

Supporting Information

Adsorption of Ir₄ cluster on single-well carbon nanotubes: the zigzag types are more suitable

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Table S1. The formation energies (eV) for different adsorption modes of SWNT-Ir₄ systems.

modes	substrates					
	(7, 0)	(8, 0)	(10, 0)	(7, 7)	(8, 8)	(10, 10)
T-1	4.80	4.16	5.07	3.58	3.80	4.31
T-2	5.31	4.06	5.33	3.73	4.09	4.53
T-3	5.85	4.94	5.65	3.99	4.13	4.57
S-1	4.28	3.56	4.07	3.15	2.99	3.84
S-2	4.66	4.03	4.66	3.26	3.22	4.11
S-4	4.82	4.25	4.63	3.21	3.28	3.54

Table S2. The adsorption energies (eV) of CO and NO molecules on different SWNT-Ir₄ (T-3) systems.

Molecules	free	substrates					
		(7, 0)	(8, 0)	(10, 0)	(7, 7)	(8, 8)	(10, 10)
CO	2.83	2.52	2.31	2.34	2.91	2.67	2.37
NO	3.15	3.11	2.82	3.07	3.47	3.53	3.19

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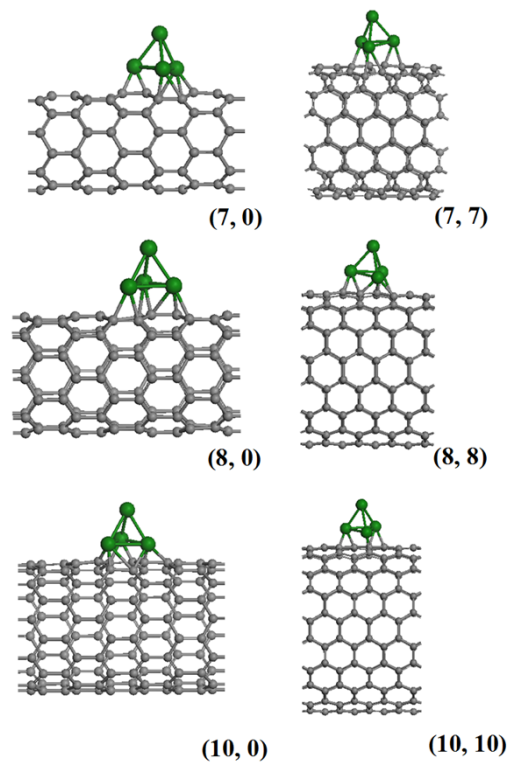


Fig.S1. The relaxed configurations of different SWNTs supported tetrahedron isomer of Ir_4 cluster in the most stable T-3 model.

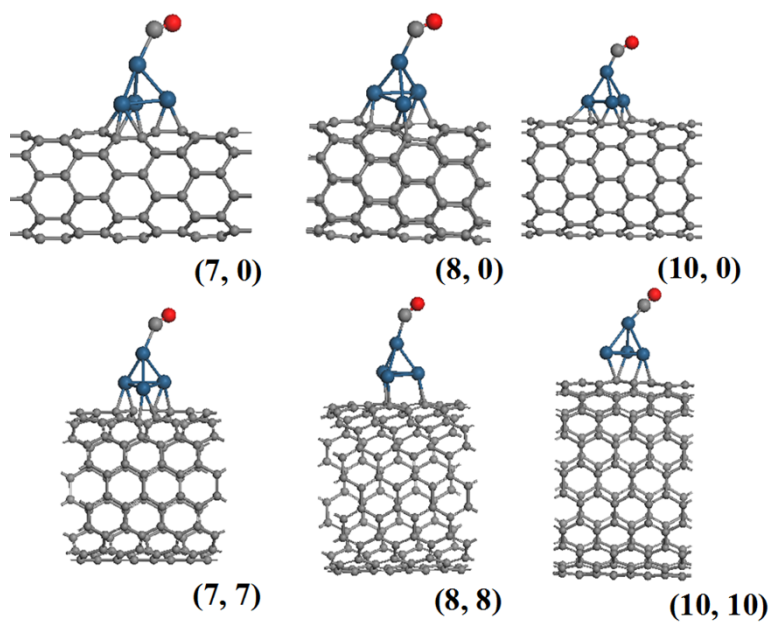


Fig.S2. The relaxed configurations of CO adsorbed on different SWNTs supported tetrahedron isomer of Ir_4 cluster in T-3 model.

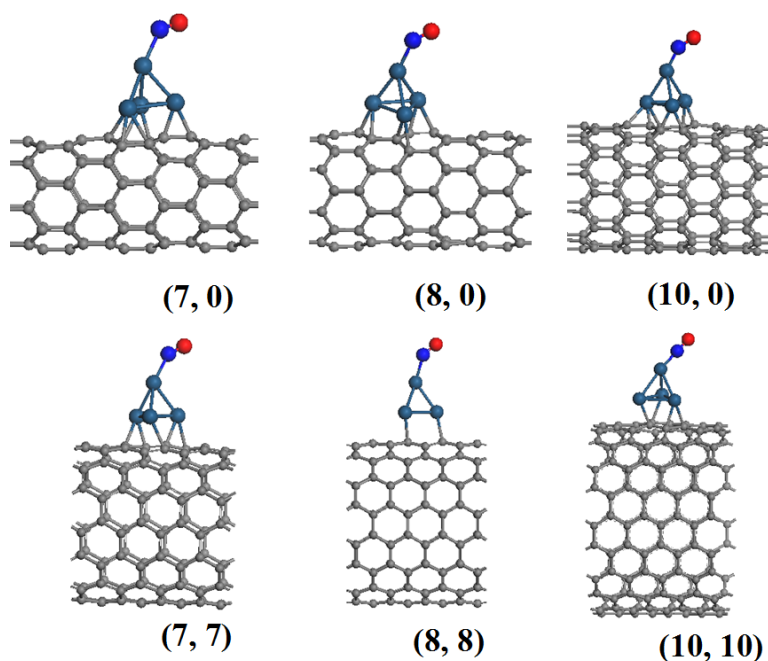


Fig.S3. The relaxed configurations of NO adsorbed on different SWNTs supported tetrahedron isomer of Ir₄ cluster in T-3 model.

The cartesian coordinations of relaxed structures in Fig S1, Fig S2 and Fig S3 are listed as followings:

(7, 0)-Ir₄

C1	9.099885051	14.544350211	0.242124117
C2	9.095253233	14.546207428	1.659020025
C3	8.054084433	15.237401188	2.369183413
C4	6.823799262	15.392726031	0.238827845
C5	6.822974769	15.394041182	1.652392858
C6	5.645148776	14.991073965	2.365427112
C7	8.049707677	15.255159505	3.786460092
C8	4.766215370	14.105259707	0.238656654
C9	4.769089443	14.102786699	1.657815308
C10	4.361768932	12.926439541	2.367219525
C11	5.643242130	15.008300792	3.782572276
C12	4.484612123	11.691644489	0.236767359
C13	4.486817719	11.689130298	1.655396050
C14	5.139805089	10.625009033	2.367497104
C15	4.372967149	12.928110154	3.786503238
C16	6.180533417	9.948508631	0.236697463
C17	6.180051497	9.943624364	1.653717942
C18	7.414105832	9.778168643	2.366646187
C19	5.144654648	10.622287777	3.785698739
C20	8.595023587	10.184455098	0.238376174
C21	8.592793534	10.184104443	1.656427247

C22	9.470428386	11.065803719	2.368928857
C23	7.415719272	9.769577230	3.783608231
C24	9.882655688	12.243485457	0.241503908
C25	9.879920410	12.244295804	1.660494734
C26	9.739313120	13.480254574	2.371653305
C27	9.466482699	11.063627894	3.786841887
C28	9.732388805	13.482692931	3.789669542
C29	9.098624760	14.560108136	4.499296395
C30	9.096174242	14.545436144	5.907071984
C31	8.074654594	15.272037905	6.617603071
C32	6.814892855	15.440704592	4.486031382
C33	6.792315110	15.535564397	5.925127695
C34	5.602193186	15.019275832	6.617263264
C35	8.074963679	15.266892699	8.055474004
C36	4.766915388	14.109472456	4.490172554
C37	4.769160385	14.099262609	5.906087514
C38	4.395293789	12.924930746	6.624786973
C39	5.586957582	15.064936261	8.029565398
C40	4.504852405	11.688336633	4.500487775
C41	4.513427847	11.684886851	5.916563069
C42	5.151601091	10.614981461	6.630806810
C43	4.422647803	12.941399327	8.043057738
C44	6.182417484	9.929882114	4.498206488
C45	6.184932969	9.923726196	5.916050025
C46	7.420117810	9.753885745	6.628737814
C47	5.162533227	10.623325763	8.048923474
C48	8.593947701	10.172332141	4.495751776
C49	8.597020039	10.162329408	5.916103512
C50	9.469680597	11.048772308	6.627363559
C51	7.422863514	9.749129105	8.047257260
C52	9.860004273	12.243768275	4.500645990
C53	9.856979004	12.234552728	5.918479891
C54	9.697920001	13.463671129	6.629429269
C55	9.470497077	11.048365401	8.046845755
C56	9.708410828	13.465174721	8.049278991
C57	9.103638866	14.544515555	8.773342099
C58	9.081318755	14.531765169	10.182949651
C59	8.040030647	15.224421079	10.904898472
C60	6.796532818	15.524758332	8.751902037
C61	6.809993939	15.515484436	10.205775865
C62	5.611078961	15.083533698	10.897080831
C63	8.052635412	15.230727091	12.314461410
C64	4.741788368	14.149764318	8.749160410
C65	4.797159454	14.131812024	10.172815736

C66	4.412177433	12.950315806	10.882860157
C67	5.624428535	15.038641844	12.319754568
C68	4.550872991	11.707796053	8.760842445
C69	4.535751661	11.709865122	10.172951989
C70	5.160868816	10.635403294	10.888380014
C71	4.390966041	12.947272719	12.301847054
C72	6.189266471	9.918486309	8.760537382
C73	6.190828934	9.930984233	10.178270160
C74	7.424128451	9.765349495	10.892201205
C75	5.156524729	10.640012327	12.305102542
C76	8.600288081	10.160631730	8.758878195
C77	8.600976260	10.169653358	10.179572292
C78	9.476077469	11.058097500	10.890506285
C79	7.422731431	9.775793749	12.309459289
C80	9.858281622	12.233303449	8.758745418
C81	9.878601132	12.236190957	10.178710320
C82	9.744997457	13.473769537	10.890623830
C83	9.481380601	11.058042468	12.309683891
C84	9.742111543	13.472025142	12.309228012
C85	9.090901472	14.534962191	13.023151362
C86	9.096561512	14.538119107	14.438738748
C87	8.057826064	15.226709748	15.154142272
C88	6.819684499	15.400400201	13.032295944
C89	6.822702167	15.396406443	14.444622439
C90	5.641445228	14.996086968	15.153868496
C91	8.058346367	15.227794713	16.567360810
C92	4.758953762	14.131872795	13.018547711
C93	4.762893941	14.116724573	14.439753119
C94	4.355014245	12.936655999	15.146186183
C95	5.642712260	14.991651004	16.569852443
C96	4.510615297	11.708448507	13.014296368
C97	4.494796373	11.701693161	14.431916601
C98	5.142098768	10.636424419	15.145955310
C99	4.355485990	12.931482408	16.566218341
C100	6.188458723	9.947785395	13.019922870
C101	6.185091025	9.951239428	14.436438738
C102	7.416973501	9.785665877	15.149707637
C103	5.137327003	10.630864876	16.563816444
C104	8.602484736	10.176445093	13.021428049
C105	8.598776513	10.182823614	14.439954647
C106	9.480681295	11.063258823	15.150706829
C107	7.415030484	9.786984941	16.566307338
C108	9.885801823	12.237774019	13.020391669
C109	9.887997437	12.239891393	14.439991988

C110	9.750328699	13.477829219	15.150766653
C111	9.477470879	11.065438391	16.569688436
C112	9.750940038	13.480301845	16.570175418
Ir1	-9.118480923	-9.101359081	6.974873334
Ir2	-8.304016226	-6.901535608	7.926985208
Ir3	-6.709179918	-8.862263577	7.744208479
Ir4	-8.601770394	-8.896897590	9.462171901

(8, 0)-Ir₄

C1	9.845612448	14.563202085	1.969974926
C2	9.910932912	14.608171987	3.409930748
C3	8.822441135	15.306246450	4.096268097
C4	8.791325767	15.239583841	1.267564749
C5	7.567151722	15.497204054	1.980333531
C6	7.564047395	15.472232033	3.377532279
C7	6.338144524	15.293434268	4.097119287
C8	6.339860357	15.299691645	1.264085421
C9	5.270535546	14.656074596	1.978971632
C10	5.288131890	14.623460275	3.390467433
C11	4.417734147	13.736090261	4.111083431
C12	4.476455164	13.701604004	1.271462848
C13	4.114635084	12.519263614	1.988838700
C14	4.042700556	12.542149526	3.413567431
C15	4.235516241	11.311834757	4.119597214
C16	4.179667202	11.273814084	1.279872929
C17	4.748390972	10.163044935	1.985912428
C18	4.836110772	10.229080922	3.404527977
C19	5.773588541	9.411429665	4.117036232
C20	5.764471503	9.444630836	1.278963682
C21	6.982699918	9.191361461	1.994510076
C22	6.984444265	9.114324231	3.410211616
C23	8.204451342	9.356747696	4.120480636
C24	8.208644360	9.374026594	1.278818538
C25	9.283404418	9.998768185	1.989244797
C26	9.245563517	10.034152731	3.406066273
C27	10.019862376	11.000121780	4.123411516
C28	10.032332866	10.994692912	1.285272763
C29	10.347221657	12.191458479	2.002395038
C30	10.429385568	12.176211369	3.417621189
C31	10.353173476	13.416827481	4.129747586
C32	10.396322259	13.432675612	1.284207450
C33	9.837758930	14.539168330	6.251367371
C34	9.890607975	14.566915797	7.693841749
C35	8.815032316	15.253666096	8.394922645

C36	8.835742468	15.316439187	5.530795636
C37	7.591674814	15.664321374	6.226084041
C38	7.580137193	15.488546391	7.678585987
C39	6.326852950	15.357581625	8.381305667
C40	6.363971386	15.246221564	5.511649795
C41	5.243166507	14.691731792	6.243158910
C42	5.303536230	14.643408055	7.658980575
C43	4.544085149	13.668578240	8.379319747
C44	4.440553689	13.735895744	5.543119184
C45	4.105999172	12.533365982	6.248430109
C46	4.078642262	12.520638233	7.669869966
C47	4.160167757	11.273393461	8.369374640
C48	4.231581395	11.301289203	5.535895357
C49	4.797667661	10.194110733	6.244044597
C50	4.793950373	10.199478689	7.664844014
C51	5.781399492	9.448055144	8.381211758
C52	5.770516669	9.413193654	5.539347480
C53	6.985913490	9.149047696	6.252803230
C54	6.987173113	9.137444270	7.671092511
C55	8.210230715	9.358624811	8.382531219
C56	8.205498193	9.373142568	5.537590637
C57	9.283296557	9.993857101	6.250594558
C58	9.254536929	10.030519464	7.669778887
C59	10.013513286	11.012139919	8.387193865
C60	10.040762642	10.979269175	5.541916555
C61	10.347997947	12.178792262	6.255701744
C62	10.429750201	12.179106715	7.674863989
C63	10.461165355	13.424354407	8.384856743
C64	10.404535980	13.412093158	5.543512111
C65	9.778264184	14.483310441	10.515207735
C66	9.796940276	14.506369668	11.930356012
C67	8.788976914	15.240680780	12.636047934
C68	8.802949625	15.256385169	9.809642268
C69	7.581595295	15.538715582	10.511313753
C70	7.575319201	15.524189148	11.921668233
C71	6.348402984	15.299241499	12.635416546
C72	6.361472115	15.280783735	9.790469650
C73	5.305127303	14.625376997	10.509298347
C74	5.289292120	14.647604691	11.920810546
C75	4.504081451	13.686540252	12.632813999
C76	4.471096892	13.705684387	9.797833520
C77	4.070337006	12.524484037	10.500704884
C78	4.109402724	12.511038798	11.923105195
C79	4.169653563	11.269235565	12.634632321

C80	4.205592651	11.288129420	9.791611465
C81	4.786382923	10.190768529	10.505945046
C82	4.753837308	10.167478051	11.929720527
C83	5.762643171	9.439536622	12.639676995
C84	5.765297633	9.418774087	9.800236528
C85	6.981355702	9.160423557	10.512113378
C86	6.979705806	9.179744309	11.927978581
C87	8.202522513	9.389956842	12.642490518
C88	8.204462905	9.378703000	9.800629845
C89	9.257672431	10.038262273	10.515501287
C90	9.273923539	10.021226723	11.932604993
C91	10.042787227	10.994696405	12.645944797
C92	10.043251505	10.998113295	9.803211313
C93	10.487295718	12.160161787	10.511831807
C94	10.449808965	12.168725014	11.934603911
C95	10.394119238	13.415826446	12.640446650
C96	10.413862375	13.405840085	9.805549720
Ir1	-4.129085162	-7.462891678	5.653559917
Ir2	-4.279703390	-9.727103469	6.784613760
Ir3	-4.672831461	-9.514287087	4.271755553
Ir4	-6.385939453	-8.613686614	5.920424434

(10, 0)-Ir₄

C1	10.711008031	15.120086437	1.334373226
C2	10.707213063	15.122786518	2.753325252
C3	9.803740810	15.976364881	3.452928235
C4	9.805050801	15.965469506	0.627119132
C5	8.675736781	16.481442913	1.331964013
C6	8.676404964	16.489760805	2.745846613
C7	7.444476076	16.616210399	3.458116005
C8	7.441695960	16.604273416	0.626559125
C9	6.234164875	16.326213025	1.336222642
C10	6.236476894	16.327208165	2.753798120
C11	5.182364243	15.679038536	3.464521776
C12	5.173828726	15.683524392	0.629805667
C13	4.357365518	14.753785393	1.337480314
C14	4.362152878	14.751396033	2.759263897
C15	3.857844899	13.619399225	3.467257688
C16	3.852345067	13.623156336	0.628738703
C17	3.711491130	12.393043495	1.336903540
C18	3.712551463	12.391214083	2.758424186
C19	3.949594364	11.175010204	3.467103929
C20	3.949643572	11.178089241	0.627975402
C21	4.555226552	10.096286426	1.336711997

C22	4.555025318	10.094000857	2.758285081
C23	5.468549487	9.257910564	3.466619637
C24	5.469642149	9.261198769	0.629245115
C25	6.599168699	8.752503075	1.337650063
C26	6.599131361	8.750601780	2.759058932
C27	7.830539378	8.622039792	3.468173861
C28	7.831392729	8.624918994	0.629668447
C29	9.040798833	8.890635839	1.338744149
C30	9.040818218	8.889730974	2.759929951
C31	10.103511689	9.526307637	3.469084177
C32	10.105277268	9.526856708	0.630736184
C33	10.921247769	10.457235858	1.338915613
C34	10.919628569	10.458541056	2.761739004
C35	11.411028015	11.594027434	3.469775092
C36	11.419167720	11.590985549	0.630792764
C37	11.551872864	12.821922489	1.339345212
C38	11.546157783	12.824347689	2.760322848
C39	11.298494688	14.038723952	3.465959031
C40	11.311402262	14.035751806	0.629326821
C41	10.687769936	15.127802426	5.586793198
C42	10.679538420	15.126515148	7.010786082
C43	9.842333694	16.032884372	7.708845442
C44	9.805404625	15.996863849	4.869258994
C45	8.694501927	16.556830257	5.565614086
C46	8.748239420	16.680082348	6.994726481
C47	7.414323463	16.761349286	7.722417169
C48	7.449197534	16.642119314	4.872880016
C49	6.235748472	16.345612060	5.589924414
C50	6.226085859	16.350647443	7.003976190
C51	5.201432222	15.670547165	7.718531752
C52	5.188997036	15.678543735	4.885941210
C53	4.373583608	14.746603116	5.595268639
C54	4.379385172	14.742063618	7.015478892
C55	3.868367386	13.615239899	7.725014737
C56	3.861488534	13.617546662	4.888195288
C57	3.715591632	12.388787959	5.596645184
C58	3.716341901	12.387190999	7.017740937
C59	3.949288221	11.171104900	7.727245620
C60	3.949569966	11.172775069	4.887793569
C61	4.553710668	10.090537961	5.596856185
C62	4.553578817	10.088798901	7.018644561
C63	5.467569268	9.253409245	7.727245853
C64	5.468277938	9.255640937	4.888944377
C65	6.597932997	8.746753133	5.597624878

C66	6.597992826	8.745131839	7.019268476
C67	7.829737563	8.615940011	7.728522742
C68	7.830441847	8.619790445	4.889170858
C69	9.040042244	8.884986766	5.598687085
C70	9.040280933	8.882450042	7.019797142
C71	10.103708566	9.518964164	7.729269967
C72	10.103448816	9.524529627	4.890690464
C73	10.915531305	10.457389801	5.599516080
C74	10.915948307	10.455237720	7.021796223
C75	11.401165123	11.592968928	7.730151319
C76	11.405691014	11.596193325	4.892365842
C77	11.526160775	12.827372740	5.600167156
C78	11.520725427	12.827606172	7.021885376
C79	11.270139635	14.037984582	7.728609734
C80	11.284390502	14.041918105	4.887829961
C81	10.723851317	15.134625027	9.869265503
C82	10.715374539	15.133350417	11.289248433
C83	9.830572286	16.007884392	12.009258505
C84	9.901508778	16.077726090	9.163519524
C85	8.725052187	16.620474115	9.858778944
C86	8.709666133	16.590745323	11.329887425
C87	7.453948871	16.654371254	12.017474405
C88	7.428090369	16.669039401	9.156514932
C89	6.254934509	16.318331226	9.858335546
C90	6.259516953	16.328696425	11.289851630
C91	5.201379835	15.679303943	11.988751558
C92	5.201927404	15.667214794	9.143799614
C93	4.384057513	14.744133034	9.852655679
C94	4.383421985	14.748179405	11.277079081
C95	3.868882072	13.622789554	11.984540537
C96	3.868445619	13.615617558	9.146543991
C97	3.717920683	12.389215407	9.856019707
C98	3.719207011	12.391908589	11.277225674
C99	3.952309999	11.176755417	11.986931812
C100	3.949771109	11.171393441	9.148010006
C101	4.554029020	10.090085389	9.857499143
C102	4.554991585	10.092276436	11.279082519
C103	5.468824832	9.257296223	11.987742671
C104	5.467990933	9.253461793	9.149719374
C105	6.597872880	8.745275511	9.858387458
C106	6.598441331	8.746808619	11.280023817
C107	7.830159927	8.618808599	11.989197482
C108	7.830157979	8.615620372	9.149732737
C109	9.040229849	8.880919141	9.859072846

C110	9.040679892	8.882895379	11.280347445
C111	10.103952859	9.520455832	11.989249594
C112	10.104270419	9.518130086	9.150393539
C113	10.916220251	10.452683643	9.858713261
C114	10.917555447	10.453606617	11.280901293
C115	11.408596832	11.589948758	11.988563065
C116	11.401180542	11.592546740	9.151429277
C117	11.524613318	12.823387535	9.860474371
C118	11.531910510	12.822505317	11.280549497
C119	11.290633798	14.036042781	11.991763554
C120	11.277025253	14.039506646	9.153817756
C121	10.712431283	15.122415745	14.124705978
C122	10.712943271	15.120619390	15.543370317
C123	9.807220076	15.966766746	16.251259588
C124	9.817438864	15.985914363	13.423043422
C125	8.683648213	16.501044290	14.134060906
C126	8.679371925	16.486694718	15.546360641
C127	7.442742615	16.605726142	16.252675160
C128	7.447232155	16.628482980	13.427865069
C129	6.239712831	16.331655935	14.126803465
C130	6.235320331	16.327881935	15.544328201
C131	5.174538954	15.684948841	16.248982596
C132	5.186842142	15.684990547	13.412134499
C133	4.364108886	14.756722624	14.116428815
C134	4.357621593	14.756706022	15.538938665
C135	3.852636911	13.624707731	16.246480076
C136	3.862320404	13.624075346	13.407535638
C137	3.714969153	12.395549295	14.115956898
C138	3.712225071	12.395001014	15.537755951
C139	3.950004618	11.179275120	16.246787728
C140	3.952349712	11.178382614	13.408022549
C141	4.556005290	10.097073937	14.117153119
C142	4.556041181	10.097579748	15.538896423
C143	5.469528571	9.261961282	16.247101240
C144	5.469536556	9.259540645	13.409896838
C145	6.598975714	8.751544636	14.118439686
C146	6.599464933	8.752810754	15.539854602
C147	7.830864971	8.624798268	16.248782406
C148	7.830832972	8.621325954	13.410226391
C149	9.040453219	8.887498831	14.119374266
C150	9.041029062	8.889545908	15.540391706
C151	10.104916805	9.525924621	16.249088388
C152	10.104689457	9.522605265	13.410593503
C153	10.920083606	10.454483553	14.118370201

C154	10.921582213	10.455702221	15.540908777
C155	11.419023533	11.589814828	16.248730418
C156	11.412946142	11.589577572	13.410125746
C157	11.545638265	12.820544625	14.119120072
C158	11.551435059	12.820543442	15.539698532
C159	11.311494511	14.034808053	16.248935941
C160	11.300127326	14.035165543	13.413168018
Ir1	-5.297664414	-6.174875812	8.806100301
Ir2	-4.521778822	-8.577524894	8.428990406
Ir3	-6.807004181	-7.836958911	7.602753532
Ir4	-6.383425703	-8.054857705	10.085649344

(7, 7)-Ir₄

C1	11.590210784	14.757099924	0.463301027
C2	7.959662871	16.769398706	0.456435682
C3	10.613368708	15.803128708	0.459836528
C4	10.032068368	16.214743857	1.685441592
C5	6.535886393	16.569467469	0.463932031
C6	5.872330059	16.294609899	1.689737243
C7	8.683220978	16.706407444	1.671673364
C8	4.197894357	14.966257600	0.468171057
C9	4.690674623	15.480631585	1.695216722
C10	3.084664450	10.944120707	0.466932268
C11	3.442544422	13.747434469	0.467516122
C12	3.200797203	13.074497375	1.696300597
C13	3.532181354	9.583627377	0.466864851
C14	3.899914676	8.972817924	1.696577013
C15	3.018390809	11.654017234	1.696420478
C16	5.501185627	7.564524527	0.466675089
C17	4.898566483	7.946202131	1.696437055
C18	9.651441333	7.450088732	0.466035611
C19	6.853256620	7.092501854	0.466423515
C20	7.562461763	7.018496739	1.696095136
C21	10.847491078	8.239164797	0.465784511
C22	11.342836017	8.750578767	1.695543275
C23	8.983430888	7.200433373	1.695798668
C24	12.317823099	10.649750756	0.466190505
C25	12.085991846	9.974845040	1.695365075
C26	12.480012113	12.073219384	0.466444683
C27	12.398336235	12.783649724	1.695060860
C28	11.947842789	14.143904958	1.694587958
C29	11.583785253	14.759664768	2.924936559
C30	7.967651178	16.817794401	2.896972524
C31	10.632107998	15.826413154	2.922489979

C32	10.083774157	16.287717542	4.161343469
C33	6.538633614	16.565623363	2.917366245
C34	5.876538563	16.282560936	4.156493407
C35	8.721838461	16.859304387	4.146377043
C36	4.198244749	14.959130753	2.925555709
C37	4.691606127	15.462659424	4.155002163
C38	3.083028846	10.944005953	2.926177630
C39	3.440215719	13.744087295	2.926107792
C40	3.197483289	13.073211513	4.155710285
C41	3.531309627	9.583756502	2.926245549
C42	3.899524532	8.973090820	4.156166044
C43	3.015676146	11.653180421	4.156210824
C44	5.501126305	7.564659278	2.926183421
C45	4.898459341	7.946616924	4.155953566
C46	9.651546972	7.449160542	2.925535833
C47	6.853208326	7.092425540	2.925937656
C48	7.562569960	7.018734776	4.155692750
C49	10.847326754	8.238347657	2.925233761
C50	11.342802693	8.750532168	4.154979646
C51	8.983441836	7.200499627	4.155516309
C52	12.312131942	10.650471845	2.924679086
C53	12.084721902	9.974848519	4.154502332
C54	12.469309572	12.073610305	2.924015327
C55	12.392925990	12.781722918	4.154186601
C56	11.944255899	14.139303143	4.154447235
C57	11.587086671	14.751553193	5.385346407
C58	7.944056325	16.968804517	5.413233946
C59	10.626556625	15.808413310	5.393041083
C60	10.023586743	16.182890582	6.620099286
C61	6.523337941	16.568272322	5.391473330
C62	5.874993837	16.273720920	6.628201267
C63	8.709233855	16.779868020	6.635205528
C64	4.202027840	14.953417241	5.384346168
C65	4.701675216	15.464405789	6.620635996
C66	3.082079314	10.943714201	5.386460213
C67	3.439086901	13.743238690	5.386039471
C68	3.198052758	13.073969332	6.616771132
C69	3.531167403	9.583817500	5.386081102
C70	3.899911321	8.973003254	6.615708946
C71	3.016365066	11.653424089	6.616290233
C72	5.501202953	7.564914626	5.385621597
C73	4.898589164	7.946624101	6.615434899
C74	9.651687017	7.449906570	5.385277952
C75	6.853195587	7.092808088	5.385475012

C76	7.562582031	7.019054829	6.615154818
C77	10.847706018	8.238724086	5.385171130
C78	11.343930731	8.750916721	6.614647356
C79	8.983456981	7.201185716	6.615027149
C80	12.315648947	10.649486416	5.384288925
C81	12.089486838	9.974113394	6.614418030
C82	12.475040305	12.071919670	5.383684037
C83	12.406117232	12.780237737	6.614110565
C84	11.952603147	14.136467551	6.614284090
C85	11.588874761	14.748378259	7.844109170
C86	7.959206188	16.850709240	7.854676292
C87	10.599593535	15.782130560	7.842158922
C88	10.009268538	16.195002165	9.072014627
C89	6.532668226	16.576298544	7.850228564
C90	5.872244456	16.299200963	9.073189626
C91	8.677113294	16.717143637	9.077704519
C92	4.200809197	14.958164654	7.849363481
C93	4.693585623	15.480829651	9.075563422
C94	3.083875631	10.944102251	7.846083062
C95	3.440929388	13.745131942	7.847176284
C96	3.201061015	13.075109735	9.076901060
C97	3.532038432	9.583850574	7.845614297
C98	3.900342575	8.972958598	9.075151538
C99	3.018685759	11.653899464	9.075920140
C100	5.501229264	7.564746144	7.845081693
C101	4.898767164	7.946253783	9.074937915
C102	9.651611753	7.450642915	7.844625880
C103	6.853265228	7.092797479	7.844881808
C104	7.562499291	7.019072744	9.074583546
C105	10.847964060	8.239544484	7.844440643
C106	11.343702424	8.751435617	9.074281564
C107	8.983364313	7.201404961	9.074326987
C108	12.321116332	10.648597794	7.844301860
C109	12.089759134	9.974316604	9.074366394
C110	12.484780018	12.071657457	7.844499327
C111	12.410595725	12.781556967	9.074137106
C112	11.957328880	14.139992305	9.073500720
Ir1	-8.843485220	-7.477911984	4.434314422
Ir2	-7.578804310	-5.279351302	4.547672754
Ir3	-6.457955081	-7.328450699	3.570385724
Ir4	-6.923696427	-7.201563718	6.081099404

(8, 8)-Ir₄

C1	12.219726735	16.251031011	0.811995265
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C2	11.073061298	17.117749050	0.806390210
C3	10.410841372	17.420365238	2.008724002
C4	12.678034247	15.698277429	2.034036055
C5	8.295340403	17.659981682	0.800558775
C6	9.006978228	17.694627921	2.020880829
C7	4.556646458	15.738711446	0.808677771
C8	6.900573930	17.333552381	0.805211551
C9	6.248001948	17.044876797	2.036995915
C10	3.729407611	14.569365714	0.809233874
C11	3.429402529	13.924249663	2.039066756
C12	5.063578431	16.238045737	2.037934527
C13	3.041851401	11.824466947	0.810349379
C14	3.082199437	12.534665363	2.039750792
C15	4.686489502	7.980256568	0.811816895
C16	3.237119987	10.406166241	0.810885967
C17	3.470920549	9.733394578	2.040829339
C18	5.849807573	7.144468018	0.812394383
C19	6.499336858	6.853388463	2.042360364
C20	4.202642924	8.502775034	2.041379599
C21	8.609542255	6.542345705	0.813418121
C22	7.898618418	6.548737498	2.042944219
C23	12.358302896	8.404369664	0.815112995
C24	10.014328125	6.820781990	0.814014983
C25	10.669841173	7.097997148	2.043951261
C26	13.160977414	9.590449383	0.815711289
C27	13.443453760	10.243975136	2.045536753
C28	11.856002061	7.900691090	2.044504296
C29	13.785057883	12.350221159	0.815835582
C30	13.756886544	11.641035158	2.045990767
C31	13.586273547	13.767930624	0.815182202
C32	13.364510079	14.445129266	2.043058070
C33	12.212071468	16.245447223	3.252182808
C34	11.097541186	17.154730365	3.218579976
C35	10.440981451	17.552972471	4.461293885
C36	12.651945250	15.693466322	4.511784887
C37	8.291631135	17.672884078	3.256299905
C38	8.990680034	17.703831760	4.487755158
C39	4.555564712	15.739222333	3.267146913
C40	6.896297886	17.332811381	3.264595306
C41	6.250793576	17.035040592	4.495136039
C42	3.728780501	14.569849781	3.268437257
C43	3.428663390	13.924303515	4.498409745
C44	5.064365989	16.236220172	4.497073117
C45	3.041960872	11.824624870	3.269697270

C46	3.081757306	12.534816428	4.499142656
C47	4.686546545	7.980311779	3.271326546
C48	3.237116100	10.406259507	3.270327944
C49	3.470962441	9.733465536	4.500258057
C50	5.849788234	7.144465846	3.271909065
C51	6.499394243	6.853447456	4.501871033
C52	4.202684027	8.502934770	4.500856931
C53	8.609557780	6.542363932	3.272884386
C54	7.898666868	6.548924303	4.502454011
C55	12.358401378	8.404436742	3.274385020
C56	10.014281202	6.820910394	3.273448641
C57	10.669922067	7.097881469	4.503397010
C58	13.160745739	9.590715781	3.274871227
C59	13.442688625	10.243862991	4.505002519
C60	11.856228399	7.900363721	4.503934346
C61	13.781415266	12.351978770	3.275929029
C62	13.753323241	11.641422791	4.505528510
C63	13.578457997	13.769525041	3.275795012
C64	13.340334540	14.440239602	4.507648973
C65	12.223045275	16.256483554	5.753346477
C66	11.183543104	17.281148468	5.724371609
C67	10.486041355	17.587697835	6.991334815
C68	12.659106815	15.700277698	6.978820102
C69	8.297204618	17.635529194	5.728943816
C70	9.013542116	17.684469059	6.963445198
C71	4.556289115	15.737411017	5.727562516
C72	6.908238382	17.307030148	5.728056890
C73	6.257770247	17.025591721	6.957854003
C74	3.728118498	14.569342925	5.728138096
C75	3.428468929	13.924045728	6.958329078
C76	5.066434892	16.232817135	6.957723448
C77	3.041459793	11.824598491	5.729112406
C78	3.081444034	12.534555553	6.958820672
C79	4.686573505	7.980392439	5.730818628
C80	3.237029872	10.406348498	5.729767118
C81	3.470897846	9.733528903	6.959764239
C82	5.849872701	7.144635423	5.731408288
C83	6.499454969	6.853555392	6.961363417
C84	4.202738834	8.502999851	6.960347873
C85	8.609632195	6.542440669	5.732411586
C86	7.898695229	6.548793793	6.961951692
C87	12.358648638	8.403766489	5.733943392
C88	10.014433498	6.820667487	5.732990932
C89	10.670061641	7.097633548	6.962957556

C90	13.161006782	9.589902764	5.734537409
C91	13.443405533	10.242499769	6.964601088
C92	11.856421704	7.899933778	6.963583149
C93	13.776936333	12.350991595	5.736664783
C94	13.754108685	11.639465743	6.965359656
C95	13.566287564	13.766358460	5.738691767
C96	13.338507027	14.441002503	6.970233313
C97	12.238074136	16.267242828	8.207951005
C98	11.163791092	17.239171940	8.224613142
C99	10.430902923	17.441985780	9.428925692
C100	12.675514540	15.701551789	9.422383754
C101	8.305233037	17.637000096	8.186397719
C102	9.015651179	17.674889757	9.417896783
C103	4.557602900	15.736786399	8.188125384
C104	6.911652707	17.312664101	8.187756465
C105	6.253870351	17.036268127	9.416590213
C106	3.728744487	14.568844005	8.188107923
C107	3.429219940	13.923745138	9.417958115
C108	5.066048833	16.235366656	9.416916880
C109	3.041589362	11.824493727	8.188802469
C110	3.081846391	12.534505859	9.418414821
C111	4.686635999	7.980465072	8.190307825
C112	3.236997216	10.406217893	8.189366440
C113	3.470937452	9.733425084	9.419330042
C114	5.849863738	7.144598796	8.190895562
C115	6.499362655	6.853373173	9.420852061
C116	4.202701508	8.502896584	9.419873443
C117	8.609631452	6.542293029	8.191906665
C118	7.898661932	6.548797525	9.421442769
C119	12.358666525	8.403622745	8.193535798
C120	10.014399022	6.820689816	8.192513827
C121	10.669912234	7.097810178	9.422501448
C122	13.161303744	9.589520012	8.194217466
C123	13.443603903	10.242738132	9.424037985
C124	11.856201970	7.900343483	9.423139093
C125	13.781290185	12.349530085	8.194924234
C126	13.756603419	11.639607413	9.424647975
C127	13.575938539	13.765333170	8.196013228
C128	13.358975801	14.443129080	9.424608662
Ir1	-3.576935324	-5.120924393	4.772869203
Ir2	-3.138621087	-7.594411747	4.421900659
Ir3	-5.500509939	-6.639821025	4.092682430
Ir4	-4.523743705	-6.809753425	6.422458844

(10, 10)-Ir₄

C1	12.056264051	17.568635008	0.246277738
C2	10.934353782	18.450616764	0.245443986
C3	10.320272171	18.815501364	1.462660960
C4	12.537795408	17.050208114	1.475613416
C5	8.257583049	19.397869732	0.245526665
C6	8.972957615	19.302525761	1.454416507
C7	4.131346903	18.473596979	0.246297392
C8	6.819649158	19.388502039	0.245339835
C9	6.115494240	19.263720736	1.468717993
C10	2.967831577	17.642026689	0.246781961
C11	2.459077184	17.146947782	1.476832492
C12	4.764580689	18.800646095	1.474003442
C13	1.249880494	15.385646526	0.247070067
C14	1.593077458	16.008700351	1.476861848
C15	0.657548759	11.209886213	0.246953263
C16	0.758701791	14.042870624	0.247030020
C17	0.620896745	13.345339222	1.476794399
C18	1.058923345	9.836067842	0.246920500
C19	1.365030323	9.194581441	1.476667270
C20	0.570181734	11.915881874	1.476744901
C21	2.673619557	7.506014343	0.246864150
C22	2.179603233	8.017282465	1.476630819
C23	6.494721467	5.715319255	0.246781254
C24	3.816160921	6.644846719	0.246834586
C25	4.443033852	6.308713436	1.476574976
C26	7.924749432	5.695695007	0.246750658
C27	8.628715783	5.800691978	1.476477903
C28	5.794062009	5.839683358	1.476542233
C29	10.627517814	6.552856873	0.246695165
C30	9.992066957	6.233899763	1.476432543
C31	13.484626751	9.661331574	0.246612208
C32	11.792550692	7.384607638	0.246663165
C33	12.298998502	7.883444831	1.476376758
C34	13.954351614	11.012137000	0.246588375
C35	14.082203018	11.711735347	1.476715441
C36	13.151185070	9.033038783	1.476344914
C37	14.030034854	13.845487312	0.246636532
C38	14.119150543	13.141173075	1.477072934
C39	13.632135911	15.218744362	0.246721603
C40	13.330624942	15.862454639	1.476588448
C41	12.057806389	17.583262772	2.701073856
C42	10.959690232	18.493975440	2.688908246
C43	10.383528317	18.943385641	3.919237202

C44	12.531749733	17.064340208	3.935423142
C45	8.260377033	19.462793562	2.669356165
C46	8.987511571	19.441544472	3.921495055
C47	4.133928717	18.474394083	2.705667407
C48	6.820324405	19.400596135	2.691936699
C49	6.123233088	19.251689815	3.931009431
C50	2.969598775	17.642864766	2.706279016
C51	2.461361416	17.146329643	3.936522406
C52	4.771536952	18.793708381	3.934565943
C53	1.250065325	15.386103656	2.706631206
C54	1.594108611	16.009241158	3.936422143
C55	0.657486325	11.209913750	2.706487603
C56	0.758587813	14.043210778	2.706604867
C57	0.620621924	13.345459573	3.936267285
C58	1.058897569	9.836077173	2.706440793
C59	1.365013245	9.194573469	3.936174939
C60	0.570018590	11.915985420	3.936240609
C61	2.673633584	7.506026700	2.706374002
C62	2.179606096	8.017306400	3.936138840
C63	6.494737720	5.715321777	2.706279904
C64	3.816169539	6.644852996	2.706340801
C65	4.443053661	6.308715985	3.936079285
C66	7.924756328	5.695676377	2.706243401
C67	8.628741659	5.800643372	3.935982853
C68	5.794071462	5.839685673	3.936046956
C69	10.627523628	6.552774967	2.706165272
C70	9.992087670	6.233791501	3.935940688
C71	13.484106543	9.661267971	2.706219259
C72	11.792499791	7.384480446	2.706106138
C73	12.298920023	7.883218819	3.935890202
C74	13.952839299	11.012141109	2.706316741
C75	14.079328611	11.712459985	3.936192211
C76	13.150774150	9.032834792	3.935864404
C77	14.024563764	13.847379546	2.707176411
C78	14.113386362	13.141808230	3.936559844
C79	13.625021999	15.220879471	2.707970519
C80	13.318879279	15.868969252	3.936466904
C81	12.051387408	17.602690366	5.165337546
C82	10.977531302	18.551879651	5.166599991
C83	10.393209007	18.928037107	6.421361027
C84	12.532296552	17.064522198	6.394747782
C85	8.234620956	19.429388516	5.166031041
C86	8.991442927	19.402658786	6.431193904
C87	4.139844831	18.468534738	5.166746861

C88	6.821372943	19.358981280	5.171294716
C89	6.123628328	19.247528472	6.405238270
C90	2.973717584	17.640668822	5.166312465
C91	2.460900859	17.145876040	6.395728292
C92	4.771222563	18.792436190	6.399537191
C93	1.250114584	15.386015536	5.165996914
C94	1.593784686	16.008980887	6.395659755
C95	0.657350926	11.209882598	5.165948080
C96	0.758509703	14.043380119	5.165974098
C97	0.620518097	13.345406467	6.395694131
C98	1.058869412	9.836120181	5.165918799
C99	1.364995696	9.194568964	6.395648684
C100	0.569964356	11.915955394	6.395671498
C101	2.673640380	7.506017764	5.165869753
C102	2.179598531	8.017303154	6.395620638
C103	6.494750736	5.715313643	5.165783805
C104	3.816175775	6.644865847	5.165838022
C105	4.443050944	6.308716050	6.395574455
C106	7.924772683	5.695651301	5.165752923
C107	8.628741254	5.800638801	6.395500733
C108	5.794074349	5.839684993	6.395541657
C109	10.627542164	6.552655957	5.165699758
C110	9.992101353	6.233787744	6.395479648
C111	13.483675305	9.661174485	5.165606470
C112	11.792515945	7.384340046	5.165670046
C113	12.298944327	7.883207555	6.395423540
C114	13.951508808	11.012268070	5.165568642
C115	14.079399096	11.712459030	6.394915417
C116	13.150826373	9.032865212	6.395386739
C117	14.019046653	13.848751678	5.165432181
C118	14.113490004	13.141932666	6.394458310
C119	13.618089446	15.222748191	5.165354331
C120	13.319583570	15.868635418	6.394099628
C121	12.059784304	17.582183894	7.630270706
C122	10.961418558	18.489170097	7.642205018
C123	10.319670986	18.809715778	8.865334805
C124	12.538800827	17.049337120	8.856036293
C125	8.256265854	19.437517735	7.663804844
C126	8.968943694	19.292241443	8.873058943
C127	4.133080590	18.472549254	7.626706827
C128	6.821780532	19.388821663	7.636938623
C129	6.117104231	19.260104290	8.859560407
C130	2.968733852	17.641938756	7.625976900
C131	2.458579885	17.146451613	8.855219046

C132	4.764368121	18.799264240	8.856440250
C133	1.249728677	15.385873491	7.625447671
C134	1.592727553	16.008401942	8.855245869
C135	0.657423115	11.209891887	7.625421799
C136	0.758384501	14.043065144	7.625411032
C137	0.620786967	13.345292524	8.855221093
C138	1.058866368	9.836066367	7.625403522
C139	1.365012636	9.194573997	8.855149381
C140	0.570124838	11.915851737	8.855197134
C141	2.673625308	7.506022603	7.625360925
C142	2.179593937	8.017280273	8.855123909
C143	6.494738640	5.715320757	7.625285191
C144	3.816166468	6.644851520	7.625331974
C145	4.443034368	6.308711613	8.855073562
C146	7.924759994	5.695672632	7.625259473
C147	8.628722794	5.800688683	8.855001656
C148	5.794060292	5.839683091	8.855042869
C149	10.627541342	6.552763644	7.625231556
C150	9.992071841	6.233889680	8.854982299
C151	13.484176297	9.661294788	7.625015814
C152	11.792534898	7.384470376	7.625226492
C153	12.299035973	7.883447199	8.854930606
C154	13.952938867	11.012209837	7.624851788
C155	14.082290525	11.711822259	8.854459552
C156	13.151224409	9.033032644	8.854900852
C157	14.024818698	13.847364286	7.623871817
C158	14.119295465	13.141212357	8.854066807
C159	13.625489788	15.220988045	7.622955280
C160	13.331187440	15.862212445	8.854821246
Ir1	-6.509205725	-4.831548004	3.404418247
Ir2	-5.097524240	-3.048308930	4.540093661
Ir3	-4.139126108	-5.371936019	4.148159892
Ir4	-5.969058932	-5.012252047	5.864933119

(7, 0)-Ir₄-CO

C1	9.113014651	14.543459422	0.246847917
C2	9.112938313	14.555029370	1.664804409
C3	8.068760554	15.247486638	2.371782579
C4	6.835447496	15.386077487	0.244063057
C5	6.834164271	15.386884834	1.655061821
C6	5.661325952	14.968958102	2.367778057
C7	8.064778671	15.281165903	3.787917435
C8	4.785485169	14.082687640	0.244509609
C9	4.791387795	14.074985549	1.661268059

C10	4.381255516	12.897995877	2.369501756
C11	5.665385223	14.977917800	3.781794453
C12	4.487726512	11.669120636	0.238134604
C13	4.485969916	11.661057464	1.657081737
C14	5.120271035	10.585603650	2.368965690
C15	4.388372509	12.895990628	3.786761983
C16	6.167362476	9.914367135	0.237932659
C17	6.165732901	9.910391354	1.657017074
C18	7.401003449	9.757817579	2.372270209
C19	5.120153473	10.580826011	3.790451540
C20	8.578621742	10.179322815	0.246417004
C21	8.576635910	10.176159878	1.663778459
C22	9.444937762	11.065739716	2.376992976
C23	7.400658810	9.756216013	3.788633377
C24	9.873960205	12.235343211	0.249913153
C25	9.858139752	12.241622307	1.667487508
C26	9.739086495	13.481087120	2.377405677
C27	9.443586788	11.065340782	3.793755328
C28	9.719330900	13.483640778	3.795890662
C29	9.100155274	14.568305567	4.505602507
C30	9.116830463	14.577353570	5.916680350
C31	8.108837701	15.345808671	6.618191239
C32	6.823169076	15.453705813	4.480440858
C33	6.801972764	15.544699249	5.921536910
C34	5.608691708	15.007662277	6.601971147
C35	8.107054401	15.333431096	8.065570896
C36	4.793825568	14.072140590	4.490528735
C37	4.788522450	14.064972709	5.898117802
C38	4.415814916	12.901963390	6.625838484
C39	5.597575236	15.081163030	8.024968931
C40	4.490823482	11.655459124	4.502432166
C41	4.502477862	11.658475987	5.921356080
C42	5.138328724	10.590480771	6.636159035
C43	4.409152145	12.936953623	8.049895316
C44	6.165177394	9.899470175	4.503397931
C45	6.171014392	9.898375855	5.923220573
C46	7.409292978	9.733133416	6.634936671
C47	5.161681301	10.624134384	8.054473833
C48	8.573720852	10.172438277	4.502156222
C49	8.578088316	10.160748842	5.920970585
C50	9.433342485	11.061666095	6.631990701
C51	7.417882963	9.735431967	8.052578443
C52	9.841228169	12.245844110	4.505964382
C53	9.820686163	12.246227057	5.921699648

C54	9.698234918	13.480072443	6.633425465
C55	9.450848873	11.050208265	8.049033681
C56	9.695366952	13.467049947	8.055766386
C57	9.108758426	14.550904951	8.782096556
C58	9.108700194	14.542407307	10.197497218
C59	8.073087768	15.229619253	10.925227278
C60	6.814194999	15.506241652	8.777399713
C61	6.833918629	15.531077749	10.227326471
C62	5.620421427	15.077079965	10.912292948
C63	8.066131778	15.214059664	12.327502881
C64	4.770176787	14.136022935	8.755541422
C65	4.763714453	14.158708991	10.179038445
C66	4.430303361	12.958051530	10.885654217
C67	5.628642643	15.049281574	12.332733903
C68	4.527139436	11.699346647	8.762560463
C69	4.566672359	11.720029944	10.174136907
C70	5.162450179	10.629046290	10.889769437
C71	4.408026351	12.945913905	12.306023009
C72	6.189957856	9.924934893	8.767717899
C73	6.190956850	9.924425640	10.184238901
C74	7.424125247	9.753523660	10.898245991
C75	5.159141342	10.634057856	12.306097508
C76	8.596573222	10.148859798	8.762383066
C77	8.604190948	10.148414546	10.183672745
C78	9.477814933	11.038970122	10.893137767
C79	7.421114759	9.757599148	12.314371162
C80	9.844489934	12.231552078	8.762006804
C81	9.852541469	12.225805780	10.181264764
C82	9.729717762	13.458131382	10.900996736
C83	9.472210664	11.048283125	12.313708027
C84	9.758924062	13.461518818	12.319741579
C85	9.104228948	14.519319090	13.035107884
C86	9.113567259	14.530584687	14.449719731
C87	8.070768336	15.217714542	15.161017074
C88	6.828566305	15.412414423	13.041923047
C89	6.833485691	15.385454564	14.451003217
C90	5.650617504	14.988616008	15.162940214
C91	8.072962914	15.228990480	16.572923129
C92	4.784585356	14.122890742	13.030802027
C93	4.775055830	14.108219431	14.449520787
C94	4.378814444	12.922182158	15.151841995
C95	5.657033337	14.974562206	16.576291100
C96	4.513176001	11.702186400	13.013738916
C97	4.501561420	11.689219051	14.432822710

C98	5.130141457	10.610323898	15.144231907
C99	4.371421750	12.911989610	16.570406903
C100	6.185684482	9.933894789	13.021617734
C101	6.179018214	9.932720871	14.438198836
C102	7.410399523	9.770446686	15.154440723
C103	5.128270567	10.603266492	16.564210581
C104	8.597623989	10.164863744	13.027765376
C105	8.592846558	10.169789936	14.446217249
C106	9.468539669	11.054138328	15.159262564
C107	7.405807923	9.766655302	16.571007846
C108	9.885640974	12.224129598	13.027762192
C109	9.882921503	12.227221744	14.447277500
C110	9.759017104	13.466721795	15.159050168
C111	9.461071618	11.059631221	16.577694703
C112	9.755121742	13.471900184	16.578277428
Ir1	-9.157435164	-9.037547712	6.956835640
Ir2	-8.348712004	-6.785358455	7.826761290
Ir3	-6.714617846	-8.723881767	7.649366949
Ir4	-8.575355881	-8.747719442	9.441490128
C	6.875926040	21.156101372	8.788726233
O	7.333542892	21.539343195	9.790067303

(8, 0)-Ir₄-CO

C1	9.737741784	14.535572210	1.979174910
C2	9.835081855	14.614274332	3.411533539
C3	8.765916355	15.364504097	4.093303636
C4	8.744742861	15.293560557	1.273758128
C5	7.525233863	15.592054193	1.985657650
C6	7.518763602	15.584786519	3.386676421
C7	6.315485856	15.320878993	4.120924916
C8	6.299682421	15.363391011	1.278795045
C9	5.269331351	14.671125601	1.995819354
C10	5.207699277	14.743099660	3.413213185
C11	4.526223995	13.701813700	4.115694390
C12	4.498068539	13.701412195	1.277176973
C13	4.109823188	12.518890432	1.983530044
C14	4.228185635	12.501969557	3.399608176
C15	4.253853237	11.259915771	4.116011451
C16	4.278256405	11.289385082	1.276857430
C17	4.867060357	10.196476661	1.994022230
C18	4.772347686	10.122509280	3.414558116
C19	5.795461385	9.404487459	4.117482939
C20	5.803870022	9.377551451	1.279236026
C21	7.002234490	9.027022813	1.983912424

C22	7.008375663	9.148344491	3.398385374
C23	8.237011580	9.304320827	4.117823464
C24	8.214050414	9.318237974	1.282625551
C25	9.209783530	10.052049303	2.003450427
C26	9.325153000	9.917516697	3.412612256
C27	9.988351477	10.970981403	4.113617732
C28	9.984886938	11.019715729	1.284342042
C29	10.461357942	12.170420521	1.992504299
C30	10.206763015	12.186847197	3.392291737
C31	10.263575994	13.414797485	4.120004404
C32	10.291768412	13.411097747	1.276132170
C33	9.739968577	14.557483512	6.246573178
C34	9.794244087	14.591823108	7.687620755
C35	8.757958689	15.341546332	8.394317406
C36	8.770742521	15.390724923	5.529257852
C37	7.538784028	15.807366778	6.231575645
C38	7.533172910	15.651940328	7.693718424
C39	6.309059251	15.368024082	8.399713497
C40	6.255615189	15.514496578	5.534078037
C41	5.393796297	14.607404915	6.254326700
C42	5.251111297	14.728306331	7.660313077
C43	4.462612072	13.758146055	8.363169124
C44	4.595116982	13.668057748	5.533951527
C45	4.144082395	12.514875461	6.240656269
C46	4.225549364	12.528734979	7.659654951
C47	4.342714634	11.298151952	8.381466868
C48	4.247659682	11.267904673	5.541333457
C49	4.854606855	10.183201174	6.252791122
C50	4.845752172	10.164243561	7.672627803
C51	5.793393075	9.352698627	8.375553998
C52	5.811228418	9.398075791	5.535260491
C53	7.010306050	9.052494031	6.244555628
C54	7.011244463	9.085941624	7.666108056
C55	8.232021325	9.313787769	8.383735090
C56	8.240245982	9.261835914	5.540559073
C57	9.247078537	9.987211269	6.254095746
C58	9.305527583	9.937285365	7.671924537
C59	10.023772119	10.957474243	8.374495095
C60	9.976064320	10.984726070	5.533853166
C61	10.380596577	12.159142456	6.239870488
C62	10.259598127	12.174610432	7.661384774
C63	10.277932741	13.411685228	8.381276586
C64	10.229071576	13.388561652	5.528680466
C65	9.736902546	14.531733390	10.508223727

C66	9.711392301	14.506560692	11.924589272
C67	8.732874685	15.274934793	12.640834643
C68	8.728295960	15.273629668	9.808873972
C69	7.516894062	15.563817141	10.527392799
C70	7.522242252	15.582187365	11.934876242
C71	6.295799035	15.369839767	12.647025951
C72	6.273656744	15.447406824	9.811905190
C73	5.218174021	14.763481878	10.505543925
C74	5.243916643	14.709630404	11.927167897
C75	4.476491656	13.724741003	12.633023085
C76	4.594142607	13.697639455	9.783180987
C77	4.218914223	12.518504133	10.502903258
C78	4.150917775	12.527146925	11.921986422
C79	4.291906486	11.294743833	12.636687010
C80	4.265743105	11.276201434	9.798222008
C81	4.832944851	10.169174433	10.505290074
C82	4.855951680	10.187352806	11.927069313
C83	5.806409933	9.384278522	12.637965271
C84	5.814562540	9.400849366	9.795662124
C85	7.019677675	9.098947424	10.511500057
C86	7.014139182	9.074006865	11.930364004
C87	8.232677789	9.303952948	12.642712978
C88	8.249340050	9.281912883	9.803560274
C89	9.307933847	9.942478202	10.510628266
C90	9.275451169	9.986016302	11.932761282
C91	10.017023247	10.986575525	12.642813186
C92	9.999500323	10.972650397	9.796599122
C93	10.329319024	12.169656398	10.507794155
C94	10.384341487	12.166982659	11.926400997
C95	10.297331184	13.407348640	12.635983552
C96	10.298643547	13.413280636	9.795673054
Ir1	-3.982890794	-7.494863872	5.643709274
Ir2	-4.254671235	-9.753627359	6.776828291
Ir3	-4.660763062	-9.509216300	4.262084472
Ir4	-6.303704575	-8.523579826	5.939237924
C	12.123708248	20.143271404	6.525173796
O	12.495065257	20.440388091	7.577242197

(10, 0)-Ir₄-CO

C1	10.710522138	15.109361146	1.332186627
C2	10.708169640	15.112827722	2.749635708
C3	9.804745500	15.967668065	3.447586048
C4	9.804024833	15.955082223	0.626205406
C5	8.674518163	16.472393744	1.330315267

C6	8.675564083	16.481709593	2.742309150
C7	7.442674671	16.610966554	3.453678066
C8	7.439926039	16.596960921	0.626715723
C9	6.231869937	16.320267466	1.335673466
C10	6.234171241	16.322071331	2.751639478
C11	5.179581972	15.675341603	3.462953174
C12	5.171064145	15.678709910	0.630223328
C13	4.354708607	14.749385796	1.337594859
C14	4.359598377	14.747422292	2.758745022
C15	3.855432083	13.615708565	3.467099689
C16	3.849924537	13.619207360	0.628688368
C17	3.709647319	12.389257734	1.336755686
C18	3.710744471	12.387634660	2.758394917
C19	3.948310887	11.171750519	3.467276826
C20	3.948217496	11.174662521	0.627726539
C21	4.554046009	10.092817620	1.336505557
C22	4.553915346	10.090723223	2.758410533
C23	5.467491474	9.254733927	3.466689891
C24	5.468268903	9.257560420	0.629036915
C25	6.597653448	8.748181695	1.337497925
C26	6.597760662	8.746635664	2.759140937
C27	7.829393780	8.617310565	3.468162317
C28	7.829789597	8.619322419	0.629426199
C29	9.039372433	8.883735169	1.338500603
C30	9.039698218	8.883359410	2.759819253
C31	10.103363283	9.518978622	3.468760235
C32	10.104250583	9.518464071	0.630254937
C33	10.920991748	10.448018576	1.338350902
C34	10.920063219	10.449957563	2.760937837
C35	11.412839838	11.585016819	3.468308492
C36	11.418999762	11.580789462	0.629955799
C37	11.552012779	12.811575070	1.337927846
C38	11.547583081	12.814698040	2.758024058
C39	11.300919690	14.029535424	3.462364967
C40	11.310869948	14.024981177	0.628127587
C41	10.694884455	15.121670145	5.580383470
C42	10.691151977	15.121398997	7.002482336
C43	9.849128141	16.034608821	7.697014029
C44	9.808627557	15.990660136	4.861227192
C45	8.696526861	16.555375351	5.552733996
C46	8.754157330	16.684220713	6.978943879
C47	7.398194940	16.765880836	7.722657249
C48	7.447606923	16.640560812	4.866457381
C49	6.231194877	16.345588500	5.586322946

C50	6.214853714	16.350722354	7.000891689
C51	5.192422593	15.670981875	7.716721597
C52	5.185464428	15.676636125	4.883790383
C53	4.369504027	14.744583489	5.594323006
C54	4.373703371	14.740739732	7.014922876
C55	3.864101308	13.613658199	7.725252414
C56	3.858761312	13.614694936	4.887969824
C57	3.713503666	12.386182858	5.596851857
C58	3.714066035	12.385363368	7.018315227
C59	3.948219401	11.169409676	7.727747103
C60	3.948302195	11.170211513	4.888152150
C61	4.553065512	10.088187098	5.597204805
C62	4.553088606	10.087035385	7.019115516
C63	5.467316328	9.251802589	7.727287613
C64	5.467443281	9.253070619	4.889262717
C65	6.597313563	8.743976704	5.597753072
C66	6.597614686	8.742870435	7.019283107
C67	7.829740315	8.612852679	7.728103492
C68	7.829794530	8.615732294	4.889247942
C69	9.039946817	8.879948357	5.598341373
C70	9.040655514	8.877923509	7.019360609
C71	10.105596210	9.513289490	7.728335453
C72	10.104126227	9.518009562	4.890203333
C73	10.918179383	10.450181776	5.598354331
C74	10.919651115	10.448707114	7.020655060
C75	11.407637407	11.585960309	7.728220867
C76	11.409157695	11.588096625	4.890613922
C77	11.532192052	12.819976509	5.597376729
C78	11.528924451	12.821290299	7.019107558
C79	11.281056284	14.033575326	7.724399563
C80	11.289699811	14.034162417	4.883383651
C81	10.735644461	15.119785150	9.874603751
C82	10.720098952	15.122553357	11.294491655
C83	9.834680621	16.000884502	12.017949687
C84	9.909253349	16.064892272	9.176691933
C85	8.736847793	16.594071315	9.858838371
C86	8.709705544	16.596533074	11.353910794
C87	7.448850274	16.663243419	12.030508226
C88	7.421701090	16.684569476	9.160757014
C89	6.243214189	16.325217270	9.860225303
C90	6.251303839	16.335727968	11.292988811
C91	5.194941656	15.682714924	11.990483768
C92	5.193765099	15.671720085	9.144277331
C93	4.377667576	14.745575953	9.853576075

C94	4.377813550	14.749831547	11.277873725
C95	3.865234662	13.622316118	11.984955475
C96	3.864195621	13.615321460	9.147404592
C97	3.715588896	12.388367251	9.856438913
C98	3.717010241	12.391131876	11.277687859
C99	3.951332440	11.175412978	11.986884363
C100	3.948703181	11.170291696	9.148436731
C101	4.553729310	10.088852372	9.857482188
C102	4.554592140	10.090917556	11.279022109
C103	5.468301816	9.255407513	11.987169087
C104	5.467717951	9.252118942	9.149712328
C105	6.597628437	8.743196056	9.857926744
C106	6.597880312	8.744374124	11.279390689
C107	7.829624814	8.614757769	11.988232944
C108	7.830112961	8.612517907	9.149204307
C109	9.040644252	8.876190634	9.858030616
C110	9.040561596	8.877509693	11.279331163
C111	10.104670103	9.513303575	11.988199887
C112	10.106029331	9.512124935	9.149315826
C113	10.919879931	10.445463901	9.857344887
C114	10.920096327	10.445380062	11.279931380
C115	11.411624988	11.580490079	11.988330184
C116	11.407596904	11.584591202	9.150049967
C117	11.532917189	12.815080474	9.859436080
C118	11.537128575	12.812816096	11.280744770
C119	11.294394908	14.025161415	11.994779080
C120	11.288834546	14.031922730	9.152669510
C121	10.712881460	15.111712741	14.127557051
C122	10.712219216	15.109814427	15.544669917
C123	9.806056636	15.956794438	16.252043874
C124	9.818952239	15.977980970	13.428139671
C125	8.682126071	16.497137937	14.139095834
C126	8.678032216	16.479573567	15.549238867
C127	7.440522003	16.599841889	16.254734996
C128	7.442742297	16.631149643	13.436818029
C129	6.234755435	16.332453687	14.132087440
C130	6.231663486	16.324790693	15.547517927
C131	5.171109400	15.681328147	16.250647583
C132	5.181618119	15.686817379	13.414545382
C133	4.360262274	14.756231314	14.117377306
C134	4.354187624	14.754284773	15.539701404
C135	3.850064423	13.621485187	16.246590599
C136	3.859120716	13.622942838	13.407796447
C137	3.713081478	12.393649981	14.115672752

C138	3.710328119	12.392185032	15.537570729
C139	3.948657456	11.176249708	16.246368593
C140	3.951280891	11.176551814	13.407718264
C141	4.555249564	10.094675459	14.116591145
C142	4.555049883	10.094630324	15.538428977
C143	5.468255466	9.258491092	16.246532544
C144	5.468710053	9.257114424	13.409394050
C145	6.597854679	8.747881146	14.117725186
C146	6.598008440	8.748683866	15.539266262
C147	7.829336236	8.619211495	16.248255084
C148	7.829779611	8.616601663	13.409403868
C149	9.039451530	8.880885370	14.118490523
C150	9.039612678	8.882507653	15.539750030
C151	10.103926043	9.517436048	16.248685108
C152	10.104523647	9.514683445	13.409615594
C153	10.920394364	10.445293985	14.117948499
C154	10.921270103	10.446186354	15.540423833
C155	11.418775102	11.579430630	16.248461968
C156	11.414318225	11.579612599	13.410072394
C157	11.546444115	12.809864648	14.120203677
C158	11.551276923	12.809745843	15.539892557
C159	11.310728859	14.023867184	16.248895119
C160	11.301462508	14.024601665	13.415720166
Ir1	-5.297942047	-6.069366035	8.818583490
Ir2	-4.498921477	-8.491016357	8.433117440
Ir3	-6.800621899	-7.761686977	7.606166652
Ir4	-6.377366251	-7.956988548	10.091525738
O	10.433975299	21.903469800	7.062618270
C	10.231231759	21.360668676	8.076418028

(7, 7)-Ir₄-CO

C1	11.590329419	14.753524059	0.463910784
C2	7.963404381	16.774878731	0.455830018
C3	10.615724438	15.802901283	0.461147722
C4	10.033057299	16.213530702	1.685983661
C5	6.539332156	16.571371949	0.463675623
C6	5.870632261	16.298716652	1.688640998
C7	8.690643289	16.713531920	1.668705291
C8	4.201514112	14.963843430	0.467776667
C9	4.690708236	15.480894294	1.694500271
C10	3.087413536	10.942104317	0.466605667
C11	3.446319269	13.745213205	0.466748702
C12	3.203197767	13.072662170	1.695632057
C13	3.533864534	9.581402350	0.466687353

C14	3.901011575	8.970562701	1.696535042
C15	3.020975488	11.652299696	1.696048228
C16	5.500943218	7.561022655	0.466624327
C17	4.898761934	7.943224126	1.696399435
C18	9.650347633	7.444681434	0.466118536
C19	6.852591822	7.088117898	0.466432442
C20	7.561666933	7.013837001	1.696118704
C21	10.846226988	8.233727194	0.465926338
C22	11.341554198	8.745093364	1.695643781
C23	8.982539965	7.195264546	1.695916985
C24	12.315565051	10.644442075	0.466329464
C25	12.084388777	9.969303865	1.695436349
C26	12.477428083	12.067855896	0.466489473
C27	12.396291935	12.777985509	1.695204315
C28	11.946483384	14.138639866	1.694786154
C29	11.582713737	14.753070594	2.925592697
C30	7.969795065	16.833866056	2.894984303
C31	10.629214045	15.819617710	2.927403967
C32	10.085408106	16.269918203	4.160690505
C33	6.531528999	16.575805370	2.915479833
C34	5.868642246	16.290056160	4.151760092
C35	8.733105810	16.853436642	4.147777485
C36	4.195966207	14.959871724	2.924460640
C37	4.686187142	15.464302339	4.154164923
C38	3.085116727	10.942462158	2.925985775
C39	3.440968473	13.743448243	2.925276329
C40	3.199054258	13.072378090	4.155577647
C41	3.532815994	9.581963032	2.926103573
C42	3.900643844	8.970948996	4.155901846
C43	3.017952796	11.652102414	4.155910598
C44	5.501012909	7.561325563	2.926119969
C45	4.898701540	7.943739554	4.155803493
C46	9.650648054	7.443916046	2.925656859
C47	6.852616786	7.088221528	2.925944769
C48	7.561823988	7.014169321	4.155685916
C49	10.846357625	8.232982704	2.925465724
C50	11.341763928	8.745159840	4.155204619
C51	8.982629070	7.195470097	4.155603417
C52	12.310927655	10.644774800	2.924725369
C53	12.083799251	9.969585971	4.154827878
C54	12.468063663	12.067792621	2.923796818
C55	12.392570368	12.775457990	4.154332414
C56	11.943487537	14.132666031	4.154280117
C57	11.587397048	14.745654839	5.385277405

C58	7.956765589	16.958212192	5.419138101
C59	10.627435089	15.803242508	5.388249001
C60	10.033470859	16.187627082	6.618697078
C61	6.526766310	16.574543251	5.390871421
C62	5.877569552	16.272440989	6.630703663
C63	8.720987740	16.786393663	6.636956176
C64	4.203005184	14.953446261	5.383990691
C65	4.706193899	15.463668926	6.620566073
C66	3.084560022	10.942051566	5.386067384
C67	3.441690276	13.742316936	5.386188758
C68	3.201910921	13.071909018	6.616606628
C69	3.532779627	9.581977511	5.385760628
C70	3.901060846	8.970649857	6.615372056
C71	3.019654555	11.651683433	6.616043393
C72	5.501057431	7.561525389	5.385450872
C73	4.898772265	7.943554442	6.615241222
C74	9.650750290	7.444710237	5.385381641
C75	6.852596022	7.088562661	5.385412880
C76	7.561762667	7.014372322	6.615120863
C77	10.846688468	8.233475994	5.385350781
C78	11.342588718	8.745702396	6.614908675
C79	8.982524244	7.196078611	6.615074486
C80	12.314558921	10.644093885	5.384718034
C81	12.087941481	9.968925759	6.614814118
C82	12.474318355	12.066686242	5.384403525
C83	12.405221053	12.775233009	6.614734397
C84	11.953127184	14.132143540	6.615093688
C85	11.590630990	14.746090547	7.844460499
C86	7.964801387	16.851697492	7.854860824
C87	10.606245610	15.785097720	7.840913596
C88	10.014746407	16.198151881	9.072638292
C89	6.539457695	16.571985480	7.849404703
C90	5.878721108	16.295488766	9.074082467
C91	8.682010594	16.719549701	9.077504824
C92	4.206117666	14.955343759	7.848977065
C93	4.699646580	15.477590611	9.074822763
C94	3.086876530	10.942014743	7.845718669
C95	3.445696087	13.742706350	7.846847192
C96	3.205581139	13.072662936	9.076144236
C97	3.533788386	9.581596192	7.845334726
C98	3.901467728	8.970501920	9.074954142
C99	3.022163189	11.651614631	9.075499081
C100	5.500980105	7.561177413	7.844935339
C101	4.898942747	7.943036334	9.074810945

C102	9.650500259	7.445331359	7.844715516
C103	6.852584296	7.088398616	7.844834152
C104	7.561579773	7.014290674	9.074573447
C105	10.846624172	8.234266061	7.844602172
C106	11.342076455	8.746042502	9.074455956
C107	8.982390238	7.196193865	9.074403392
C108	12.318977607	10.643540239	7.844747014
C109	12.087600131	9.969166975	9.074572005
C110	12.482689188	12.066640756	7.845273873
C111	12.408211469	12.776509521	9.074590411
C112	11.956462517	14.136489428	9.074239373
Ir1	-8.857427702	-7.452799890	4.443087671
Ir2	-7.608732417	-5.232529924	4.568076085
Ir3	-6.470473238	-7.266728677	3.558838782
Ir4	-6.926720743	-7.170770088	6.093003501
C	7.902741629	22.665907041	5.461305440
O	8.302520241	23.234425436	6.408990101

(8, 8)-Ir₄-COC1 12.187380427 16.220662542 0.812333786

C2	11.075987796	17.132437342	0.812971209
C3	10.450801602	17.489096733	2.032249475
C4	12.635927286	15.666354751	2.043742996
C5	8.333481478	17.753892838	0.813661806
C6	9.051051054	17.805289914	2.032291585
C7	4.640136210	15.742889364	0.810292430
C8	6.936446607	17.412562489	0.812892855
C9	6.292968406	17.106658708	2.043787489
C10	3.829251622	14.559898309	0.807909575
C11	3.531510680	13.911279320	2.036996941
C12	5.136218455	16.257271729	2.040412708
C13	3.136984936	11.808965878	0.805492695
C14	3.183168711	12.520308375	2.035379442
C15	4.706966347	7.929107765	0.802927556
C16	3.311122242	10.386964746	0.804162165
C17	3.531201331	9.709207441	2.033702977
C18	5.854663027	7.072638610	0.802481780
C19	6.499225378	6.772657837	2.032166610
C20	4.234935501	8.462072067	2.032825636
C21	8.605442521	6.445358508	0.802436366
C22	7.895367087	6.455395192	2.032136187
C23	12.339407638	8.328461370	0.803973304
C24	10.010121395	6.723737721	0.802818685
C25	10.663969419	7.004346224	2.032703460
C26	13.128039631	9.525127953	0.805254867

C27	13.404325061	10.182786227	2.035112554
C28	11.842893059	7.818318840	2.033520869
C29	13.727031796	12.297139732	0.807578523
C30	13.706280926	11.584250814	2.036658635
C31	13.521851322	13.715959802	0.809959002
C32	13.303232006	14.397028718	2.040173069
C33	12.203690125	16.237734552	3.270557595
C34	11.147397988	17.233699562	3.266549390
C35	10.495019904	17.566640457	4.510044110
C36	12.617033395	15.651615114	4.492522465
C37	8.312327191	17.876810150	3.267799977
C38	9.042258566	17.895570453	4.510939664
C39	4.635594498	15.745005268	3.267837058
C40	6.928850636	17.433061423	3.271006306
C41	6.301186358	17.087826247	4.493316894
C42	3.826047932	14.561767196	3.266729876
C43	3.531509708	13.911380726	4.496629792
C44	5.140057714	16.253386214	4.496261376
C45	3.136689647	11.809318582	3.264880900
C46	3.183566696	12.520842487	4.494912720
C47	4.707127765	7.929178439	3.262412613
C48	3.311168354	10.387305103	3.263632071
C49	3.531174545	9.709091725	4.493061854
C50	5.854696231	7.072723422	3.261971354
C51	6.499355739	6.772685946	4.491699084
C52	4.234940513	8.462280054	4.492277708
C53	8.605445540	6.445447720	3.261928143
C54	7.895260041	6.455478469	4.491667508
C55	12.339583688	8.328715320	3.263415800
C56	10.010016508	6.723854853	3.262304819
C57	10.664086872	7.004524650	4.492145305
C58	13.128668317	9.525188857	3.264580263
C59	13.404455582	10.183257445	4.494578637
C60	11.842903724	7.818141726	4.492849043
C61	13.731516481	12.297244745	3.266359985
C62	13.706521654	11.584010698	4.496197407
C63	13.528171012	13.715836628	3.267468358
C64	13.295443942	14.394160382	4.495902248
C65	12.150515200	16.190723647	5.732740488
C66	11.095150419	17.126669641	5.738886907
C67	10.502534204	17.589604195	6.967842537
C68	12.612283760	15.649033351	6.965365158
C69	8.310349209	17.758418723	5.739183742
C70	9.042764371	17.922126157	6.967758532

C71	4.641819846	15.741954575	5.728484795
C72	6.952194582	17.376256278	5.733116183
C73	6.303435063	17.085201342	6.966043079
C74	3.830581548	14.560073010	5.726445638
C75	3.533552440	13.910245146	6.955861158
C76	5.138785486	16.251492838	6.960651826
C77	3.136919280	11.808996274	5.724137817
C78	3.183903915	12.520226778	6.954290521
C79	4.707019601	7.929141289	5.721912351
C80	3.311161771	10.387277525	5.723018887
C81	3.531006135	9.709145712	6.952585384
C82	5.854667833	7.072730216	5.721487790
C83	6.499227385	6.772693667	6.951163558
C84	4.234836538	8.462058625	6.951756831
C85	8.605488416	6.445446103	5.721436714
C86	7.895390772	6.455424782	6.951128137
C87	12.339647558	8.328661951	5.722790218
C88	10.010108654	6.723767674	5.721791529
C89	10.664083885	7.004290537	6.951626042
C90	13.128399915	9.524871861	5.723834334
C91	13.403843611	10.182792005	6.953999062
C92	11.843095489	7.818147850	6.952389357
C93	13.726137593	12.297409562	5.726012239
C94	13.704048271	11.583891773	6.955513437
C95	13.519069867	13.715090824	5.727894857
C96	13.295135243	14.391449818	6.960036149
C97	12.172310498	16.216407075	8.192240224
C98	11.097305090	17.162706723	8.200894599
C99	10.445470367	17.460124818	9.422815919
C100	12.621353953	15.656752153	9.423424793
C101	8.324955600	17.790893724	8.201942916
C102	9.041746746	17.776808327	9.422720294
C103	4.639486833	15.742026391	8.189347050
C104	6.944513260	17.404910140	8.193217447
C105	6.300042956	17.093926686	9.424176668
C106	3.829055832	14.558966340	8.186659837
C107	3.533179044	13.910227333	9.415712042
C108	5.137983787	16.253466686	9.419510450
C109	3.136984812	11.808990776	8.183855459
C110	3.183699970	12.519884274	9.413994286
C111	4.706958336	7.929142159	8.181378408
C112	3.310954427	10.386962774	8.182579353
C113	3.531011278	9.709007120	9.412168213
C114	5.854673862	7.072690916	8.180947761

C115	6.499288311	6.772668659	9.410661952
C116	4.234779627	8.462028491	9.411305245
C117	8.605461993	6.445413454	8.180899400
C118	7.895320663	6.455435451	9.410627779
C119	12.339618284	8.328321084	8.182388332
C120	10.010163129	6.723766310	8.181262938
C121	10.664095005	7.004263917	9.411182320
C122	13.128226389	9.525027958	8.183613404
C123	13.403576657	10.182619087	9.413746564
C124	11.842968901	7.818071436	9.411990087
C125	13.726959169	12.295840739	8.186322624
C126	13.704040798	11.583962725	9.415414907
C127	13.521544189	13.714406795	8.188867845
C128	13.297998229	14.393726146	9.418859762
Ir1	-4.309438659	-4.141531520	5.083419197
Ir2	-3.543927730	-6.470845381	4.320343793
Ir3	-6.002580513	-5.925137995	4.320358024
Ir4	-4.768867080	-6.171803007	6.555408702
C129	10.829882160	23.855618213	5.634622351
O1	10.842607442	24.656009269	6.496680536

(10, 10)-Ir₄-CO

C1	12.027798213	15.459162463	0.220791193
C2	10.911564728	16.346287942	0.219459454
C3	10.310675187	16.724436749	1.445903606
C4	12.510187383	14.943350917	1.449870233
C5	8.250501719	17.324314368	0.209015583
C6	8.970012185	17.260497418	1.432792035
C7	4.166582202	16.302782563	0.211717667
C8	6.827261731	17.285483458	0.211560349
C9	6.124588067	17.146779194	1.441411151
C10	3.022906936	15.442267447	0.212522214
C11	2.523837271	14.937584382	1.442809239
C12	4.787284757	16.645391374	1.441683131
C13	1.345792405	13.154315745	0.213633628
C14	1.677967157	13.782991814	1.443304319
C15	0.815263047	8.968885492	0.214703982
C16	0.876388365	11.803391661	0.214043152
C17	0.748895379	11.103534091	1.443867245
C18	1.234152973	7.600652977	0.215095618
C19	1.547003597	6.962609060	1.444952709
C20	0.717775765	9.673606377	1.444312286
C21	2.868268069	5.284254258	0.215720071
C22	2.371095405	5.791945109	1.445355903

C23	6.705123808	3.530023031	0.216753184
C24	4.017979867	4.432218339	0.216135868
C25	4.647602401	4.102102511	1.445996859
C26	8.135210025	3.527380687	0.217171087
C27	8.837487192	3.641363932	1.447027279
C28	6.003326603	3.646641936	1.446389991
C29	10.826008189	4.419085587	0.217764536
C30	10.195025199	4.091631459	1.447407959
C31	13.633099713	7.569546349	0.218838124
C32	11.979840301	5.265825609	0.218148540
C33	12.479664656	5.770843740	1.448027640
C34	14.072005362	8.931048524	0.219273213
C35	14.181651663	9.633717806	1.449425498
C36	13.312964471	6.934774865	1.448411167
C37	14.071842808	11.765896377	0.220242297
C38	14.179521223	11.063679372	1.450239061
C39	13.639138017	13.129230238	0.220838960
C40	13.321267976	13.765716134	1.450464179
C41	12.028978179	15.477255401	2.677081886
C42	10.945368366	16.399553876	2.664211158
C43	10.397032441	16.902442602	3.903813064
C44	12.524332638	14.963099765	3.913688487
C45	8.241383849	17.411126059	2.645884651
C46	9.004467464	17.455880919	3.871863321
C47	4.170825061	16.297594840	2.674076110
C48	6.816275504	17.302649917	2.665423449
C49	6.133684078	17.147638654	3.909368717
C50	3.025063086	15.440964726	2.673516421
C51	2.523694237	14.936001379	3.902423587
C52	4.798498364	16.634396597	3.904398321
C53	1.345425807	13.154184914	2.673069689
C54	1.677260677	13.782692665	3.902871501
C55	0.815376927	8.968929314	2.674189854
C56	0.876156792	11.803365618	2.673509830
C57	0.748274501	11.103463004	3.903405253
C58	1.234320713	7.600748676	2.674597381
C59	1.547061667	6.962649018	3.904456973
C60	0.717571332	9.673616258	3.903823175
C61	2.868348269	5.284335735	2.675230310
C62	2.371177155	5.792047487	3.904857641
C63	6.705134303	3.530066080	2.676252375
C64	4.018026386	4.432273336	2.675642016
C65	4.647641267	4.102166264	3.905499128
C66	8.135225079	3.527416285	2.676667639

C67	8.837482218	3.641404314	3.906532220
C68	6.003345969	3.646709689	3.905887838
C69	10.826008370	4.419029622	2.677271151
C70	10.195011606	4.091649286	3.906926948
C71	13.632827887	7.569255727	2.678367929
C72	11.979864332	5.265691399	2.677669628
C73	12.479634585	5.770746384	3.907595632
C74	14.070882834	8.930774835	2.678840533
C75	14.180929117	9.633835800	3.908620496
C76	13.312917221	6.934626565	3.908043949
C77	14.065617286	11.766570882	2.680127256
C78	14.178185531	11.063750728	3.908931777
C79	13.630906396	13.129488640	2.681170173
C80	13.320783820	13.771664461	3.910381369
C81	12.070030944	15.501650347	5.141222776
C82	11.001251285	16.478787252	5.150769080
C83	10.336639599	16.756032908	6.389869722
C84	12.530108375	14.958151071	6.368349509
C85	8.262004050	17.541362011	5.143105095
C86	9.003307467	17.330088719	6.380635944
C87	4.172887937	16.292256852	5.131977290
C88	6.821296121	17.320425018	5.132511634
C89	6.135165861	17.143975081	6.356523402
C90	3.025725905	15.439424526	5.132244416
C91	2.524114820	14.935781557	6.362065173
C92	4.799002017	16.634341758	6.360308736
C93	1.344555448	13.154225026	5.132704863
C94	1.677047841	13.782487763	6.362304956
C95	0.815083808	8.968860562	5.133682921
C96	0.875436408	11.803259730	5.133049198
C97	0.748094590	11.103425661	6.362908605
C98	1.234208293	7.600737486	5.134085717
C99	1.546928920	6.962615924	6.363955218
C100	0.717307316	9.673520039	6.363331772
C101	2.868375269	5.284376281	5.134731247
C102	2.371111422	5.792012519	6.364356317
C103	6.705146388	3.530111230	5.135756242
C104	4.018044436	4.432334957	5.135141446
C105	4.647632127	4.102171432	6.365002925
C106	8.135211168	3.527459697	5.136175381
C107	8.837469753	3.641403128	6.366051773
C108	6.003337722	3.646704298	6.365395478
C109	10.825981902	4.419057768	5.136812542
C110	10.194990450	4.091668599	6.366453703

C111	13.632934808	7.569322380	5.137851300
C112	11.979808965	5.265735325	5.137248436
C113	12.479605676	5.770935172	6.367107453
C114	14.071326383	8.930966138	5.138231690
C115	14.182455576	9.634021103	6.367736024
C116	13.312946506	6.934867050	6.367518065
C117	14.069009605	11.767671375	5.138400593
C118	14.181732079	11.064292156	6.367740227
C119	13.637439354	13.131765689	5.138393251
C120	13.328773350	13.770262028	6.368410236
C121	12.042607981	15.468570743	7.602231923
C122	10.923462447	16.361648981	7.606940519
C123	10.297722845	16.704073048	8.832766742
C124	12.520585755	14.944567329	8.826657544
C125	8.258361827	17.357960733	7.610112105
C126	8.958756527	17.202761941	8.828129555
C127	4.171653412	16.296314839	7.589636701
C128	6.829194335	17.293940400	7.594723364
C129	6.129231394	17.144090067	8.817268812
C130	3.025486045	15.440296651	7.590814389
C131	2.523548758	14.937044881	8.821298882
C132	4.790973433	16.644314561	8.819522215
C133	1.345182188	13.153992143	7.592226602
C134	1.677809479	13.782738088	8.821720892
C135	0.815029548	8.968850199	7.593218904
C136	0.875779245	11.803229447	7.592604425
C137	0.748529077	11.103458120	8.822479402
C138	1.234063357	7.600660241	7.593606842
C139	1.546831145	6.962521385	8.823456959
C140	0.717517261	9.673578581	8.822873924
C141	2.868284715	5.284303593	7.594226657
C142	2.371020181	5.791916062	8.823853809
C143	6.705120795	3.530056567	7.595257706
C144	4.018003644	4.432265174	7.594641979
C145	4.647589349	4.102086433	8.824495140
C146	8.135209071	3.527403718	7.595678278
C147	8.837474299	3.641361118	8.825536831
C148	6.003318509	3.646636732	8.824890308
C149	10.825979121	4.419114539	7.596301949
C150	10.194998149	4.091664652	8.825928067
C151	13.633063740	7.569703230	7.597262775
C152	11.979794464	5.265861690	7.596719802
C153	12.479633518	5.771062418	8.826540103
C154	14.072190765	8.931195121	7.597545747

C155	14.183263647	9.633813774	8.827567878
C156	13.312969208	6.935055517	8.826911478
C157	14.072731297	11.766706473	7.597708895
C158	14.183242966	11.063871542	8.828091769
C159	13.641310499	13.129827540	7.597574850
C160	13.330958374	13.766855905	8.828309843
Ir1	-8.179211326	-10.875491789	3.124116354
Ir2	-6.897131074	-9.077745201	4.676741899
Ir3	-6.176594082	-11.549120833	4.624053874
Ir4	-8.339436284	-10.892295215	5.767790979
C	11.692424637	22.221076368	5.781632050
O	12.417621991	22.776655012	6.514229212

(7, 0)-Ir₄-NO

C1	9.097250288	14.528686287	0.247574021
C2	9.074379459	14.521498757	1.663829456
C3	8.049382657	15.239872728	2.370984984
C4	6.817503530	15.379292994	0.246730921
C5	6.814128499	15.392990234	1.657268169
C6	5.642809427	14.968017352	2.371983161
C7	8.035986092	15.237728918	3.784281905
C8	4.765712510	14.089022117	0.243438964
C9	4.764917639	14.084360636	1.662099514
C10	4.355403450	12.907250281	2.369774115
C11	5.622861411	15.006699700	3.787099718
C12	4.488142202	11.671037120	0.241948630
C13	4.495276336	11.670806600	1.661473750
C14	5.147830691	10.608585077	2.376491632
C15	4.372059153	12.909359845	3.789301657
C16	6.185223709	9.935093404	0.245791045
C17	6.180671757	9.916773269	1.663926648
C18	7.415396987	9.752075755	2.377255439
C19	5.154441268	10.608128215	3.795822805
C20	8.603418893	10.151189425	0.248657344
C21	8.592001707	10.166716429	1.667318742
C22	9.469950081	11.046325078	2.381131072
C23	7.418475851	9.733033935	3.794713377
C24	9.865819046	12.223601710	0.256968170
C25	9.883165473	12.224806209	1.676288118
C26	9.709900247	13.459738412	2.383810363
C27	9.447155390	11.055464443	3.799188354
C28	9.718415302	13.480015464	3.803649277
C29	9.097730106	14.567707234	4.505989826
C30	9.078973849	14.553592618	5.918317874

C31	8.107667504	15.372781708	6.619004239
C32	6.799852575	15.436818509	4.484406683
C33	6.788941972	15.542719884	5.923460680
C34	5.594082484	15.006726064	6.600618842
C35	8.115325147	15.373392288	8.070902421
C36	4.751461204	14.095508831	4.492020054
C37	4.754430828	14.075159783	5.901033607
C38	4.375872038	12.915693170	6.630612255
C39	5.589129221	15.100671989	8.031292388
C40	4.518623580	11.676452845	4.509554884
C41	4.527565737	11.677838014	5.928968998
C42	5.172469715	10.613512568	6.645380646
C43	4.489466653	12.943974845	8.052443938
C44	6.186059201	9.909186438	4.508850683
C45	6.184280301	9.897849453	5.928928145
C46	7.420255595	9.734689264	6.639184209
C47	5.146882650	10.583687263	8.066062209
C48	8.596057522	10.145402172	4.505296464
C49	8.591123137	10.159525906	5.924731139
C50	9.463685712	11.044135392	6.636764855
C51	7.417273521	9.740446873	8.054006714
C52	9.818853805	12.241149120	4.515230149
C53	9.851167132	12.232985679	5.931928630
C54	9.652848547	13.459396301	6.639011398
C55	9.450894291	11.048045467	8.057088828
C56	9.684908781	13.467774458	8.061877442
C57	9.094514896	14.546659993	8.783348648
C58	9.058246412	14.489407998	10.195326874
C59	8.079395796	15.237414171	10.936008870
C60	6.813747106	15.510896872	8.793398909
C61	6.839113363	15.553061866	10.241392965
C62	5.625562221	15.073119830	10.911439048
C63	8.089804772	15.258694163	12.338106724
C64	4.733624634	14.165064269	8.757396663
C65	4.876888681	14.081124202	10.163446267
C66	4.411567546	12.929946849	10.880787005
C67	5.645243943	15.000846125	12.324609268
C68	4.626504501	11.714305845	8.777927695
C69	4.470246589	11.676106316	10.185166579
C70	5.170921028	10.645806260	10.899541193
C71	4.386907370	12.935139183	12.305311907
C72	6.180115503	9.884296473	8.768636222
C73	6.200647026	9.948303898	10.185562951
C74	7.426696757	9.736088197	10.898905123

C75	5.150379293	10.622420135	12.315419378
C76	8.595949309	10.147690675	8.768048448
C77	8.598096188	10.156291933	10.187331084
C78	9.460586427	11.051722677	10.902602084
C79	7.424023490	9.775204229	12.313861733
C80	9.830452696	12.232125334	8.771339230
C81	9.896484718	12.219382521	10.190307500
C82	9.753287307	13.455007178	10.900740093
C83	9.504187579	11.019545029	12.322863285
C84	9.696698439	13.438191615	12.318208924
C85	9.113503622	14.534196485	13.035759905
C86	9.088776828	14.510079558	14.450991919
C87	8.061459385	15.220192153	15.162954113
C88	6.836195281	15.368365859	13.047912848
C89	6.826226182	15.405732863	14.453834534
C90	5.651616349	14.972032742	15.162690762
C91	8.053656090	15.206875725	16.573708146
C92	4.750357318	14.122134460	13.022268965
C93	4.783977828	14.086404153	14.442089062
C94	4.345158211	12.919051353	15.149465343
C95	5.634484903	14.985072724	16.575894369
C96	4.523457028	11.700817661	13.021748499
C97	4.487897002	11.683728174	14.440349171
C98	5.155730255	10.631028055	15.153916712
C99	4.368576237	12.911344216	16.570430299
C100	6.189292419	9.935791910	13.026425584
C101	6.189897369	9.936077075	14.443835348
C102	7.420878859	9.753794420	15.157138895
C103	5.136329997	10.607895469	16.572273361
C104	8.612257929	10.148345329	13.030150834
C105	8.601602941	10.158693523	14.449075752
C106	9.479193161	11.039735678	15.164125965
C107	7.418838421	9.768191414	16.574454948
C108	9.868835158	12.210914904	13.034191525
C109	9.891055951	12.214021845	14.453477846
C110	9.740245162	13.451437394	15.162916187
C111	9.479674455	11.039247470	16.583925900
C112	9.743264694	13.459128453	16.582350893
Ir1	-9.191159504	-8.986763728	6.952488380
Ir2	-8.357389650	-6.704096644	7.765770572
Ir3	-6.718884700	-8.647879067	7.567091613
Ir4	-8.529496660	-8.648551070	9.427406482
N	6.909413572	21.222990320	8.651498622
O	7.402310520	21.599637133	9.654411099

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C1	9.739822345	14.407007277	1.978385121
C2	9.825219203	14.491677517	3.405800076
C3	8.723863303	15.218326004	4.095288463
C4	8.703585387	15.100798813	1.272675076
C5	7.486169313	15.395496141	1.991547085
C6	7.470884240	15.425753939	3.392631139
C7	6.233571833	15.334985346	4.113085594
C8	6.252605143	15.275435732	1.275525017
C9	5.122821112	14.748224946	1.986280126
C10	5.096179920	14.781151244	3.411366807
C11	4.374979943	13.751758702	4.116891021
C12	4.363537254	13.760367114	1.282554095
C13	4.021590930	12.563639599	1.989961673
C14	3.973776684	12.570680530	3.414195417
C15	4.188170473	11.343405989	4.118438155
C16	4.194204910	11.330418506	1.280186893
C17	4.811252122	10.251391589	1.987931010
C18	4.845406607	10.285417699	3.411729211
C19	5.850835050	9.552604380	4.128636661
C20	5.836983106	9.542182423	1.278453592
C21	7.044782074	9.251607055	1.994463169
C22	7.046510086	9.217743048	3.413313605
C23	8.274739289	9.391903082	4.115652583
C24	8.274077062	9.413938271	1.281348876
C25	9.395663019	9.956575062	1.985142523
C26	9.392669178	9.943739242	3.404727380
C27	10.143775759	10.937566584	4.118019015
C28	10.159107871	10.942074699	1.286307847
C29	10.640196418	12.103785114	1.985280214
C30	10.628650121	12.098964914	3.430599346
C31	10.385734560	13.333238049	4.127295461
C32	10.396421290	13.349033937	1.276459154
C33	9.815300312	14.471504858	6.241637617
C34	9.849510707	14.512387167	7.685327390
C35	8.680188993	15.106079845	8.396543291
C36	8.713645401	15.204299971	5.553258095
C37	7.484789092	15.578409524	6.257221240
C38	7.475943797	15.477408082	7.699999048
C39	6.215389653	15.424978199	8.388259089
C40	6.232939190	15.314802927	5.529060315
C41	5.136656362	14.739254626	6.238143765
C42	5.126623095	14.760058211	7.676523337

C43	4.319475168	13.785793844	8.382032837
C44	4.336582703	13.770839774	5.542157144
C45	3.958912519	12.573372888	6.247052185
C46	3.936077731	12.570667611	7.683081024
C47	4.042662093	11.303321677	8.367685058
C48	4.247634615	11.369950588	5.541291684
C49	4.883378546	10.324869169	6.256104164
C50	4.876377632	10.355520712	7.670641898
C51	5.881522464	9.628263010	8.388394554
C52	5.856172737	9.553823818	5.545112540
C53	7.059284160	9.247516728	6.254322102
C54	7.065072048	9.265657381	7.670524397
C55	8.298857614	9.354881636	8.378132993
C56	8.285202651	9.384381593	5.537357991
C57	9.402886963	9.931205320	6.246932358
C58	9.388085122	9.955865338	7.670598523
C59	10.158850871	10.932749306	8.381650745
C60	10.158514352	10.919579157	5.544802091
C61	10.527903356	12.108598339	6.247459781
C62	10.547598488	12.118459144	7.683307980
C63	10.397605794	13.349346645	8.392900755
C64	10.377844033	13.331010806	5.527493569
C65	9.725137445	14.411727599	10.515860487
C66	9.729731284	14.412233696	11.924541136
C67	8.700812047	15.106879407	12.642916394
C68	8.683666304	15.102509217	9.801922098
C69	7.491316154	15.428574923	10.516368515
C70	7.494340508	15.397198214	11.929123561
C71	6.261243732	15.274682864	12.644022449
C72	6.250380077	15.321159197	9.808343002
C73	5.154994811	14.713766451	10.515465643
C74	5.157146266	14.713454292	11.932910765
C75	4.372239288	13.756744312	12.641959338
C76	4.296806224	13.805926226	9.810274584
C77	4.027002407	12.584697881	10.504826339
C78	4.037046302	12.567500189	11.929035261
C79	4.201104168	11.336213845	12.634828134
C80	4.225803706	11.363899136	9.789665729
C81	4.872512279	10.306322152	10.503936433
C82	4.852714342	10.283732170	11.924384036
C83	5.843128700	9.540648294	12.640708249
C84	5.860876440	9.560277488	9.795949295
C85	7.054925064	9.223375627	10.509694117
C86	7.050736605	9.230349264	11.929270403

C87	8.276833776	9.389898520	12.642013493
C88	8.291039263	9.366205609	9.801876055
C89	9.380837553	9.960599484	10.513117857
C90	9.376540417	9.967646753	11.934575432
C91	10.157018764	10.932522710	12.641834744
C92	10.169139526	10.922098970	9.806079876
C93	10.519117750	12.110874146	10.510986458
C94	10.520902704	12.114834881	11.930055059
C95	10.389803807	13.351994862	12.640175594
C96	10.382212159	13.346620494	9.799409825
Ir1	-4.026275309	-7.481888755	5.583783901
Ir2	-4.172678056	-9.773314492	6.739761151
Ir3	-4.641428111	-9.536525248	4.197253086
Ir4	-6.294004548	-8.671147093	5.994416300
N	11.922375715	20.108272532	6.447335206
O	12.306652062	20.470692504	7.494864406

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C1	10.709701413	15.100888908	1.328111476
C2	10.709705959	15.105163014	2.744559327
C3	9.807186298	15.961632633	3.441421996
C4	9.802423619	15.946868233	0.622866751
C5	8.673345791	16.465472512	1.327002620
C6	8.675714304	16.476211306	2.737819322
C7	7.442267594	16.608256796	3.448422930
C8	7.437728607	16.591286764	0.625723631
C9	6.229549244	16.315643413	1.334913992
C10	6.232689930	16.318566065	2.749672085
C11	5.178382608	15.672774332	3.462485050
C12	5.167940310	15.674490096	0.631456140
C13	4.352253317	14.745327323	1.339191365
C14	4.358304661	14.744066809	2.759977693
C15	3.854769783	13.612296094	3.468941692
C16	3.847412260	13.615093467	0.630480224
C17	3.708164406	12.385355669	1.338409869
C18	3.710070260	12.384225336	2.760223244
C19	3.948260784	11.168456540	3.468882974
C20	3.946876030	11.170918742	0.629060181
C21	4.553173158	10.089040903	1.337497669
C22	4.553487845	10.087244719	2.759576763
C23	5.466981755	9.251327086	3.467420368
C24	5.466910120	9.253603721	0.629656444
C25	6.596257019	8.743720144	1.337818227
C26	6.596686137	8.742540508	2.759511798

C27	7.828497724	8.612599234	3.468165202
C28	7.828171499	8.613732479	0.629322947
C29	9.037860419	8.877210044	1.338114578
C30	9.038563825	8.877361590	2.759425702
C31	10.103017636	9.512399310	3.467893884
C32	10.102878871	9.510844796	0.629337433
C33	10.920280774	10.440058961	1.336992914
C34	10.920123365	10.442576648	2.759445236
C35	11.414208072	11.577419841	3.465943436
C36	11.417988160	11.572163031	0.628021696
C37	11.551412619	12.803130325	1.335037897
C38	11.548632483	12.806879218	2.754740772
C39	11.303531729	14.022535134	3.457860519
C40	11.309317009	14.016268640	0.624938151
C41	10.703421842	15.118140143	5.574800084
C42	10.703831881	15.117556045	6.995732003
C43	9.856861475	16.039330886	7.687232863
C44	9.814085184	15.987695426	4.852860718
C45	8.701458650	16.558433748	5.538103164
C46	8.761129370	16.694323023	6.960856241
C47	7.387035100	16.769624958	7.717967086
C48	7.448643022	16.642357232	4.859736701
C49	6.229865012	16.347197129	5.582909446
C50	6.207805089	16.350058615	6.997460721
C51	5.188998890	15.669478685	7.718922644
C52	5.184861707	15.675597843	4.883233781
C53	4.369211133	14.742602938	5.595825114
C54	4.372520829	14.737928070	7.017352302
C55	3.863464570	13.610269951	7.727743862
C56	3.858841636	13.611875307	4.889921078
C57	3.714039203	12.383323638	5.598711203
C58	3.714617559	12.382552262	7.020429518
C59	3.949036380	11.166524575	7.729510124
C60	3.948757027	11.167451867	4.889757683
C61	4.553707417	10.085311722	5.598464243
C62	4.553896330	10.084355738	7.020393794
C63	5.467760095	9.249153324	7.727974534
C64	5.467338001	9.250097405	4.890073252
C65	6.597210159	8.740721466	5.598153991
C66	6.597674192	8.739869550	7.019527523
C67	7.829931578	8.609113417	7.727726895
C68	7.829446763	8.611519673	4.889246289
C69	9.039837076	8.874926641	5.597681171
C70	9.040872898	8.873156138	7.018596079

C71	10.106917348	9.507597863	7.726832655
C72	10.104513203	9.512014468	4.889169837
C73	10.920238791	10.443654803	5.596353025
C74	10.922517169	10.442456424	7.018786152
C75	11.412904039	11.578991011	7.725307948
C76	11.412032194	11.580989145	4.888085031
C77	11.537719506	12.813643908	5.593845011
C78	11.536174895	12.815196693	7.015612136
C79	11.291095935	14.029294690	7.719567741
C80	11.295311196	14.028364477	4.878785907
C81	10.744493012	15.103915683	9.876378041
C82	10.719476774	15.111969896	11.295609203
C83	9.833060912	15.994591292	12.019368157
C84	9.915176195	16.050324011	9.183395479
C85	8.742275018	16.561231414	9.855622900
C86	8.702519658	16.603200445	11.366475544
C87	7.437923555	16.671840826	12.037779531
C88	7.411225224	16.688673366	9.164552480
C89	6.232925151	16.328555661	9.874034811
C90	6.239897776	16.341156176	11.300725912
C91	5.186297562	15.684555378	11.995533462
C92	5.189706498	15.672579159	9.151801435
C93	4.373214763	14.743496719	9.858360136
C94	4.371946054	14.748906132	11.281755240
C95	3.861085445	13.619526090	11.987579999
C96	3.862567229	13.612595521	9.150481134
C97	3.714674903	12.385490280	9.858569009
C98	3.715185675	12.388411044	11.279893357
C99	3.950385249	11.172319195	11.988314006
C100	3.949020955	11.167656782	9.150070626
C101	4.554089833	10.086061377	9.858534402
C102	4.554359947	10.088038345	11.280116314
C103	5.467669907	9.252196250	11.987534560
C104	5.467860237	9.249542140	9.150375621
C105	6.597513412	8.739956237	9.857966644
C106	6.597158374	8.740813705	11.279318205
C107	7.828828340	8.609875774	11.987597515
C108	7.829998806	8.608572977	9.148786572
C109	9.040631871	8.870873567	9.856878674
C110	9.039852335	8.871534621	11.278203020
C111	10.104454158	9.506112142	11.986760669
C112	10.106928690	9.505824438	9.147745503
C113	10.922168721	10.438190823	9.855219606
C114	10.921086172	10.437256204	11.278159617

C115	11.412309415	11.571693380	11.986914471
C116	11.412367770	11.576296302	9.147630231
C117	11.538863411	12.806417395	9.857038377
C118	11.539167878	12.803565376	11.279279045
C119	11.293720542	14.015134230	11.995300347
C120	11.298792915	14.023509917	9.149908066
C121	10.709444742	15.102705699	14.126369503
C122	10.708953481	15.100929428	15.542585574
C123	9.803177447	15.948752757	16.249764103
C124	9.816077203	15.971423301	13.427235897
C125	8.677559585	16.494454608	14.139327397
C126	8.674689813	16.474017462	15.548594496
C127	7.437025440	16.595272036	16.254871119
C128	7.434903513	16.634536976	13.442134519
C129	6.227143566	16.333401912	14.136596090
C130	6.226312143	16.322293460	15.550284929
C131	5.166489454	15.677899983	16.252904070
C132	5.173783546	15.687605829	13.419063690
C133	4.354656637	14.754585725	14.120283998
C134	4.349411134	14.751256083	15.542146263
C135	3.846718264	13.617613587	16.248550764
C136	3.854771529	13.620184873	13.410138307
C137	3.710412315	12.390429494	14.117183264
C138	3.707752618	12.388486341	15.539231388
C139	3.947013274	11.172531326	16.247551644
C140	3.949808170	11.173358540	13.408941749
C141	4.554184861	10.091102099	14.117321493
C142	4.553756865	10.090872958	15.539249186
C143	5.466808410	9.254469963	16.246900468
C144	5.467558305	9.253611413	13.409844121
C145	6.596480073	8.743430156	14.117674736
C146	6.596301331	8.744053349	15.539264714
C147	7.827671978	8.613465366	16.248017960
C148	7.828353086	8.611226454	13.408881864
C149	9.037988129	8.874117366	14.117632689
C150	9.037821992	8.875541415	15.539053432
C151	10.102411716	9.509573034	16.247902038
C152	10.103429196	9.506929840	13.408245702
C153	10.919391781	10.436941612	14.116768574
C154	10.919936277	10.437714253	15.539177714
C155	11.417247707	11.570534409	16.246932139
C156	11.413455496	11.570713311	13.408756639
C157	11.544408882	12.800584544	14.119340905
C158	11.548995184	12.800595057	15.538244369

C159	11.307955632	14.014973294	16.246279882
C160	11.298771524	14.015383089	13.415634565
Ir1	-5.289825860	-5.958805242	8.828437988
Ir2	-4.472914979	-8.402704561	8.437376709
Ir3	-6.784118100	-7.665830885	7.599980400
Ir4	-6.374055724	-7.860125727	10.092958888
O	10.480009485	22.100453160	7.092776410
N	10.249920035	21.494961839	8.082170426

(7, 7)-Ir₄-NO

C1	11.587169991	14.749876632	0.465137875
C2	7.964052011	16.777198523	0.457652870
C3	10.613718349	15.800743705	0.463148633
C4	10.029588799	16.210596996	1.687776256
C5	6.542728277	16.572271105	0.463992590
C6	5.871724721	16.304361888	1.689065895
C7	8.691676131	16.718345799	1.670828418
C8	4.207421927	14.964582788	0.468001546
C9	4.693970570	15.484145813	1.695217969
C10	3.091678654	10.943206541	0.467340239
C11	3.452148691	13.746159328	0.467190580
C12	3.208124108	13.074185004	1.696226019
C13	3.536750469	9.582174115	0.467405465
C14	3.903331483	8.971047962	1.697267752
C15	3.025573956	11.653693545	1.696674076
C16	5.501613570	7.559629942	0.467333232
C17	4.899906039	7.942594566	1.697117071
C18	9.650606856	7.440707455	0.466866885
C19	6.852781170	7.085485906	0.467166764
C20	7.561848492	7.010740010	1.696856386
C21	10.846327292	8.229873521	0.466702328
C22	11.341546207	8.741372221	1.696421305
C23	8.982796132	7.191506034	1.696684997
C24	12.313810201	10.641274508	0.467082248
C25	12.083670396	9.965938981	1.696265229
C26	12.474304026	12.064627953	0.467192417
C27	12.393261320	12.774268008	1.696140610
C28	11.942781522	14.134480654	1.695688255
C29	11.578761732	14.748207502	2.926294526
C30	7.968420318	16.848175394	2.896326128
C31	10.622952981	15.813390297	2.929732611
C32	10.077937171	16.258993261	4.159704843
C33	6.527768604	16.588326379	2.915676393
C34	5.862942954	16.301583445	4.150503783

C35	8.736066194	16.853895817	4.147135046
C36	4.197323228	14.964078052	2.925874854
C37	4.683815991	15.470098645	4.155893293
C38	3.089064871	10.943922942	2.926586584
C39	3.444412431	13.745640900	2.926000427
C40	3.202522438	13.074184889	4.156227446
C41	3.535765567	9.582913919	2.926758929
C42	3.902880931	8.971466784	4.156564749
C43	3.021879734	11.653702448	4.156512759
C44	5.501743393	7.560138635	2.926842335
C45	4.899819871	7.943180080	4.156500948
C46	9.650927902	7.440063768	2.926426228
C47	6.852897396	7.085738382	2.926672441
C48	7.561998765	7.011144923	4.156418192
C49	10.846606396	8.229211802	2.926291597
C50	11.341795408	8.741544807	4.156045849
C51	8.982847539	7.191813212	4.156347606
C52	12.310105184	10.641404434	2.925622515
C53	12.083370322	9.966335373	4.155772596
C54	12.466243283	12.064540999	2.924769625
C55	12.390719946	12.772323750	4.155286872
C56	11.940072510	14.129080054	4.155134272
C57	11.583655980	14.743010256	5.386038411
C58	7.962983536	16.952078231	5.419874673
C59	10.623143216	15.800976235	5.386938776
C60	10.036673424	16.192479295	6.619591102
C61	6.528135942	16.583399287	5.389226547
C62	5.881681281	16.274537746	6.627558819
C63	8.725322016	16.792068931	6.637014917
C64	4.204224458	14.955816676	5.384958474
C65	4.710799369	15.465043775	6.619688531
C66	3.088128170	10.943150975	5.386596442
C67	3.445261996	13.743984419	5.387193964
C68	3.206376881	13.072458113	6.617241735
C69	3.535432458	9.582871734	5.386374588
C70	3.903046459	8.970906576	6.615964920
C71	3.023823822	11.652671385	6.616666203
C72	5.501731043	7.560191927	5.386151123
C73	4.899706450	7.942806462	6.615894019
C74	9.650979742	7.440893893	5.386145263
C75	6.852758144	7.086033028	5.386130703
C76	7.561870261	7.011220668	6.615842801
C77	10.846753788	8.229769329	5.386128385
C78	11.342309781	8.742212150	6.615712838

C79	8.982670869	7.192345219	6.615811008
C80	12.313513966	10.641094990	5.385622663
C81	12.086852216	9.965866419	6.615625002
C82	12.472482489	12.063901995	5.385420344
C83	12.402389835	12.772728919	6.615471692
C84	11.950244167	14.129980943	6.615927780
C85	11.588645114	14.744214082	7.845549914
C86	7.966437392	16.850252265	7.855754413
C87	10.607888900	15.786947780	7.841801433
C88	10.015015200	16.198599722	9.074199425
C89	6.545153690	16.568393310	7.848503540
C90	5.885495625	16.292767022	9.073363987
C91	8.682134786	16.718808955	9.078144871
C92	4.212275147	14.955316034	7.847943357
C93	4.706416716	15.476474336	9.074525240
C94	3.090809149	10.942954129	7.846395218
C95	3.451182978	13.742996455	7.846968629
C96	3.211462709	13.073452744	9.076607222
C97	3.536442461	9.582143677	7.845982767
C98	3.903581639	8.970750424	9.075629454
C99	3.026914975	11.652566544	9.076161493
C100	5.501515859	7.559724322	7.845588229
C101	4.899925349	7.942194146	9.075498902
C102	9.650632501	7.441400881	7.845458663
C103	6.852740124	7.085725900	7.845530959
C104	7.561680678	7.011074792	9.075283561
C105	10.846560270	8.230571830	7.845357681
C106	11.341767533	8.742424053	9.075194017
C107	8.982564372	7.192370857	9.075152053
C108	12.317005892	10.640700239	7.845502119
C109	12.086239316	9.966099754	9.075264250
C110	12.479517575	12.063994805	7.846019403
C111	12.404398789	12.773285636	9.075432235
C112	11.952794933	14.133489560	9.075354943
Ir1	-8.866907315	-7.426060104	4.445226427
Ir2	-7.631219939	-5.194815425	4.574685487
Ir3	-6.478056431	-7.223463385	3.546533597
Ir4	-6.927782672	-7.147729299	6.094074829
N	7.885376750	22.653935477	5.421865101
O	8.280929702	23.204454081	6.381051354

(8, 8)-Ir₄-NO

C1	12.187104474	16.209951262	0.806241738
C2	11.074244528	17.117961882	0.805395659

C3	10.448500711	17.468740823	2.025517166
C4	12.636510466	15.655782590	2.036563054
C5	8.330704432	17.737183223	0.805625769
C6	9.046816016	17.783983157	2.025210828
C7	4.634605138	15.741654540	0.808019036
C8	6.934130424	17.398854055	0.806826261
C9	6.289958839	17.093129148	2.036847948
C10	3.821190863	14.562961117	0.808709734
C11	3.523277937	13.916561265	2.038007504
C12	5.131458623	16.250628216	2.037688857
C13	3.128749276	11.818176246	0.809244587
C14	3.174353300	12.527576518	2.038796851
C15	4.706481044	7.944190284	0.809818361
C16	3.305174161	10.397604740	0.809629212
C17	3.526521775	9.721205754	2.039382756
C18	5.856017524	7.089988313	0.809898991
C19	6.501724656	6.790661227	2.039633048
C20	4.233071172	8.476133928	2.039573141
C21	8.609479321	6.464073679	0.809859079
C22	7.898622968	6.474223287	2.039612043
C23	12.347720593	8.339359855	0.809400913
C24	10.014716739	6.741078731	0.809711133
C25	10.669267161	7.020423418	2.039438991
C26	13.138329632	9.533186309	0.809022029
C27	13.414688412	10.188675755	2.038531894
C28	11.850152097	7.831274586	2.039160213
C29	13.736580733	12.299079859	0.808337473
C30	13.716378939	11.588288274	2.037695027
C31	13.528592776	13.715091758	0.807536055
C32	13.307968317	14.391674768	2.037169568
C33	12.202940074	16.220591870	3.263533747
C34	11.144001074	17.209195998	3.255543796
C35	10.493369708	17.541359375	4.497899106
C36	12.616454576	15.639150108	4.486943434
C37	8.307596400	17.849531816	3.255811166
C38	9.037195310	17.869272091	4.498371970
C39	4.630872224	15.741332928	3.265740687
C40	6.925383623	17.412814013	3.263710493
C41	6.299521842	17.071523214	4.487750209
C42	3.818376191	14.563185244	3.267518078
C43	3.523934890	13.915966398	4.498002323
C44	5.136083356	16.244128003	4.493981453
C45	3.128584474	11.818301758	3.268579497
C46	3.175079202	12.527717780	4.498430789

C47	4.706597421	7.944242904	3.269283899
C48	3.305248844	10.397778477	3.269074024
C49	3.526552610	9.721099572	4.498777759
C50	5.856039811	7.090047437	3.269377752
C51	6.501843682	6.790699661	4.499141596
C52	4.233101330	8.476327507	4.499019959
C53	8.609481691	6.464134881	3.269341464
C54	7.898526513	6.474308192	4.499120243
C55	12.347827538	8.339494987	3.268828569
C56	10.014651453	6.741166330	3.269183684
C57	10.669367440	7.020592026	4.498880539
C58	13.138802405	9.533147695	3.268314032
C59	13.414462186	10.188978849	4.498121336
C60	11.850137934	7.831098534	4.498524727
C61	13.740264368	12.298015075	3.267142380
C62	13.715982237	11.587730485	4.497620951
C63	13.533618135	13.713399212	3.265234725
C64	13.299194933	14.387115677	4.493606384
C65	12.149217685	16.175164555	5.727678688
C66	11.092637271	17.104838455	5.730753779
C67	10.499553732	17.568989699	6.957450692
C68	12.612386017	15.639490748	6.962210860
C69	8.306967821	17.735279168	5.730431092
C70	9.039242145	17.900030564	6.957613767
C71	4.637936691	15.738273066	5.727254165
C72	6.949704493	17.357163217	5.727648673
C73	6.302267249	17.072072477	6.962112990
C74	3.823383241	14.561456917	5.727613699
C75	3.525920275	13.915550586	6.957753187
C76	5.135317070	16.244842956	6.959053435
C77	3.129052534	11.818031256	5.728191987
C78	3.175434654	12.527519470	6.958064344
C79	4.706535054	7.944238858	5.728808628
C80	3.305360135	10.397779108	5.728591933
C81	3.526450005	9.721197378	6.958423778
C82	5.856020409	7.090084097	5.728900797
C83	6.501733964	6.790722888	6.958637952
C84	4.233034125	8.476147345	6.958566897
C85	8.609526519	6.464163091	5.728855713
C86	7.898643583	6.474276207	6.958611560
C87	12.347830617	8.339494622	5.728312444
C88	10.014711338	6.741107652	5.728690595
C89	10.669343664	7.020396455	6.958415103
C90	13.138387091	9.532892428	5.727868606

C91	13.413999789	10.188807251	6.957718894
C92	11.850288967	7.831153194	6.958166239
C93	13.734586375	12.298383510	5.727218014
C94	13.713814324	11.588109844	6.957318188
C95	13.524163298	13.712985603	5.726781265
C96	13.299403971	14.386701161	6.958628036
C97	12.172154220	16.206189377	8.187052776
C98	11.094596112	17.148538491	8.193676008
C99	10.443548994	17.445761367	9.415419600
C100	12.622792739	15.649554669	9.418195822
C101	8.323531808	17.773790001	8.194451123
C102	9.039220595	17.761249242	9.415329643
C103	4.634664373	15.740770308	8.188084532
C104	6.943292677	17.391187697	8.188024169
C105	6.297654281	17.083953873	9.418843572
C106	3.821474241	14.562070636	8.187881829
C107	3.524872696	13.916097594	9.417112311
C108	5.133871248	16.249437836	9.417274677
C109	3.128925636	11.818235442	8.187919088
C110	3.174922311	12.527578918	9.417560694
C111	4.706485786	7.944243333	8.188299742
C112	3.305107470	10.397618703	8.188168606
C113	3.526399304	9.721064508	9.417922330
C114	5.856047203	7.090043176	8.188380888
C115	6.501790756	6.790695628	9.418128090
C116	4.232963306	8.476129401	9.418072826
C117	8.609478804	6.464132781	8.188335820
C118	7.898580177	6.474283125	9.418101406
C119	12.347870805	8.339241068	8.187910241
C120	10.014755512	6.741121341	8.188180271
C121	10.669362826	7.020382818	9.417934235
C122	13.138423588	9.533167209	8.187632633
C123	13.414074046	10.188821446	9.417291555
C124	11.850194766	7.831079094	9.417687379
C125	13.736301215	12.297935107	8.187528327
C126	13.714432745	11.588361562	9.416786601
C127	13.528026654	13.713785075	8.187661852
C128	13.303162865	14.390951890	9.416544924
Ir1	-4.321164724	-4.163886068	5.057397182
Ir2	-3.546592567	-6.502115410	4.307246530
Ir3	-6.014330621	-5.957781328	4.306347507
Ir4	-4.775338434	-6.193755639	6.536971822
N	10.816763931	23.784455207	5.580302189
O	10.824361329	24.534442478	6.491673802

(10, 10)-Ir₄-NO

C1	12.053842236	15.446091200	0.218184662
C2	10.941682521	16.338551700	0.215555830
C3	10.341082554	16.719314350	1.442070142
C4	12.532748224	14.927934698	1.447734725
C5	8.281799218	17.313735631	0.207583582
C6	8.999762253	17.245135933	1.429812909
C7	4.192928173	16.313442231	0.210565009
C8	6.857545793	17.282354266	0.211021893
C9	6.153603352	17.147552893	1.442316570
C10	3.045700203	15.457290390	0.211077587
C11	2.544900066	14.953956140	1.441183399
C12	4.814226900	16.652930462	1.441169647
C13	1.360185724	13.175338457	0.212058770
C14	1.695012319	13.802521015	1.441813034
C15	0.810493446	8.991959961	0.213170643
C16	0.885277555	11.826212131	0.212522114
C17	0.754592323	11.126995077	1.442379912
C18	1.222458457	7.621431447	0.213514998
C19	1.532404979	6.981992703	1.443360406
C20	0.716708930	9.697152162	1.442782716
C21	2.847900683	5.299055292	0.214080187
C22	2.352318723	5.808347797	1.443721875
C23	6.678421065	3.530929912	0.215007550
C24	3.994668184	4.443185754	0.214451611
C25	4.623119697	4.110750390	1.444305293
C26	8.108501076	3.522706925	0.215380451
C27	8.811230995	3.633993666	1.445225838
C28	5.977106044	3.650263100	1.444656826
C29	10.802378911	4.405027735	0.215912897
C30	10.170340967	4.079698854	1.445561143
C31	13.619420169	7.547085082	0.216885585
C32	11.958736443	5.248508543	0.216251143
C33	12.459749754	5.752325689	1.446115727
C34	14.064089032	8.906640550	0.217274779
C35	14.177034175	9.608809028	1.447407267
C36	13.296712330	6.913522024	1.446449745
C37	14.078469900	11.741623496	0.218322523
C38	14.182141592	11.038701821	1.448160783
C39	13.652719872	13.107400818	0.219056293
C40	13.337604927	13.745760800	1.448413077
C41	12.053772183	15.464956566	2.674893306
C42	10.975339107	16.393730445	2.661908097

C43	10.424536784	16.896739467	3.900795516
C44	12.545087447	14.945631680	3.911015748
C45	8.274035778	17.402650298	2.644992778
C46	9.036411053	17.456521714	3.865534590
C47	4.196053437	16.307330541	2.672635858
C48	6.845489697	17.302768055	2.664770792
C49	6.162014765	17.151829797	3.906160524
C50	3.048161374	15.455012340	2.672112263
C51	2.545827770	14.951580244	3.901371097
C52	4.826233278	16.642165880	3.902137062
C53	1.360044056	13.174907001	2.671659397
C54	1.695182346	13.801736896	3.901558500
C55	0.810397661	8.991906953	2.672619661
C56	0.885113611	11.826114873	2.672040131
C57	0.754140945	11.126789880	3.901881363
C58	1.222409472	7.621460385	2.673000239
C59	1.532324760	6.981949616	3.902846899
C60	0.716475815	9.697095684	3.902258912
C61	2.847896804	5.299049358	2.673583450
C62	2.352295482	5.808373842	3.903211314
C63	6.678441166	3.530935142	2.674505880
C64	3.994661978	4.443197869	2.673955673
C65	4.623128367	4.110756522	3.903799369
C66	8.108513363	3.522693885	2.674875673
C67	8.811240799	3.633977021	3.904732311
C68	5.977111562	3.650282328	3.904149802
C69	10.802412032	4.404924500	2.675415224
C70	10.170346571	4.079662336	3.905085625
C71	13.618959104	7.546876475	2.676397100
C72	11.958742854	5.248334299	2.675763521
C73	12.459678768	5.752240768	3.905687358
C74	14.062628714	8.906386777	2.676810338
C75	14.175974517	9.608988708	3.906587427
C76	13.296478780	6.913457873	3.906091765
C77	14.071711260	11.742326307	2.677938816
C78	14.180412180	11.038761086	3.906821133
C79	13.643997763	13.107376823	2.678806219
C80	13.336519468	13.751187598	3.907969385
C81	12.092141390	15.484545051	5.139490275
C82	11.027000173	16.464756475	5.149361499
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C93	1.359930740	13.174664305	5.131387567
C94	1.695319933	13.801637210	6.360986134
C95	0.810213059	8.991857902	5.132123056
C96	0.884764770	11.825818754	5.131594732
C97	0.754214922	11.126745195	6.361438942
C98	1.222338205	7.621412252	5.132492280
C99	1.532341733	6.981985719	6.362362624
C100	0.716420454	9.696977139	6.361812976
C101	2.847893906	5.299074406	5.133074928
C102	2.352310322	5.808372630	6.362720132
C103	6.678437494	3.530947909	5.134006407
C104	3.994670779	4.443221180	5.133447022
C105	4.623125468	4.110772495	6.363298675
C106	8.108512432	3.522703413	5.134383750
C107	8.811219427	3.633988989	6.364250205
C108	5.977105396	3.650276664	6.363652288
C109	10.802380089	4.404930865	5.134965690
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C117	14.075076861	11.743237227	5.136254655
C118	14.184321983	11.039373479	6.365676025
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C124	12.543333177	14.927707790	8.824665044
C125	8.289530552	17.352653323	7.608399681
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C127	4.199708648	16.307091030	7.588423959
C128	6.862170202	17.293084609	7.593581548
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C131	2.545106262	14.953703283	8.819550220
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C136	0.885048363	11.825943253	7.591114410
C137	0.754446140	11.126882259	8.820986766
C138	1.222395206	7.621426264	7.592034547
C139	1.532377935	6.981961409	8.821872265
C140	0.716655911	9.697120993	8.821339035
C141	2.847902137	5.299064750	7.592578361
C142	2.352320813	5.808356768	8.822220058
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C144	3.994665355	4.443204357	7.592951388
C145	4.623114300	4.110741432	8.822798342
C146	8.108492335	3.522696211	7.593887164
C147	8.811211887	3.634004758	8.823735853
C148	5.977098720	3.650259359	8.823152006
C149	10.802363015	4.405049502	7.594454214
C150	10.170302936	4.079758146	8.824088296
C151	13.619274120	7.547339075	7.595313237
C152	11.958664707	5.248547604	7.594832550
C153	12.459715292	5.752575449	8.824637706
C154	14.064132050	8.906834595	7.595566066
C155	14.178800378	9.608913889	8.825603551
C156	13.296757469	6.913812224	8.824971946
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Ir2	-6.814056284	-9.097878062	4.678463111
Ir3	-6.135792591	-11.577456204	4.648130882
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