491500	2.26846000	-0.01385000
C	1.83492400	-2.26853300	0.01314600
C	-2.79648100	0.08115600	-0.00753800
C	-3.09935600	1.42758100	0.00520800

C	2.79646900	-0.08122000	0.00694500
C	3.09935800	-1.42764100	-0.00577100
C	-1.83334200	3.10322100	-1.30198800
C	-1.65581200	3.11798800	1.24924700
C	1.83327700	-3.10340100	1.30121700
C	-1.27076200	2.62485800	-2.48666900
C	-1.35923300	3.35976200	-3.66546700
C	-2.01185700	4.59345800	-3.70612900
C	-2.58243000	5.06408600	-2.52001900
C	-2.49563000	4.33518700	-1.33961600
C	-2.32300400	2.80726800	2.43532800
C	-2.08950200	3.53644800	3.59777500
C	-1.18215200	4.59731500	3.61897800
C	-0.51078100	4.90033100	2.43047000
C	-0.74314200	4.17800300	1.26605000
C	2.49546300	-4.33542200	1.33876500
C	2.58219100	-5.06440800	2.51912100
C	2.01164700	-4.59381600	3.70525700
C	1.35913400	-3.36005700	3.66467700
C	1.27073400	-2.62506700	2.48592900
C	-2.07752100	5.40064700	-4.97158500
C	-0.95438700	5.40386300	4.86588100
C	2.07721300	-5.40110300	4.97065600
C	0.95476800	-5.40358800	-4.86687800
C	0.74320000	-4.17793900	-1.26700500
C	0.51094000	-4.90018400	-2.43148700
C	1.18245900	-4.59711900	-3.61991100
C	2.08984400	-3.53629800	-3.59854000
C	2.32325100	-2.80719600	-2.43601500
C	1.65592100	-3.11795700	-1.25003500
C	-10.46096300	1.13711300	0.04726300
C	-11.46623400	0.19531300	0.04431100
C	-11.27473400	-1.26532400	0.01768800
C	-12.62061300	-1.86992800	0.01766900
C	-13.58584800	-0.85501000	0.04507500
C	-12.89942800	0.45583800	0.06378800
O	-10.21911600	-1.87996400	-0.00136500
C	-13.55064900	1.67332100	0.09605100
C	-12.94044500	-3.21761800	-0.00514400
C	-14.28433500	-3.54459700	0.00016200
C	-15.26218900	-2.54395700	0.02794400
C	-14.93932900	-1.19714900	0.05047700
C	10.46097000	-1.13706000	-0.04669800
C	11.46622400	-0.19524300	-0.04367600
C	11.27469900	1.26538900	-0.01693100
C	12.62057000	1.87001200	-0.01665000
C	13.58582300	0.85511100	-0.04408100
C	12.89942300	-0.45574500	-0.06303300
O	10.21907000	1.88001300	0.00202200
C	13.55066200	-1.67321600	-0.09542000
C	12.94037900	3.21770300	0.00638500
C	14.28426400	3.54470300	0.00128800
C	15.26213700	2.54408100	-0.02651800
C	14.93930000	1.19727100	-0.04927500
C	4.49025300	-1.63868300	-0.00095700
C	5.21531100	-0.43588500	0.00742400
S	4.17779000	0.95882000	0.02339200
S	5.51690200	-3.04566000	-0.02399700
C	6.92761400	-2.01351400	-0.02664900
C	6.60519800	-0.64514400	-0.00653800
C	-4.49024800	1.63864000	0.00052900
C	-5.21532400	0.43585300	-0.00777200
S	-4.17782100	-0.95886800	-0.02385500
S	-5.51687200	3.04563300	0.02382500
C	-6.92759600	2.01350800	0.02670400
C	-6.60520500	0.64513300	0.00648300
C	8.29691100	-2.24822400	-0.03982400
C	9.05003400	-1.06528600	-0.03193300
S	8.00415600	0.35944000	-0.00516900
C	-8.29688700	2.24824100	0.04011900
C	-9.05003000	1.06531500	0.03232100
S	-8.00418000	-0.35942500	0.00535500
F	-14.68183700	-4.81269000	-0.02082800
F	-16.53797900	-2.92003900	0.03202100
F	16.53792100	2.92018300	-0.03039000
F	14.68174500	4.81279800	0.02250600
C	-12.89417700	2.93673200	0.11686100
N	-12.40470100	3.99262500	0.13492900
C	-14.96859100	1.80262500	0.11362900
N	-16.12153800	1.95928600	0.12911700
C	12.89420300	-2.93663000	-0.11646100

N	12.40474600	-3.99252800	-0.13471000
C	14.96860600	-1.80250300	-0.11289600
N	16.12155400	-1.95916400	-0.12830100
H	-1.07115700	-2.27437600	0.00043300
H	1.07114500	2.27429700	-0.00110500
H	-0.75843700	1.66777000	-2.49560800
H	-0.91003100	2.96290000	-4.57268100
H	-3.10337000	6.01855300	-2.51809200
H	-2.93656100	4.73965100	-0.43270900
H	-3.03024900	1.98320700	2.45866000
H	-2.62522800	3.27275900	4.50651600
H	0.20535200	5.71849800	2.41456000
H	-0.21637900	4.45113000	0.35609600
H	2.93637700	-4.73985700	0.43183600
H	3.10305400	-6.01891800	2.51713400
H	0.90996400	-2.96321600	4.57191700
H	0.75849800	-1.66793100	2.49493000
H	-1.95912900	4.76801700	-5.85526300
H	-3.02928600	5.93298900	-5.05625500
H	-1.28145600	6.15413400	-4.99850600
H	-1.61242900	6.28054500	4.89234500
H	-1.15884000	4.81576200	5.76462100
H	0.07477600	5.76952300	4.92214300
H	1.28090800	-6.15433400	4.99762900
H	3.02881900	-5.93375200	5.05517800
H	1.95912500	-4.76848900	5.85438800
H	-0.07470900	-5.76827600	-4.92378700
H	1.16037200	-4.81578200	-5.76554500
H	1.61198100	-6.28090800	-4.89279700
H	0.21633300	-4.45110400	-0.35712300
H	-0.20523100	-5.71832100	-2.41571000
H	2.62568900	-3.27257400	-4.50720100
H	3.03053100	-1.98316300	-2.45922800
H	-10.78319900	2.17361200	0.06398700
H	-12.17584600	-3.98661600	-0.02642500
H	-15.74724100	-0.47761400	0.07074000
H	10.78322500	-2.17355400	-0.06337300
H	12.17576500	3.98668600	0.02767400
H	15.74722500	0.47775200	-0.06954500
H	8.76571000	-3.22560800	-0.05552400
H	-8.76566800	3.22563200	0.05591900

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C	12.46777600	3.39962300	-0.19575200
C	13.47026700	2.41900300	-0.20742800
C	14.80723300	2.81522700	-0.24050400
C	15.09634400	4.18059600	-0.26053600
C	14.08635100	5.14406200	-0.24861400
C	12.74855400	4.75471100	-0.21581600
C	11.14542400	2.74285400	-0.15845300
C	11.39074200	1.29125400	-0.14676900
C	12.82816700	1.08302200	-0.17865900
C	13.52408400	-0.11366900	-0.18345100
O	10.06504100	3.31588800	-0.14036000
C	-0.98010200	0.99660500	0.37733100
C	-1.31776100	-0.37456200	0.34662000
C	-0.34802000	-1.38199800	0.34944200
C	0.98010300	-0.99663300	0.37728100
C	1.31776200	0.37453500	0.34666800
C	0.34802100	1.38197100	0.34954200
C	-2.24468900	1.88229100	0.37846600
C	2.24468900	-1.88232000	0.37838000
C	-6.55627300	-0.63065300	-0.01537400
C	-6.94217200	0.73012600	-0.00670200
C	-8.31718900	0.90720200	-0.03924300
C	-9.01342500	-0.31489900	-0.07452700
S	-7.90494600	-1.70092500	-0.06711100
N	-5.82794900	1.54337400	0.05780200
C	-2.75204200	-0.44522800	0.25529700
C	-3.32315900	0.81290100	0.23184800
C	-4.73087700	0.71289300	0.09531700
C	-5.16462000	-0.63782800	0.04279100
S	-3.85602400	-1.77339300	0.13368500
C	-5.88442200	2.99777000	0.01823600
C	6.55627800	0.63064900	-0.01525700
C	6.94217800	-0.73013000	-0.00666900
C	8.31719500	-0.90720300	-0.03921500

C	9.01343100	0.31490000	-0.07442300
S	7.90495000	1.70092600	-0.06692500
N	5.82795500	-1.54338300	0.05777400
C	2.75204500	0.44520700	0.25537000
C	3.32316200	-0.81292100	0.23184700
C	4.73088200	-0.71290400	0.09533600
C	5.16462500	0.63782000	0.04289800
S	3.85602800	1.77337900	0.13384700
C	5.88443100	-2.99777700	0.01812600
C	-2.21863500	2.80844000	-0.84927200
C	-2.34249200	2.60616600	1.73185400
C	2.34246900	-2.60627700	1.73172600
C	-2.24233500	4.19873900	-0.77965400
C	-2.19094100	4.97394400	-1.94062500
C	-2.12641800	4.39119100	-3.20381200
C	-2.11494100	2.99131000	-3.26995000
C	-2.15538700	2.21845700	-2.11998600
C	-3.35951700	2.32728400	2.64639600
C	-3.41068100	2.95906300	3.88840700
C	-2.44768500	3.89058100	4.26957600
C	-1.42118400	4.16421800	3.35849400
C	-1.36720700	3.53622900	2.12225800
C	1.36714700	-3.53632500	2.12207900
C	1.42111100	-4.16440000	3.35826900
C	2.44763200	-3.89086200	4.26936300
C	3.41066700	-2.95936800	3.88824200
C	3.35951500	-2.32750200	2.64627200
C	-2.06400800	5.22247600	-4.45344900
C	-2.50404700	4.58345200	5.60105300
C	2.50391900	-4.58376500	5.60082600
C	-5.81731200	3.62639500	-1.38458300
C	-6.62579700	2.85877200	-2.42616300
C	5.81735600	-3.62632300	-1.38473000
C	6.62587200	-2.85864800	-2.42624600
C	2.06406400	-5.22223000	-4.45372700
C	2.24232400	-4.19869900	-0.77987200
C	2.19094600	-4.97383900	-1.94088700
C	2.12646700	-4.39101500	-3.20404400
C	2.11501800	-2.99112900	-3.27010300
C	2.15544800	-2.21834100	-2.12009500
C	2.21865200	-2.80839600	-0.84941400
C	10.42042100	0.30751300	-0.10953100
C	-10.42041600	-0.30750600	-0.10963300
C	-12.46779900	-3.39959600	-0.19597400
C	-13.47028100	-2.41896600	-0.20760000
C	-14.80725100	-2.81517600	-0.24066700
C	-15.09637400	-4.18054200	-0.26074100
C	-14.08639000	-5.14401800	-0.24887000
C	-12.74858900	-4.75468100	-0.21608100
C	-11.14544000	-2.74284100	-0.15867200
C	-11.39074300	-1.29124000	-0.14691900
C	-12.82816700	-1.08299300	-0.17879200
C	-13.52406800	0.11370700	-0.18354100
O	-10.06506200	-3.31588700	-0.14061200
C	12.91498800	-1.39992100	-0.15646100
N	12.46623600	-2.47430000	-0.13494300
C	14.94453400	-0.19981200	-0.21663300
N	16.10063500	-0.33344900	-0.24299400
C	-5.35039300	8.36254900	0.57297300
C	-6.05531500	7.44330000	-0.41618300
C	-5.58204400	5.99507500	-0.32877700
C	-6.29818700	5.08296400	-1.32145100
C	5.35035100	-8.36258500	0.57254700
C	6.05531100	-7.44328300	-0.41653200
C	5.58204000	-5.99506100	-0.32906500
C	6.29822100	-5.08289900	-1.32166400
C	-12.91495400	1.39994900	-0.15651700
N	-12.46618200	2.47432000	-0.13497700
C	-14.94451800	0.19987100	-0.21670600
N	-16.10061700	0.33352900	-0.24304900
H	15.62096400	2.10215200	-0.25064200
H	11.94004000	5.47904300	-0.20565300
H	-0.64196200	-2.42503400	0.29416200
H	0.64196500	2.42501100	0.29433900
H	-8.84024800	1.85658000	-0.03730300
H	-6.82403400	3.28099600	0.50707100
H	-5.07579400	3.38003000	0.64672900
H	8.84025500	-1.85658100	-0.03733400
H	6.82403100	-3.28103000	0.50696700
H	5.07578800	-3.38007400	0.64657700
H	-2.31167400	4.69806700	0.18053800

H	-2.20777900	6.05771400	-1.85224800
H	-2.07061900	2.50113500	-4.23968600
H	-2.14046600	1.13480100	-2.20584400
H	-4.12201500	1.59381900	2.40682100
H	-4.21783400	2.71208800	4.57359300
H	-0.64618200	4.87929600	3.62384300
H	-0.55043200	3.78423200	1.45320600
H	0.55036100	-3.78425600	1.45301400
H	0.64608600	-4.87947000	3.62357300
H	4.21784700	-2.71248600	4.57342900
H	4.12205000	-1.59406200	2.40673400
H	-2.19189200	6.28510300	-4.23281600
H	-1.10099100	5.09939500	-4.96150300
H	-2.84162600	4.92748900	-5.16556400
H	-2.73278600	5.64856000	5.48201000
H	-3.27184300	4.14783600	6.24515000
H	-1.54427600	4.51789100	6.12346100
H	2.73140300	-5.64912900	5.48170100
H	3.27251100	-4.14896600	6.24452300
H	1.54448600	-4.51712000	6.12372600
H	-4.76670900	3.61951500	-1.70117200
H	-6.51617500	3.33517500	-3.40540400
H	-6.29104600	1.82200000	-2.52267700
H	-7.69475000	2.84959900	-2.18368100
H	4.76676200	-3.61942000	-1.70134800
H	6.51627600	-3.33499900	-3.40551600
H	6.29112700	-1.82187000	-2.52271500
H	7.69481900	-2.84949100	-2.18373300
H	2.19203700	-6.28486100	-4.23316200
H	1.10101200	-5.09919300	-4.96172700
H	2.84162500	-4.92714200	-5.16586100
H	2.31162900	-4.69808200	0.18029400
H	2.20776300	-6.05761400	-1.85257000
H	2.07073200	-2.50090000	-4.23981300
H	2.14055000	-1.13467900	-2.20589300
H	10.78877100	-0.71353500	-0.10451900
H	-10.78876200	0.71354400	-0.10456400
H	-15.62097500	-2.10209400	-0.25076500
H	-11.94008200	-5.47902100	-0.20595700
H	-5.70964500	9.39303100	0.49061600
H	-5.51624600	8.03392000	1.60495600
H	-4.26820500	8.37280300	0.40095700
H	-5.89831600	7.81163500	-1.43892400
H	-7.13965800	7.48023000	-0.24523200
H	-5.73192700	5.63799800	0.69931100
H	-4.50051500	5.95528200	-0.51176800
H	-6.20048800	5.51215500	-2.32786400
H	-7.37620300	5.08431900	-1.09868300
H	5.70960300	-9.39306300	0.49014600
H	5.51616700	-8.03401300	1.60455400
H	4.26816900	-8.37282700	0.40049100
H	5.89834900	-7.81156200	-1.43930000
H	7.13964800	-7.48022500	-0.24554400
H	5.73188900	-5.63804100	0.69904800
H	4.50051800	-5.95525700	-0.51209100
H	6.20055200	-5.51203300	-2.32786400
H	7.37623000	-5.08427100	-1.09886200
H	-14.34728900	-6.19766700	-0.26515700
H	-16.13481200	-4.49630700	-0.28615800
H	16.13477800	4.49637100	-0.28595900
H	14.34723900	6.19771300	-0.26486800

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C	14.94758000	1.95851900	-0.02048400
C	15.29582900	3.29975400	-0.04126500
C	14.33753300	4.31781900	-0.06095800
C	12.98724700	4.01523500	-0.06014900
C	11.28495700	2.09257600	-0.03338100
C	11.45053700	0.63131000	-0.01020500
C	12.87373900	0.34378700	0.00017100
C	13.50638300	-0.88681900	0.02587700
O	10.24213000	2.73013400	-0.04611400
C	-0.91918800	1.05324900	0.27248300
C	-1.33752600	-0.29550200	0.24665100
C	-0.42946300	-1.35887900	0.24617100
C	0.91918800	-1.05326000	0.27243200

C	1.33752600	0.29549200	0.24669100
C	0.42946400	1.35886900	0.24626300
C	-2.12860700	2.01324000	0.27835700
C	2.12860600	-2.01325200	0.27826800
C	-6.58690200	-0.24599100	-0.00662500
C	-6.89311900	1.13537000	0.00562200
C	-8.25525900	1.39202000	0.00644100
C	-9.02233300	0.21151200	-0.00593900
S	-7.99539800	-1.23665600	-0.02060300
N	-5.73221600	1.88241900	0.03903300
C	-2.77435600	-0.28141200	0.17555400
C	-3.27117000	1.00833900	0.15959400
C	-4.68484300	0.98987700	0.05407500
C	-5.19747900	-0.33389700	0.01756700
S	-3.95557000	-1.54367200	0.08303100
C	-5.70516300	3.33748500	-0.00843000
C	6.58690600	0.24599700	-0.00652800
C	6.89312400	-1.13536400	0.00564200
C	8.25526300	-1.39201300	0.00645900
C	9.02233700	-0.21150500	-0.00585000
S	7.99540100	1.23666400	-0.02044500
N	5.73222000	-1.88241600	0.03899700
C	2.77435800	0.28140600	0.17561500
C	3.27117200	-1.00834300	0.15958600
C	4.68484600	-0.98987600	0.05408400
C	5.19748300	0.33390100	0.01765800
S	3.95557200	1.54367200	0.08317700
C	5.70517100	-3.33748000	-0.00853400
C	-2.06740900	2.91925700	-0.96404300
C	-2.16102900	2.76055700	1.62143100
C	2.16100300	-2.76065200	1.62129600
C	-2.02769300	4.31014400	-0.91527800
C	-1.95137900	5.06540400	-2.08784000
C	-1.92425100	4.46215000	-3.34270900
C	-1.97780500	3.06249000	-3.38798500
C	-2.04284700	2.30892500	-2.22637200
C	-3.16469400	2.53939400	2.56590000
C	-3.15557200	3.19024900	3.79906600
C	-2.14338700	4.08401400	4.14152200
C	-1.13004400	4.29900800	3.20059900
C	-1.13620500	3.65214600	1.97299000
C	1.13616400	-3.65225300	1.97278700
C	1.12998900	-4.29920400	3.20034600
C	2.14332900	-4.08428600	4.14129400
C	3.15553000	-3.19051800	3.79890400
C	3.16466600	-2.53957200	2.56578300
C	-1.83201600	5.27175300	-4.60461300
C	-2.13630200	4.79866500	5.46253400
C	2.13617600	-4.79897900	5.46228300
C	-5.63821400	3.95335900	-1.41712200
C	-6.51467500	3.22629100	-2.43258500
C	5.63824600	-3.95329100	-1.41725500
C	6.51473700	-3.22619100	-2.43266800
C	1.83209700	-5.27148400	-4.60489500
C	2.02770000	-4.31008400	-0.91550200
C	1.95140700	-5.06527700	-2.08810700
C	1.92431000	-4.46195300	-3.34294300
C	1.97787600	-3.06229100	-3.38813900
C	2.04289800	-2.30879100	-2.22648200
C	2.06742800	-2.91919400	-0.96418800
C	10.42585300	-0.29822000	-0.00218200
C	-10.42584900	0.29822700	-0.00227500
C	-12.64275000	-2.67423000	-0.03950600
C	-13.58847300	-1.64167300	-0.01965700
C	-14.94757200	-1.95851900	-0.02065200
C	-15.29581800	-3.29975500	-0.04147800
C	-14.33752000	-4.31781700	-0.06121800
C	-12.98723500	-4.01523000	-0.06040900
C	-11.28494900	-2.09256800	-0.03357700
C	-11.45053200	-0.63130400	-0.01034600
C	-12.87373400	-0.34378400	0.00004200
C	-13.50638400	0.88681900	0.02578100
O	-10.24212000	-2.73012300	-0.04634900
C	12.83057100	-2.13920300	0.04808600
N	12.32529200	-3.18806400	0.06708700
C	14.92119900	-1.04035300	0.03431100
N	16.07160400	-1.21787600	0.04217000
C	-4.85714900	8.67147600	0.48434700
C	-5.65001200	7.78238400	-0.46500400
C	-5.23644400	6.31498800	-0.39535200
C	-6.03606800	5.43459600	-1.35222500



C	4.85706800	-8.67147700	0.48399500
C	5.64996400	-7.78235600	-0.46530100
C	5.23641700	-6.31495700	-0.39559600
C	6.03607700	-5.43453700	-1.35241200
C	-12.83057700	2.13920600	0.04801500
N	-12.32530700	3.18807100	0.06702700
C	-14.92119900	1.04034700	0.03422700
N	-16.07160600	1.21786100	0.04209500
H	15.74206000	1.22403800	-0.00624400
H	12.23672800	4.79818500	-0.07518400
H	-0.78497500	-2.38256800	0.19598500
H	0.78497700	2.38256100	0.19614600
H	-8.72098200	2.37072100	0.01730100
H	-6.61401000	3.67724600	0.50209400
H	-4.85992900	3.67449800	0.59730600
H	8.72098700	-2.37071400	0.01727000
H	6.61401100	-3.67726200	0.50198900
H	4.85992900	-3.67452200	0.59717300
H	-2.06601000	4.82638300	0.03757300
H	-1.91845300	6.14996600	-2.01525800
H	-1.96525400	2.55682400	-4.35064900
H	-2.07842500	1.22463000	-2.29680200
H	-3.96473700	1.83699100	2.35707700
H	-3.95450200	2.98829100	4.50823100
H	-0.31766700	4.98288700	3.43461900
H	-0.32808300	3.85656700	1.27905900
H	0.32804900	-3.85662300	1.27883300
H	0.31760800	-4.98309800	3.43430800
H	3.95446700	-2.98863300	4.50808100
H	3.96472800	-1.83717500	2.35701000
H	-1.94134200	6.34012200	-4.40236400
H	-0.86547400	5.12247100	-5.09902500
H	-2.60664000	4.98017900	-5.32116100
H	-2.33659900	5.86829800	5.33295900
H	-2.89631700	4.39718300	6.13738900
H	-1.16293400	4.71201800	5.95580600
H	2.33530700	-5.86881100	5.33257900
H	2.89691600	-4.39827800	6.13678300
H	1.16313500	-4.71135300	5.95603800
H	-4.59797000	3.88549400	-1.75963600
H	-6.40412500	3.69077500	-3.41739500
H	-6.24052300	2.17203800	-2.53109900
H	-7.57585000	3.27787300	-2.16285900
H	4.59800900	-3.88539800	-1.75978800
H	6.40420600	-3.69063500	-3.41749900
H	6.24059700	-2.17193200	-2.53114700
H	7.57590500	-3.27779300	-2.16292000
H	1.94142100	-6.33986400	-4.40270500
H	0.86556100	-5.12217500	-5.09931300
H	2.60673100	-4.97986800	-5.32141400
H	2.06598900	-4.82637600	0.03732100
H	1.91847000	-6.14984300	-2.01558700
H	1.96534900	-2.55657100	-4.35077500
H	2.07848600	-1.22449200	-2.29685000
H	10.73795400	-1.33779400	0.01021900
H	-10.73795000	1.33780100	0.01017600
H	-15.74205300	-1.22404100	-0.00637800
H	-12.23671400	-4.79817700	-0.07547900
H	-5.17374500	9.71679100	0.41514000
H	-4.98647400	8.35294100	1.52469200
H	-3.78537600	8.63281200	0.25931800
H	-5.52837300	8.14193100	-1.49563000
H	-6.72180600	7.86667100	-0.24032700
H	-5.35454400	5.96565500	0.63946800
H	-4.16712400	6.22825000	-0.62744400
H	-5.95174200	5.84959300	-2.36546300
H	-7.10378500	5.49632500	-1.09141200
H	5.17364800	-9.71679400	0.41474900
H	4.98637800	-8.35299000	1.52435800
H	3.78530000	-8.63278500	0.25894800
H	5.52834200	-8.14185800	-1.49594500
H	6.72175200	-7.86666900	-0.24060600
H	5.35449700	-5.96567000	0.63924200
H	4.16710300	-6.22819300	-0.62771100
H	5.95177100	-5.84948900	-2.36567000
H	7.10378700	-5.49629100	-1.09157400
F	-14.75780600	-5.57961200	-0.08065100
F	-16.57969100	-3.65096400	-0.04328300
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F	14.75782200	5.57961400	-0.08034900

# IPIC-4CI

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C		15.29582900	3.29975400	-0.04126500
C		14.33753300	4.31781900	-0.06095800
C		12.98724700	4.01523500	-0.06014900
C		11.28495700	2.09257600	-0.03338100
C		11.45053700	0.63131000	-0.01020500
C		12.87373900	0.34378700	0.00017100
C		13.50638300	-0.88681900	0.02587700
O		10.24213000	2.73013400	-0.04611400
C		-0.91918800	1.05324900	0.27248300
C		-1.33752600	-0.29550200	0.24665100
C		-0.42946300	-1.35887900	0.24617100
C		0.91918800	-1.05326000	0.27243200
C		1.33752600	0.29549200	0.24669100
C		0.42946400	1.35886900	0.24626300
C		-2.12860700	2.01324000	0.27835700
C		2.12860600	-2.01325200	0.27826800
C		-6.58690200	-0.24599100	-0.00662500
C		-6.89311900	1.13537000	0.00562200
C		-8.25525900	1.39202000	0.00644100
C		-9.02233300	0.21151200	-0.00593900
S		-7.99539800	-1.23665600	-0.02060300
N		-5.73221600	1.88241900	0.03903300
C		-2.77435600	-0.28141200	0.17555400
C		-3.27117000	1.00833900	0.15959400
C		-4.68484300	0.98987700	0.05407500
C		-5.19747900	-0.33389700	0.01756700
S		-3.95557000	-1.54367200	0.08303100
C		-5.70516300	3.33748500	-0.00843000
C		6.58690600	0.24599700	-0.00652800
C		6.89312400	-1.13536400	0.00564200
C		8.25526300	-1.39201300	0.00645900
C		9.02233700	-0.21150500	-0.00585000
S		7.99540100	1.23666400	-0.02044500
N		5.73222000	-1.88241600	0.03899700
C		2.77435800	0.28140600	0.17561500
C		3.27117200	-1.00834300	0.15958600
C		4.68484600	-0.98987600	0.05408400
C		5.19748300	0.33390100	0.01765800
S		3.95557200	1.54367200	0.08317700
C		5.70517100	-3.33748000	-0.00853400
C		-2.06740900	2.91925700	-0.96404300
C		-2.16102900	2.76055700	1.62143100
C		2.16100300	-2.76065200	1.62129600
C		-2.02769300	4.31014400	-0.91527800
C		-1.95137900	5.06540400	-2.08784000
C		-1.92425100	4.46215000	-3.34270900
C		-1.97780500	3.06249000	-3.38798500
C		-2.04284700	2.30892500	-2.22637200
C		-3.16469400	2.53939400	2.56590000
C		-3.15557200	3.19024900	3.79906600
C		-2.14338700	4.08401400	4.14152200
C		-1.13004400	4.29900800	3.20059900
C		-1.13620500	3.65214600	1.97299000
C		1.13616400	-3.65225300	1.97278700
C		1.12998900	-4.29920400	3.20034600
C		2.14332900	-4.08428600	4.14129400
C		3.15553000	-3.19051800	3.79890400
C		3.16466600	-2.53957200	2.56578300
C		-1.83201600	5.27175300	-4.60461300
C		-2.13630200	4.79866500	5.46253400
C		2.13617600	-4.79897900	5.46228300
C		-5.63821400	3.95335900	-1.41712200
C		-6.51467500	3.22629100	-2.43258500
C		5.63824600	-3.95329100	-1.41725500
C		6.51473700	-3.22619100	-2.43266800
C		1.83209700	-5.27148400	-4.60489500
C		2.02770000	-4.31008400	-0.91550200
C		1.95140700	-5.06527700	-2.08810700
C		1.92431000	-4.46195300	-3.34294300
C		1.97787600	-3.06229100	-3.38813900
C		2.04289800	-2.30879100	-2.22648200
C		2.06742800	-2.91919400	-0.96418800
C		10.42585300	-0.29822000	-0.00218200
C		-10.42584900	0.29822700	-0.00227500

C	-12.64275000	-2.67423000	-0.03950600
C	-13.58847300	-1.64167300	-0.01965700
C	-14.94757200	-1.95851900	-0.02065200
C	-15.29581800	-3.29975500	-0.04147800
C	-14.33752000	-4.31781700	-0.06121800
C	-12.98723500	-4.01523000	-0.06040900
C	-11.28494900	-2.09256800	-0.03357700
C	-11.45053200	-0.63130400	-0.01034600
C	-12.87373400	-0.34378400	0.00004200
C	-13.50638400	0.88681900	0.02578100
O	-10.24212000	-2.73012300	-0.04634900
C	12.83057100	-2.13920300	0.04808600
N	12.32529200	-3.18806400	0.06708700
C	14.92119900	-1.04035300	0.03431100
N	16.07160400	-1.21787600	0.04217000
C	-4.85714900	8.67147600	0.48434700
C	-5.65001200	7.78238400	-0.46500400
C	-5.23644400	6.31498800	-0.39535200
C	-6.03606800	5.43459600	-1.35222500
C	4.85706800	-8.67147700	0.48399500
C	5.64996400	-7.78235600	-0.46530100
C	5.23641700	-6.31495700	-0.39559600
C	6.03607700	-5.43453700	-1.35241200
C	-12.83057700	2.13920600	0.04801500
N	-12.32530700	3.18807100	0.06702700
C	-14.92119900	1.04034700	0.03422700
N	-16.07160600	1.21786100	0.04209500
H	15.74206000	1.22403800	-0.00624400
H	12.23672800	4.79818500	-0.07518400
H	-0.78497500	-2.38256800	0.19598500
H	0.78497700	2.38256100	0.19614600
H	-8.72098200	2.37072100	0.01730100
H	-6.61401000	3.67724600	0.50209400
H	-4.85992900	3.67449800	0.59730600
H	8.72098700	-2.37071400	0.01727000
H	6.61401100	-3.67726200	0.50198900
H	4.85992900	-3.67452200	0.59717300
H	-2.06601000	4.82638300	0.03757300
H	-1.91845300	6.14996600	-2.01525800
H	-1.96525400	2.55682400	-4.35064900
H	-2.07842500	1.22463000	-2.29680200
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H	-0.31766700	4.98288700	3.43461900
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H	0.32804900	-3.85662300	1.27883300
H	0.31760800	-4.98309800	3.43430800
H	3.95446700	-2.98863300	4.50808100
H	3.96472800	-1.83717500	2.35701000
H	-1.94134200	6.34012200	-4.40236400
H	-0.86547400	5.12247100	-5.09902500
H	-2.60664000	4.98017900	-5.32116100
H	-2.33659900	5.86829800	5.33295900
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H	2.33530700	-5.86881100	5.33257900
H	2.89691600	-4.39827800	6.13678300
H	1.16313500	-4.71135300	5.95603800
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H	-7.57585000	3.27787300	-2.16285900
H	4.59800900	-3.88539800	-1.75978800
H	6.40420600	-3.69063500	-3.41749900
H	6.24059700	-2.17193200	-2.53114700
H	7.57590500	-3.27779300	-2.16292000
H	1.94142100	-6.33986400	-4.40270500
H	0.86556100	-5.12217500	-5.09931300
H	2.60673100	-4.97986800	-5.32141400
H	2.06598900	-4.82637600	0.03732100
H	1.91847000	-6.14984300	-2.01558700
H	1.96534900	-2.55657100	-4.35077500
H	2.07848600	-1.22449200	-2.29685000
H	10.73795400	-1.33779400	0.01021900
H	-10.73795000	1.33780100	0.01017600
H	-15.74205300	-1.22404100	-0.00637800
H	-12.23671400	-4.79817700	-0.07547900
H	-5.17374500	9.71679100	0.41514000
H	-4.98647400	8.35294100	1.52469200
H	-3.78537600	8.63281200	0.25931800
H	-5.52837300	8.14193100	-1.49563000

H	-6.72180600	7.86667100	-0.24032700
H	-5.35454400	5.96565500	0.63946800
H	-4.16712400	6.22825000	-0.62744400
H	-5.95174200	5.84959300	-2.36546300
H	-7.10378500	5.49632500	-1.09141200
H	5.17364800	-9.71679400	0.41474900
H	4.98637800	-8.35299000	1.52435800
H	3.78530000	-8.63278500	0.25894800
H	5.52834200	-8.14185800	-1.49594500
H	6.72175200	-7.86666900	-0.24060600
H	5.35449700	-5.96567000	0.63924200
H	4.16710300	-6.22819300	-0.62771100
H	5.95177100	-5.84948900	-2.36567000
H	7.10378700	-5.49629100	-1.09157400
C1	-14.75780600	-5.57961200	-0.08065100
C1	-16.57969100	-3.65096400	-0.04328300
C1	16.57970200	3.65096100	-0.04306900
C1	14.75782200	5.57961400	-0.08034900