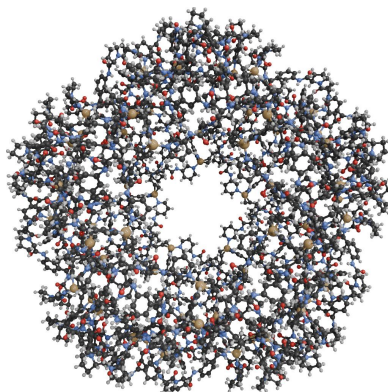




A Report On The Calculation Of The Single Point Energy Of 2425365 At The GFN2-XTB Level

osl - 14th October 2026



Abstract

The calculation of single point energy for the system '2425365' is presented, accompanied by automated analysis and image generation provided by the Digichem software package. The calculation was performed using the xTB software package at the GFN2-XTB level of theory. The total self-consistent field (SCF) energy of the system was found to be -248413.64 eV after 1 step. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -39.10 and -38.70 eV respectively, corresponding to a HOMO-LUMO band gap of 0.39 eV. The permanent dipole moment (PDM) was calculated to be 0.00 D.

Table 1: Summary of overall calculation metadata.

Date ^[a] (Duration ^[b])	CPUs (Memory)	Success (Converged)	Computational package	Level of theory	Solvent (model)	Calculations	Wavefunction	Multiplicity	T ^[c] / K	p ^[d] / atm
14/10/2026 19:59:30 (8 h, 53 m, 59 s)	16 (32 GB)	True (N/A)	xTB (6.7.1)	GFN2- XTB	Gas-phase (N/A)	Single Point	restricted	1 (singlet)	N/A	N/A

[a]: The date and time at which the calculation was completed. [b]: Total combined duration in real-time (wall-time) for all components of the calculation. [c]: Temperature used for thermochemistry analysis. [d]: Pressure used for thermochemistry analysis.

Summary Of Results

SCF Energy

Table 2: Summary of SCF energy properties.

No. of steps	1
Final energy	-248413.6428 eV
Final energy	-23,968,273 kJ·mol ⁻¹

Geometry

Table 3: Summary of geometry properties.

Formula	C ₂₂₈₀ N ₄₈₀ O ₃₆₀ Cu ₆₀ H ₂₄₀₀ ⁺⁶⁰
SMILES	<chem>[O][C]1NC2C[C]3[CH]</chem> <chem>[Cu]34[N]3[CH][CH][CH][C]</chem> <chem>([CH]3)N[C]([O])C3CCCN3[C]</chem> <chem>([O])C3C[C]5[CH][Cu]56[N]5[CH]</chem> <chem>[CH][CH][C]([CH]5)N[C]</chem> <chem>([O])C5CCCN5[C]</chem> <chem>([O])C5C[C]7[CH][Cu]78[N]7[CH]</chem> <chem>[CH][CH][C]([CH]7)N[C]</chem> <chem>([O])C7CCCN7[C]</chem> <chem>([O])C7C[C]9[CH]</chem> <chem>[Cu]9%10[N]9[CH][CH][CH][C]</chem> <chem>([CH]9)N[C]([O])C9CCCN9[C]</chem> <chem>([O])C9C[C]11[CH][Cu]11([N]</chem> <chem>%11[CH][CH][CH][C]([CH]</chem> <chem>%11)N[C]</chem> <chem>([O])C%11CCCN%11[C]2([O])</chem> <chem>[N]2[CH][CH][CH][C]([CH]2)[C]</chem> <chem>([O])N2CCCC2[C]</chem> <chem>([O])N2CCCC2[C]([O])N[C]2[CH]</chem> <chem>[CH][CH][C]([CH]2)[C]</chem> <chem>([O])NC2C[C]11[CH][Cu]</chem> <chem>%11%12[N]11[CH][CH][CH][C]</chem> <chem>([CH]11)N[C]</chem> <chem>([O])C%11CCCN%11[C]</chem> <chem>([O])C%11C[C]13[CH][Cu]</chem>
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Molar mass	46099.2120 g·mol ⁻¹	
Alignment method	Nested grid (35:10:10:10:10)	
X extension	63.35 Å	
Y extension	62.59 Å	
Z extension	57.15 Å	
Linearity ratio	0.01	
Planarity ratio	0.09	
Molecular Orbitals		
<i>Table 4: Summary of HOMO & LUMO properties.</i>		
E_{HOMO,LUMO}	0.39 eV	
E_{HOMO}	-39.10 eV	
E_{LUMO}	-38.70 eV	
Permanent Dipole Moment		
<i>Table 5: Summary of the permanent dipole moment properties.</i>		
Total	< 0.01 D	
X axis angle	90.00 °	

XY plane angle

90.00 °

Methodology

Metadata

The calculation of the single point energy was performed using the **xTB (6.7.1)** program, the **GFN2-XTB** method and using a basis set that could not be determined. It was completed on the **14th October 2026** after a total duration of **8 h, 53 m, 59 s** and **finished successfully**. The base multiplicity of the system under study was **1 (singlet)**. Finally, a **restricted wavefunction** was used, resulting in a single set of doubly occupied orbitals. The full calculation metadata is tabulated in table 1.

Analysis

The report presented here was generated using the Digichem software package. This toolset relies upon a number of third-party applications and libraries which should be cited appropriately in derivative works. In particular, the calculation results described within were parsed by the cclib library.¹ Scientific constants which were used, among other things, for the interconversion of scientific units were provided by SciPy.² Three-dimensional plots of atom positions and calculated densities, including molecular orbitals, were rendered using Visual Molecular Dynamics (VMD)³ and the Tachyon ray-tracer.⁴ Finally, two-dimensional graphs were plotted using the Matplotlib library,⁵ while this report itself was prepared using the Mako template library⁶ and the Weasyprint library⁷, the latter of which was responsible for generation of the PDF file.

Discussion

Total SCF Energy

The total energy of the system was calculated at the **self-consistent field (SCF)** level, corresponding to the energy calculated by the Hartree-Fock (HF) method, with a value of -248413.64 eV, corresponding to -23,968,273 KJmol⁻¹. A plot of the total SCF electron density is shown in figure 1.

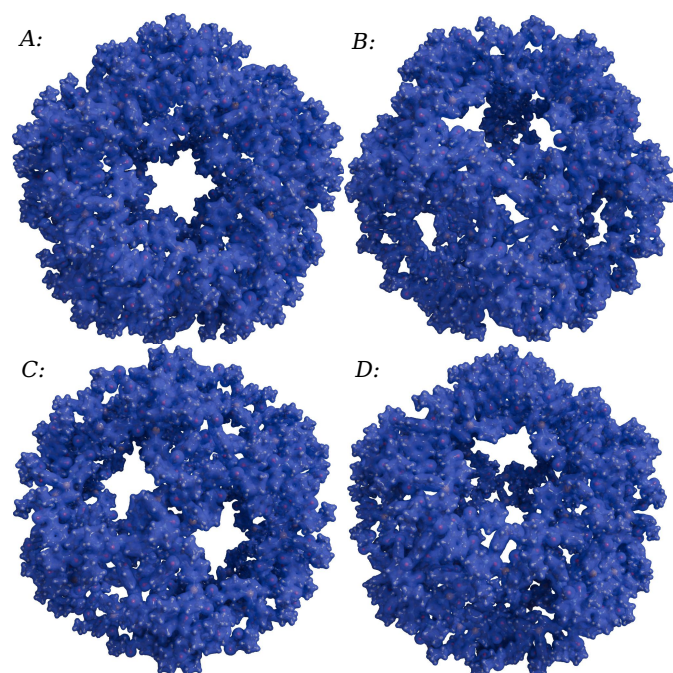


Figure 1: Plot of the total SCF electron density, plotted with an isovalue of 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Geometry

Figure 2: Labelled structure of 2425365.

The **empirical formula** of the studied system was $C_{2280}N_{480}O_{360}Cu_{60}H_{2400}^{+60}$, corresponding to a **molecular mass** of 46099.21 gmol⁻¹. The molecular structure, with atom labelling, is shown in figure 2. The molecular geometry was aligned to the cartesian (X, Y and Z) axes by the **Nested grid (35:10:10:10:10) (NEST35:10:10:10:10)** method, and the resulting atomic position are displayed in figure 3. Using this method, the **extent of the molecular system** in the X, Y and Z axes (L_X , L_Y and L_Z , corresponding to the molecular width, length and height respectively) was determined to be 63.35, 62.59 and 57.15 Å respectively. These extensions give rise to a **molecular linearity ratio** ($1-(L_Y/L_X)$) and **planarity ratio** ($1-(L_X/L_Y)$) of 0.01 and 0.09 respectively.

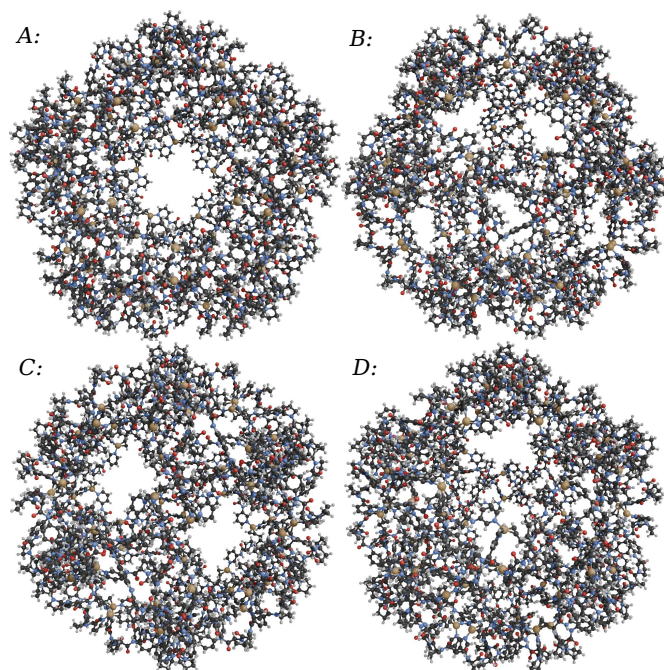


Figure 3: The molecular structure, aligned using the Nested grid (35:10:10:10:10) (NEST35:10:10:10:10) method. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Permanent Dipole Moment

The calculated **permanent dipole moment** was < 0.01 D, with a vector (x,y,z) of -0.00, 0.00, 0.00 D. The origin point of the dipole vector was (-0.00, 0.00, 0.00). The angle between the dipole moment vector and the x-axis was 90.00 °, while the angle between the dipole moment and the xy-plane was 90.00 °. A plot of the permanent dipole moment is shown in figure 4.

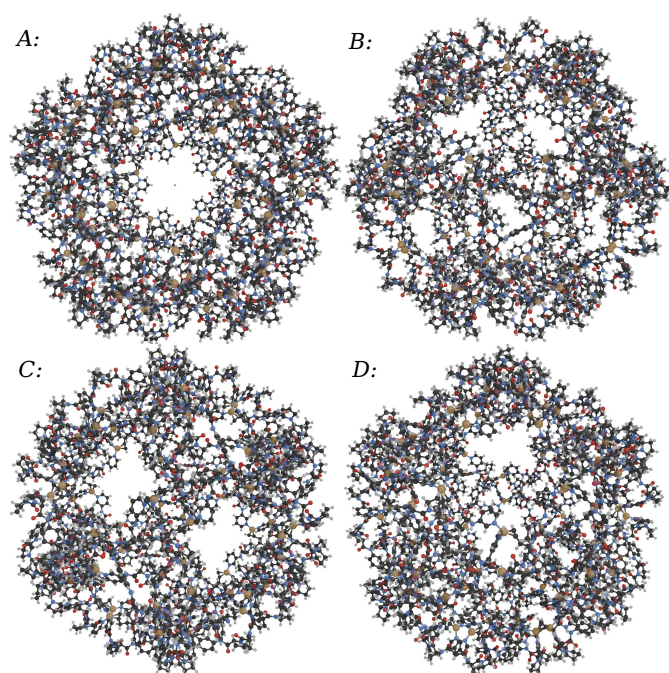


Figure 4: The permanent dipole moment (red arrow) plotted against the aligned molecular geometry with a scale of $1 \text{ \AA} = 1.0 \text{ D}$. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Molecular Orbitals

In total, 15420 doubly occupied molecular orbitals were calculated, divided into 8340 occupied orbitals and 7080 unoccupied (or virtual) orbitals. The calculated energies of the **HOMO** and **LUMO** were -39.10 and -38.70 eV respectively, corresponding to a **HOMO-LUMO band gap** of 0.39 eV (figure 8). Plots of the orbital density for the HOMO and LUMO are shown in figures 5-6 respectively, while the orbital overlap between the HOMO and LUMO is shown in figure 7.

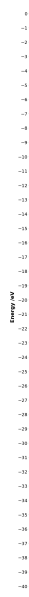


Figure 8: Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.

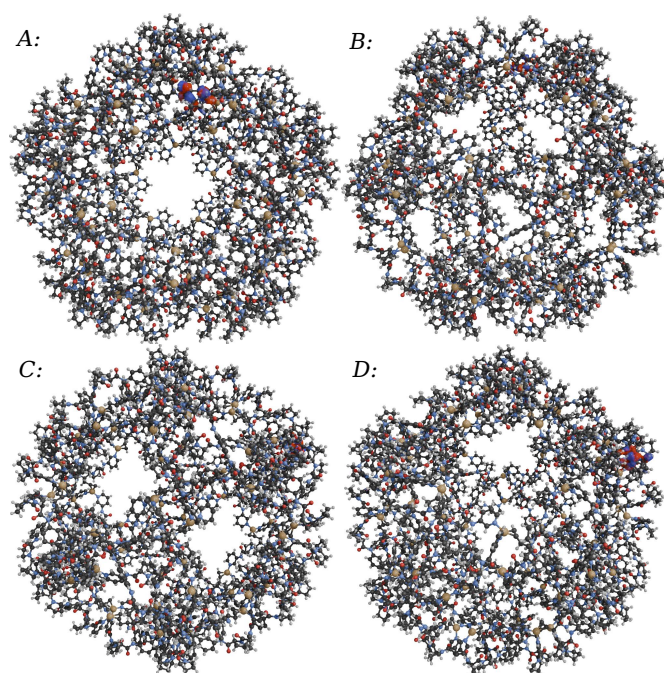


Figure 5: Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

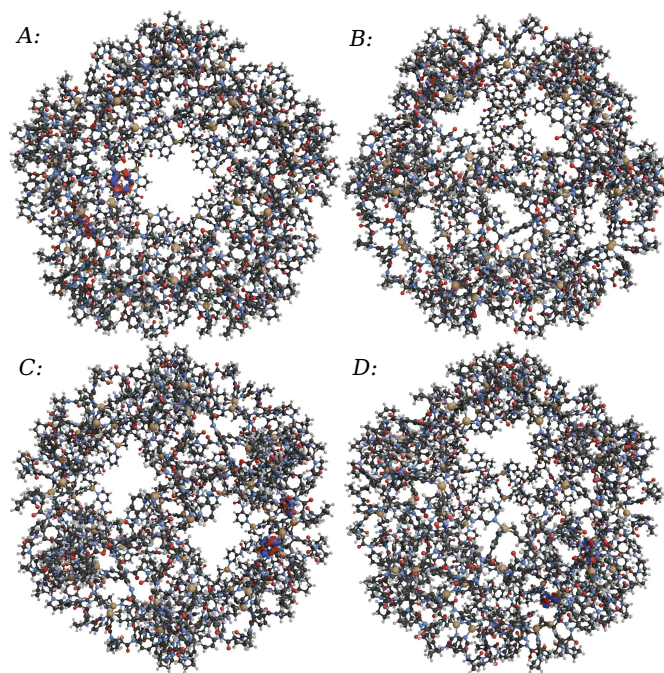


Figure 6: Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

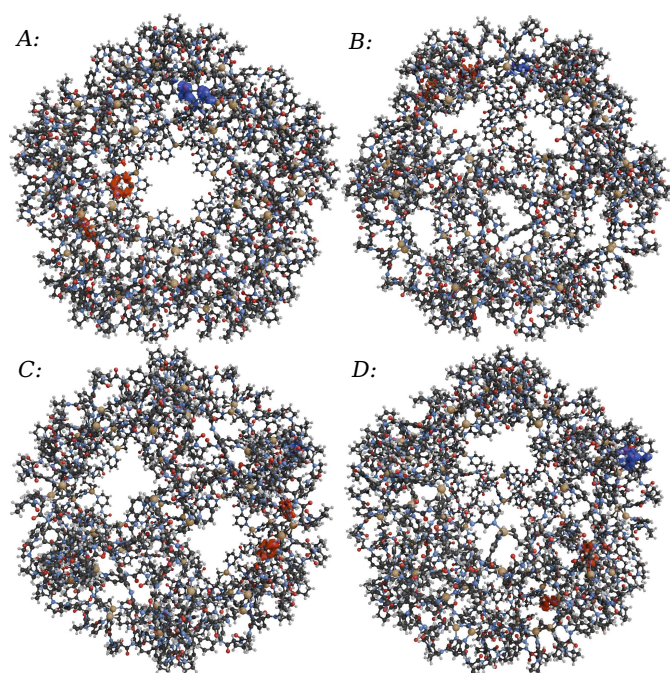


Figure 7: Orbital density plots of the HOMO (blue) and LUMO (red), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.

Tables Of Results

Atom Coordinates

Table 6: Coordinates of the atoms of the system under study, as aligned to the cartesian axes by the Nested grid (35:10:10:10) method. Atoms that are chemically equivalent have been assigned the same group numbers.

Index	Element	Group	X Coord /Å	Y Coord /Å	Z Coord /Å
1	C	C ₁	-13.3269138	18.6060316	-16.9073548
2	C	C ₂	-14.6151309	16.5759074	-18.7778957
3	C	C ₃	-15.0120007	13.8969023	-20.0510645
4	C	C ₄	-8.7039409	7.3785333	-21.1441433
5	C	C ₅	-5.7304802	7.3200308	-20.4792613
6	C	C ₁	-21.8550833	18.1967244	-1.1917647
7	C	C ₂	-21.7669996	18.8152809	-4.0527896
8	C	C ₃	-20.5305232	18.8621637	-6.8463226
9	C	C ₄	-11.7009078	19.2859905	-8.7395254
10	C	C ₅	-9.1634610	19.3333261	-6.9815235
11	C	C ₁	-10.1689500	26.4758352	-1.8695943
12	C	C ₂	-12.9961531	25.9450744	-1.0635114
13	C	C ₃	-15.4166848	24.3229530	-0.6682841
14	C	C ₄	-17.3165169	16.3324757	-4.5141610
15	C	C ₅	-15.7938546	14.5948457	-6.6199927
16	C	C ₁	-15.0871801	19.9847175	-13.6111440
17	C	C ₂	-14.0396623	22.4136396	-12.1865636
18	C	C ₃	-12.7124683	23.8197436	-9.8631081
19	C	C ₄	-12.1308891	20.8728093	-1.2848506
20	C	C ₅	-13.1851439	18.3621229	0.1239459
21	C	C ₁	-7.2704457	27.4836390	0.7342133
22	C	C ₂	-4.5375751	28.6482985	-0.0942514
23	C	C ₃	-1.6941584	28.6414180	-0.4611321
24	C	C ₁	-24.0024697	15.2224732	0.3887139
25	C	C ₁	13.2690674	5.9190912	-24.2981659
26	C	C ₄	8.7368487	15.0975979	-16.6175232
27	C	C ₅	5.7470150	14.5989161	-16.1604368
28	C	C ₁	2.0681735	14.6835837	-24.1339069
29	C	C ₂	4.0592555	12.9440375	-25.4967224
30	C	C ₃	6.2161627	10.8956815	-25.7977229
31	C	C ₁	-13.7138275	6.1167839	-23.9805223
32	C	C ₂	-11.4819148	7.4078689	-25.4619649
33	C	C ₃	-8.8726951	8.8493825	-25.8654027
34	C	C ₄	-4.6860892	13.7589566	-19.2505823
35	C	C ₅	-5.5972317	14.4695133	-16.3838005
36	C	C ₁	-1.9593989	14.1582069	-24.5220176
37	C	C ₂	-3.9406705	16.2121378	-23.6597061
38	C	C ₃	-6.2018101	17.4408102	-22.0132064
39	C	C ₄	-11.8403344	12.7456048	-16.6982699
40	C	C ₅	-12.2601284	9.7520561	-16.1444417
41	N	N ₆	-10.4804486	19.2946967	-14.5643428
42	N	N ₇	-13.5512829	18.6637012	-18.2182511
43	N	N ₈	-15.7082521	15.8573770	-18.8330793
44	N	N ₉	-10.9714242	8.0522937	-21.6744475
45	N	N ₁₀	-8.1021743	7.5115999	-19.9490400
46	N	N ₁₁	-4.7218957	8.0196515	-20.9648165
47	N	N ₆	-20.0270078	17.0722130	1.8510605
48	N	N ₇	-22.1380464	19.3146182	-1.7483567
49	N	N ₈	-22.1996111	18.2480956	-5.2311376
50	N	N ₉	-13.9065549	19.3357565	-9.7603491
51	N	N ₁₀	-11.2260149	18.3643474	-7.8346427
52	N	N ₁₁	-8.7600911	20.3897152	-6.2049772
53	N	N ₆	-6.9904058	25.0614434	-3.2506558
54	N	N ₇	-11.2555053	27.1583125	-2.2553523
55	N	N ₈	-13.7314876	25.8314389	0.0032364
56	N	N ₉	-18.1331677	17.9778903	-2.9787587
57	N	N ₁₀	-16.0510028	15.7893486	-4.4417440
58	N	N ₁₁	-15.6082915	14.9979742	-7.9857380
59	N	N ₆	-15.5394852	16.2770629	-13.6262478
60	N	N ₇	-15.6597577	21.0360248	-13.2929728
61	N	N ₈	-12.9400253	23.2252312	-12.1839668
62	N	N ₉	-11.6492372	22.7778016	-2.7293626
63	N	N ₁₀	-11.8088302	19.6259724	-1.4594534
64	N	N ₁₁	-14.4149159	18.0189886	0.3849657
65	N	N ₆	-9.0014048	24.5572624	2.2886645
66	N	N ₇	-6.7564218	28.5969555	1.0174076
67	N	N ₈	-3.9779168	28.8394891	-1.2048416
68	N	N ₆	-22.2162175	13.7406963	-2.5364309
69	N	N ₇	-25.1997389	15.0939652	0.9725798
70	N	N ₇	13.6237475	6.9190149	-24.9665003
71	N	N ₉	11.0435004	15.2138571	-17.4149487
72	N	N ₁₀	8.1609521	14.0845168	-16.1573105
73	N	N ₁₁	4.7450750	14.7109024	-17.1361345
74	N	N ₆	0.5551577	15.8213167	-20.9020218
75	N	N ₇	2.9889374	15.0316727	-25.0173312
76	N	N ₈	4.0332619	11.9167409	-26.2796667
77	N	N ₉	11.2973902	8.1514119	-21.3410171
78	N	N ₁₀	11.0596372	8.4415465	-18.0491090
79	N	N ₆	-15.2236501	5.1551068	-20.7041183
80	N	N ₇	-13.7918081	7.0365457	-24.9314445
81	N	N ₈	-10.4635728	7.0223050	-26.2315443
82	N	N ₉	-4.5818255	13.0091209	-21.5638546
83	N	N ₁₀	-4.8976652	12.9738825	-18.1793115
84	N	N ₁₁	-6.5309364	15.2948713	-15.9730451
85	N	N ₆	-0.4857938	10.7611814	-23.8774050
86	N	N ₇	-2.8051818	14.7565713	-25.2081331
87	N	N ₈	-4.0382883	17.3516097	-23.0404237
88	N	N ₉	-11.2903971	14.9565332	-17.5126007
89	N	N ₁₀	-11.0108083	11.8928946	-16.1531475
90	N	N ₁₁	-12.6114431	8.8197533	-16.9911143
91	O	O ₁₂	-13.5252763	16.0614755	-18.8720847
92	O	O ₁₃	-15.1582973	14.3958657	-21.1601910
93	O	O ₁₄	-8.1117507	7.7657483	-22.1409363
94	O	O ₁₅	-5.7305133	6.1123627	-20.4584581
95	O	O ₁₂	-20.5632876	18.8693018	-3.9519030
96	O	O ₁₃	-20.9436382	19.9866615	-7.1159140
97	O	O ₁₄	-11.4275979	20.4726177	-8.6381313
98	O	O ₁₅	-8.4639457	18.9435255	-7.8890859
99	O	O ₁₂	-12.9863593	24.9989231	-1.7810279
100	O	O ₁₃	-16.2852663	25.0743612	-1.0478788

101	O	O ₁₄	-17.8564769	16.5913891	-5.5788762	154	C	C ₁₈	-22.5709069	14.1305322	-1.3200756
102	O	O ₁₅	-16.3860009	13.6015764	-6.2993173	155	C	C ₁₈	11.4373508	4.3939513	-23.5717122
103	O	O ₁₂	-14.2154382	21.7329093	-11.1602143	156	C	C ₂₀	2.5394213	15.1785888	-17.9820907
104	O	O ₁₃	-13.5615563	24.7120218	-9.8410709	157	C	C ₁₈	1.1570754	15.0891067	-21.8456766
105	O	O ₁₄	-13.1784830	21.2108376	-0.7921914	158	C	C ₁₉	8.3988812	9.4223792	-23.2094481
106	O	O ₁₅	-12.3230910	18.3751823	1.0239582	159	C	C ₁₈	-14.3777019	5.4332387	-21.6853611
107	O	O ₁₂	-4.0691867	27.8219666	0.6555047	160	C	C ₁₉	-6.6898910	10.5902141	-23.2498145
108	O	O ₁₃	-1.5672913	29.7174592	0.0386086	161	C	C ₂₀	-7.7379724	16.8838619	-14.6303717
109	O	O ₁₂	13.5650829	8.8113989	-22.9139467	162	C	C ₁₈	-1.0518445	11.9638448	-23.7390131
110	O	O ₁₄	8.1708574	15.8206318	-17.4422414	163	C	C ₁₉	-8.4012921	15.8943541	-19.4550509
111	O	O ₁₅	5.7534593	15.3083644	-15.1577603	164	C	C ₂₀	-13.7728652	6.8594415	-17.8032748
112	O	O ₁₂	4.7000709	12.9327887	-24.4636892	165	C	C ₂₁	-10.1843386	20.5549380	-14.8905445
113	O	O ₁₃	6.9222114	11.5548299	-26.5361353	166	C	C ₂₂	-13.3885860	12.1015979	-20.8460210
114	O	O ₁₂	-11.3193138	8.0348650	-24.4277266	167	C	C ₂₃	-3.5344157	7.5941443	-21.4210569
115	O	O ₁₃	-9.3736226	9.7096741	-26.5521337	168	C	C ₂₁	-20.6126513	17.8170670	2.8026081
116	O	O ₁₄	-5.2976693	14.8005262	-19.3800808	169	C	C ₂₂	-18.2108475	19.4029292	-7.5478047
117	O	O ₁₅	-4.4293163	14.6829078	-16.0782290	170	C	C ₂₃	-7.5433597	21.0173171	-6.0282078
118	O	O ₁₂	-4.5425940	15.3273384	-23.0744900	171	C	C ₂₁	-6.5836530	26.0758462	-4.0194233
119	O	O ₁₃	-6.7970736	17.7555827	-23.0282853	172	C	C ₂₂	-16.2722656	22.2671034	-1.7713222
120	O	O ₁₄	-12.7935058	12.4402823	-17.3970177	173	C	C ₂₃	-15.7676359	14.2000427	-9.0436867
121	O	O ₁₅	-12.7286925	9.9609882	-15.0564434	174	C	C ₂₁	-16.6618168	16.1635155	-14.3491768
122	C	C ₁₆	-12.2208244	19.3145890	-16.2249376	175	C	C ₂₂	-12.7387022	23.4627045	-7.3744497
123	C	C ₁₇	-12.1230756	10.0868339	-21.3014073	176	C	C ₂₃	-15.0298933	17.6018807	1.5309952
124	C	C ₁₆	-21.4225144	18.1449498	0.2230897	177	C	C ₂₁	-9.9839330	25.1848381	2.9455289
125	C	C ₁₇	-16.0115374	19.4444150	-8.5696706	178	C	C ₂₂	0.2023836	27.5485606	0.7631708
126	C	C ₁₆	-8.9098665	26.3921928	-2.6443456	179	C	C ₂₁	-23.0782563	14.0062310	-3.5257092
127	C	C ₁₇	-17.1571574	20.1344175	-2.4930592	180	C	C ₂₃	3.5120749	15.2715375	-16.9768259
128	C	C ₁₆	-15.6923025	18.6633128	-13.8729867	181	C	C ₂₁	0.3144785	17.1020807	-21.1847146
129	C	C ₁₇	-12.3062121	23.0786908	-5.0218986	182	C	C ₂₂	8.0606405	10.3136351	-24.2224575
130	C	C ₁₆	-8.2204976	26.7092319	1.5728297	183	C	C ₂₁	-16.5151802	5.3453187	-20.9630882
131	C	C ₁₆	-23.7616258	14.7665357	-1.0048471	184	C	C ₂₂	-7.6853228	10.5001030	-24.2145650
132	C	C ₁₆	12.1564346	4.9853203	-24.6076764	185	C	C ₂₃	-6.5667726	16.2634218	-15.0115393
133	C	C ₁₇	12.1594831	13.8508413	-19.0617985	186	C	C ₂₁	-0.2970100	10.3481213	-25.1377908
134	C	C ₁₆	1.5215586	15.5828545	-23.0871625	187	C	C ₂₂	-8.0302936	16.3266566	-20.7299893
135	C	C ₁₇	9.7066643	9.3221985	-22.7577207	188	C	C ₂₃	-13.5646996	7.8289394	-16.8472906
136	C	C ₁₆	-14.7452151	5.9170839	-22.9343415	189	C	C ₂₄	-10.8674319	21.2669195	-15.8543993
137	C	C ₁₇	-6.2181649	11.8262354	-22.8254303	190	C	C ₂₅	-13.0956798	12.5622059	-22.1389610
138	C	C ₁₆	-1.4096037	12.7990974	-24.7845484	191	C	C ₂₆	-3.2221246	6.2500680	-21.5838145
139	C	C ₁₇	-9.7254066	15.5755444	-19.1726986	192	C	C ₂₄	-21.6211283	18.7309089	2.5367272
140	C	C ₁₈	-11.4563986	18.7069001	-15.2488326	193	C	C ₂₅	-18.2596017	20.7881183	-7.6238157
141	C	C ₁₉	-12.8974025	10.8584229	-20.4482012	194	C	C ₂₆	-6.4697043	20.8169200	-6.8974143
142	C	C ₂₀	-2.5095776	8.5690225	-21.7162760	195	C	C ₂₄	-7.2635605	27.2706820	-4.1282534
143	C	C ₁₈	-20.4238038	17.2597272	0.5910890	196	C	C ₂₅	-17.0432053	22.9101419	-2.7413386
144	C	C ₁₉	-17.0754229	18.7342809	-8.0230432	197	C	C ₂₆	-16.3304965	12.9215421	-9.0179751
145	C	C ₂₀	-7.2733946	21.8560356	-4.9632278	198	C	C ₂₄	-17.3351820	17.2465832	-14.8660653
146	C	C ₁₈	-8.1388710	25.2482667	-2.5953562	199	C	C ₂₅	-13.8708569	24.1846216	-7.0215512
147	C	C ₁₉	-16.3308710	20.8793143	-1.6557409	200	C	C ₂₆	-14.4151182	17.6255653	2.7758799
148	C	C ₂₀	-15.3348352	14.6966571	-10.3018290	201	C	C ₂₄	-10.1530709	26.5401774	2.9615746
149	C	C ₁₈	-15.0905148	17.5125554	-13.4020759	202	C	C ₂₅	0.4723723	28.6003778	1.6475618
150	C	C ₁₉	-11.9580083	22.9195838	-6.3586326	203	C	C ₂₄	-24.2917326	14.6446209	-3.3301388
151	C	C ₂₀	-16.3540031	17.1135609	1.5211361	204	C	C ₂₅	13.1193948	13.3006799	-21.6322311
152	C	C ₁₈	-8.1392021	25.3237861	1.6259277	205	C	C ₂₆	3.1736578	15.9174562	-15.7678399
153	C	C ₁₉	1.0482151	26.4456100	0.7448946	206	C	C ₂₄	0.6822064	17.7006371	-22.3681395

207	C	C ₂₅	9.0692294	11.0875846	-24.7981401	260	C	C ₃₂	-12.4235075	27.3169569	-1.3876274
208	C	C ₂₄	-16.9965638	5.8314412	-22.1602177	261	C	C ₃₃	-14.4180036	24.6083891	0.4387298
209	C	C ₂₅	-8.2187996	11.6765821	-24.7210739	262	C	C ₃₄	-18.0258392	16.5341461	-3.1644112
210	C	C ₂₆	-5.3891205	16.7000174	-14.3759330	263	C	C ₃₅	-15.2375770	15.6642953	-5.6753674
211	C	C ₂₄	-0.6352460	11.0868642	-26.2571178	264	C	C ₃₂	-15.0188176	22.3610596	-13.3449757
212	C	C ₂₅	-9.0224739	16.4485566	-21.6982615	265	C	C ₃₃	-11.9641211	23.3601435	-11.0971594
213	C	C ₂₆	-14.2805235	7.7078604	-15.6560298	266	C	C ₃₄	-11.1027891	21.9417062	-1.6382182
214	C	C ₂₇	-11.9247153	20.6389959	-16.5172212	267	C	C ₃₅	-12.8629410	18.5999608	-1.3388602
215	C	C ₂₈	-12.3408587	11.7734904	-23.0065568	268	C	C ₃₂	-5.8714306	29.3420474	0.1051214
216	C	C ₂₉	-1.9337932	5.9168805	-22.0070042	269	C	C ₃₃	-2.6863459	28.2085296	-1.5249161
217	C	C ₂₇	-22.0276807	18.9011978	1.2223286	270	C	C ₃₂	-25.4340574	15.7226835	2.2815268
218	C	C ₂₈	-17.2022221	21.5031410	-8.1581694	271	C	C ₃₂	14.8014444	7.7426339	-24.6759447
219	C	C ₂₉	-5.2432138	21.4184848	-6.6508033	272	C	C ₃₄	10.1878015	15.3651858	-16.2282645
220	C	C ₂₇	-8.4575703	27.4512084	-3.4282996	273	C	C ₃₅	6.8401334	13.6516174	-16.6436258
221	C	C ₂₈	-17.8857621	22.1765284	-3.5709921	274	C	C ₃₂	3.3696403	14.1442727	-26.1249406
222	C	C ₂₉	-16.4963384	12.2164567	-10.2085983	275	C	C ₃₃	4.7163883	10.6867565	-25.8852763
223	C	C ₂₇	-16.8439202	18.5374195	-14.6380738	276	C	C ₃₄	11.6648862	7.4154566	-20.1240116
224	C	C ₂₈	-14.2223196	24.3473948	-5.6899038	277	C	C ₃₂	-12.8515130	7.1043905	-26.0575204
225	C	C ₂₇	-9.2323134	27.3355565	2.2694985	278	C	C ₃₃	-9.0744396	7.3406591	-25.8850141
226	C	C ₂₇	-24.6561924	15.0111589	-2.0434658	279	C	C ₃₄	-3.7848584	13.1845977	-20.3385612
227	C	C ₂₇	11.7889037	4.6420713	-25.9075628	280	C	C ₃₅	-5.9843344	13.2775882	-17.2351367
228	C	C ₂₈	12.3906643	14.4624778	-21.3865376	281	C	C ₃₂	-3.2215815	16.1474023	-24.9915957
229	C	C ₂₉	1.8788465	16.3974604	-15.6281419	282	C	C ₃₃	-4.7085679	17.6074540	-21.7613963
230	C	C ₂₇	1.2841255	16.9292915	-23.3528276	283	C	C ₃₄	-11.6679052	14.2408501	-16.2750166
231	C	C ₂₈	10.3835234	10.9974669	-24.3561213	284	C	C ₃₅	-11.0075523	10.4863305	-16.5954249
232	C	C ₂₇	-16.0920523	6.1316178	-23.1719671	285	C	C ₃₆	-14.7515887	18.6262101	-20.2774922
233	C	C ₂₈	-7.7698414	12.9029346	-24.2811948	286	C	C ₃₇	-17.1527724	13.9547689	-18.7605061
234	C	C ₂₉	-5.4737487	17.7315611	-13.4550336	287	C	C ₃₈	-10.3110280	5.7443900	-22.1917940
235	C	C ₂₇	-1.1882826	12.3455432	-26.0862127	288	C	C ₃₉	-6.6448046	8.3714748	-18.2913852
236	C	C ₂₈	-10.3335820	16.1085481	-21.4309900	289	C	C ₃₆	-22.9642191	20.9104652	-3.2919468
237	C	C ₂₉	-15.1394350	6.6385386	-15.4628230	290	C	C ₃₇	-22.3946556	17.2966407	-7.4304785
238	C	C ₃₀	-11.8626953	10.5406435	-22.5955240	291	C	C ₃₈	-11.9479558	19.1531725	-11.2210595
239	C	C ₃₁	-1.0293295	6.9239484	-22.2452375	292	C	C ₃₉	-10.5397641	17.5610800	-5.7143632
240	C	C ₃₀	-16.0863167	20.8377653	-8.6442819	293	C	C ₃₆	-13.4254365	28.1398651	-2.2638049
241	C	C ₃₁	-5.1098944	22.2340566	-5.5326420	294	C	C ₃₇	-15.1565915	24.9274553	1.7572208
242	C	C ₃₀	-17.9378636	20.7808364	-3.4339078	295	C	C ₃₈	-19.3987447	15.8272996	-3.2061618
243	C	C ₃₁	-16.0537768	12.8113336	-11.3869241	296	C	C ₃₉	-13.8256974	15.2733294	-5.1936504
244	C	C ₃₀	-13.4448711	23.7957206	-4.6812807	297	C	C ₃₆	-16.1867360	23.3702153	-13.1884889
245	C	C ₃₀	11.9351112	14.7441556	-20.1030410	298	C	C ₃₇	-10.9587835	24.4471950	-11.5560373
246	C	C ₃₁	1.0070431	16.2742428	-16.7014905	299	C	C ₃₈	-10.6961972	22.8118661	-0.4305871
247	C	C ₃₀	10.7022468	10.1070172	-23.3315253	300	C	C ₃₉	-12.2805820	17.3529367	-2.0166311
248	C	C ₃₀	-6.7516281	12.9855953	-23.3463146	301	C	C ₃₆	-5.7445668	30.7040700	0.8141873
249	C	C ₃₁	-6.6969960	18.3031333	-13.1966377	302	C	C ₃₇	-2.2828110	28.6474558	-2.9359363
250	C	C ₃₀	-10.6948157	15.6663210	-20.1634747	303	C	C ₃₆	-26.9761381	15.6513324	2.4520801
251	C	C ₃₁	-15.2532435	5.7105777	-16.4974101	304	C	C ₃₆	14.8926600	8.7118076	-25.8813579
252	C	C ₃₂	-14.7614799	18.0834784	-18.8328437	305	C	C ₃₈	10.3829892	16.8088290	-15.7166975
253	C	C ₃₃	-15.6757594	14.3915645	-18.7766681	306	C	C ₃₉	6.6415974	12.2502532	-16.0100756
254	C	C ₃₄	-10.1614279	6.9252019	-21.2108763	307	C	C ₃₆	4.3522242	15.0002695	-26.9495132
255	C	C ₃₅	-6.7878256	8.1558061	-19.8037142	308	C	C ₃₇	4.3488221	9.6266469	-26.9655056
256	C	C ₃₂	-22.7690822	19.4023674	-3.0712674	309	C	C ₃₉	9.6606147	9.4557113	-16.3765783
257	C	C ₃₃	-21.3797055	17.7092455	-6.3301562	310	C	C ₃₆	-13.3589180	8.2806079	-26.9528729
258	C	C ₃₄	-12.5792178	18.7257243	-9.8766924	311	C	C ₃₇	-8.1829680	6.6717702	-26.9606762
259	C	C ₃₅	-10.5266408	18.8091066	-6.6201771	312	C	C ₃₈	-2.6266340	14.1639476	-20.6272890

313	C	C ₃₉	-6.1145706	11.9928949	-16.3928218	366	C	C ₄₇	-10.8198414	17.5322388	-1.9684856
314	C	C ₃₆	-4.1454156	16.4763093	-26.1700888	367	C	C ₄₄	-5.6763755	30.3109157	2.2845938
315	C	C ₃₇	-4.3571998	19.0549873	-21.3863690	368	C	C ₄₅	-3.5710611	29.1176755	-3.5526642
316	C	C ₃₈	-13.0635924	14.7343416	-15.8070827	369	C	C ₄₄	-27.3242229	14.3320181	1.7389109
317	C	C ₃₉	-9.7128081	9.9067791	-15.9860853	370	C	C ₄₄	13.4287030	9.0120653	-26.1614170
318	C	C ₄₀	-12.7053302	19.2900238	-19.2539118	371	C	C ₄₆	9.4264351	16.9630770	-14.6038400
319	C	C ₄₁	-17.0973935	16.3631951	-18.8433167	372	C	C ₄₇	7.4841071	12.3036064	-14.7829398
320	C	C ₄₂	-8.5120808	4.1212875	-21.1731408	373	C	C ₄₄	5.0223407	15.8943339	-25.8806945
321	C	C ₄₃	-8.6098077	7.0871641	-18.6384474	374	C	C ₄₅	3.0931200	10.2113813	-27.5968208
322	C	C ₄₀	-21.6598117	20.6216138	-1.2888762	375	C	C ₄₇	9.3677814	7.9527258	-16.4295116
323	C	C ₄₁	-23.6473107	18.0716746	-5.5074978	376	C	C ₄₄	-14.1007257	9.1880940	-25.9619076
324	C	C ₄₂	-9.5080133	18.1825600	-11.1134980	377	C	C ₄₅	-9.1589302	5.6797780	-27.6232663
325	C	C ₄₃	-11.3659402	16.9126251	-7.8844632	378	C	C ₄₆	-1.8979889	14.3944760	-19.3639348
326	C	C ₄₀	-11.5774623	27.4817770	-3.6462911	379	C	C ₄₇	-4.8490434	11.2535762	-16.5714479
327	C	C ₄₁	-13.8584221	26.8643719	1.0787448	380	C	C ₄₄	-4.7537919	15.1442542	-26.5652780
328	C	C ₄₂	-18.6505155	13.3600956	-3.6765934	381	C	C ₄₅	-3.5405183	19.6121492	-22.5082685
329	C	C ₄₃	-15.3126099	15.2522488	-3.2819537	382	C	C ₄₆	-13.4248227	14.0416200	-14.5483913
330	C	C ₄₀	-17.0684681	21.1778897	-12.8970110	383	C	C ₄₇	-9.4395975	10.7778989	-14.7840192
331	C	C ₄₁	-12.6210859	24.1834386	-13.2768960	384	Cu	Cu ₄₈	-14.7208476	4.3634829	-18.9523480
332	C	C ₄₂	-9.9481342	20.9738109	1.3000066	385	Cu	Cu ₄₈	-0.0637733	15.1806831	-19.1895453
333	C	C ₄₃	-10.5985742	19.0290687	-2.0424081	386	Cu	Cu ₄₈	0.1315279	9.5824325	-22.3981096
334	C	C ₄₀	-6.6166210	29.1354691	2.3623200	387	Cu	Cu ₄₈	-9.5413584	18.4588519	-13.0437122
335	C	C ₄₁	-4.4722938	29.5410540	-2.4334969	388	Cu	Cu ₄₈	-14.6768030	14.5730338	-13.1133301
336	C	C ₄₀	-26.3741627	14.2958528	0.5663429	389	Cu	Cu ₄₈	-20.5335900	12.9622017	-3.0568372
337	C	C ₄₀	12.8137765	7.6077743	-25.9744007	390	Cu	Cu ₄₈	-18.7069007	15.7088457	2.4752646
338	C	C ₄₂	8.5805114	16.7030418	-13.8253193	391	Cu	Cu ₄₈	-9.1745301	22.5857127	2.2248243
339	C	C ₄₃	8.6651002	13.1949788	-15.0810880	392	H	H ₄₉	-11.0938067	8.1971784	-22.5151889
340	C	C ₄₀	3.9356654	16.1397771	-24.8665115	393	H	H ₅₀	-4.8436409	8.8722664	-20.9873445
341	C	C ₄₁	3.3143836	11.7046019	-27.5684409	394	H	H ₄₉	-14.1012492	20.0682197	-10.1592670
342	C	C ₄₃	9.9079266	7.5549535	-17.7787247	395	H	H ₅₀	-9.3959476	20.7331068	-5.7296523
343	C	C ₄₀	-14.7222133	8.1838956	-25.0084425	396	H	H ₄₉	-18.8257963	18.3952223	-3.2753623
344	C	C ₄₁	-10.4829983	6.4031548	-27.5960490	397	H	H ₅₀	-15.3803260	15.8102425	-8.1357715
345	C	C ₄₂	-1.6182923	14.4053187	-18.2070482	398	H	H ₄₉	-12.0839049	23.4988985	-2.5490460
346	C	C ₄₃	-4.3283969	11.6421492	-17.9339505	399	H	H ₅₀	-14.9395201	18.0587360	-0.2931689
347	C	C ₄₀	-3.6639854	14.1247044	-26.2546950	400	H	H ₄₉	11.2411649	15.8991455	-17.8944627
348	C	C ₄₁	-3.3973047	18.5665818	-23.5916692	401	H	H ₅₀	4.9252626	14.3888100	-17.9116108
349	C	C ₄₂	-13.3988864	13.1972838	-13.7102896	402	H	H ₄₉	11.9226510	8.4382618	-21.8638142
350	C	C ₄₃	-9.9828381	12.1643660	-15.1114289	403	H	H ₄₉	-4.6492981	13.6501991	-22.1345924
351	C	C ₄₄	-13.2550452	18.7166720	-20.5591081	404	H	H ₅₀	-7.2779596	15.1962468	-16.3947381
352	C	C ₄₅	-17.9172986	15.2131348	-18.3438116	405	H	H ₄₉	-11.8908727	15.2815151	-18.0331183
353	C	C ₄₆	-9.3806524	4.6974058	-21.7544374	406	H	H ₅₀	-12.1976657	8.8345984	-17.7426352
354	C	C ₄₇	-7.4451931	7.2702923	-17.6691041	407	H	H ₁₈	-11.6477009	17.8174464	-15.0489012
355	C	C ₄₄	-21.8093499	21.5154513	-2.4958391	408	H	H ₁₉	-13.0987317	10.5417267	-19.5967051
356	C	C ₄₅	-23.6895298	17.1879037	-6.7174336	409	H	H ₂₀	-2.7094460	9.4659717	-21.6254657
357	C	C ₄₆	-10.5685547	18.6712549	-11.3496496	410	H	H ₁₈	-20.0033323	16.7676518	-0.0753736
358	C	C ₄₇	-10.5917689	16.4109818	-6.6785402	411	H	H ₁₉	-17.0324130	17.8071648	-7.9711501
359	C	C ₄₄	-13.0902361	27.6963037	-3.6723837	412	H	H ₂₀	-7.9706195	22.0011784	-4.3651571
360	C	C ₄₅	-14.6555833	26.2547317	2.1801758	413	H	H ₁₈	-8.4447460	24.5497579	-2.0642684
361	C	C ₄₆	-19.1905556	14.3859096	-3.4542993	414	H	H ₁₉	-15.8132706	20.4462127	-1.0130205
362	C	C ₄₇	-14.0893382	14.5631799	-3.9150730	415	H	H ₂₀	-14.9333560	15.5330336	-10.3373467
363	C	C ₄₄	-17.1790837	22.5948528	-12.3443200	416	H	H ₁₈	-14.3167604	17.5969299	-12.8927202
364	C	C ₄₅	-11.2124243	24.6647563	-12.9823582	417	H	H ₁₉	-11.1880382	22.4431608	-6.5784455
365	C	C ₄₆	-10.2441059	21.9497847	0.6732320	418	H	H ₂₀	-16.7982067	17.0656468	0.7040175

419	H	H ₁₈	-7.4458396	24.9075406	1.1680306	472	H	H ₂₆	-14.1832908	8.3546712	-14.9922118
420	H	H ₁₉	0.8785137	25.7470835	0.1529657	473	H	H ₂₇	-12.4193574	21.1013299	-17.1540998
421	H	H ₁₈	-21.9744103	13.9592600	-0.6277536	474	H	H ₂₈	-12.1508253	12.0851845	-23.8622988
422	H	H ₁₈	11.6658958	4.6155163	-22.6978957	475	H	H ₂₉	-1.6975873	5.0195984	-22.1300697
423	H	H ₂₀	2.7562715	14.7303877	-18.7699451	476	H	H ₂₇	-22.6981508	19.5095431	1.0109275
424	H	H ₁₈	1.3374312	14.1969311	-21.6560143	477	H	H ₂₈	-17.2411688	22.4323577	-8.1921459
425	H	H ₁₉	7.7352289	8.8900038	-22.8260073	478	H	H ₂₉	-4.5216549	21.2791975	-7.2227102
426	H	H ₁₈	-13.4718094	5.2931305	-21.5287259	479	H	H ₂₇	-8.9327507	28.2484475	-3.4853224
427	H	H ₁₉	-6.3268734	9.8132122	-22.8906769	480	H	H ₂₈	-18.4003026	22.6028300	-4.2148830
428	H	H ₂₀	-8.5289964	16.5707022	-15.0071200	481	H	H ₂₉	-16.8840908	11.3730314	-10.2167178
429	H	H ₁₈	-1.2193196	12.2626551	-22.8746289	482	H	H ₂₇	-17.2735269	19.2820257	-14.9919841
430	H	H ₁₉	-7.7546866	15.8131559	-18.7890677	483	H	H ₂₈	-14.9922496	24.8238816	-5.4712867
431	H	H ₂₀	-13.3037964	6.9310453	-18.6014561	484	H	H ₂₇	-9.3074366	28.2627696	2.2804638
432	H	H ₂₁	-9.4822963	20.9796459	-14.4452477	485	H	H ₂₇	-25.4783403	15.4170567	-1.8824558
433	H	H ₅₁	-14.0050877	12.5201196	-19.0642889	486	H	H ₂₇	12.2413824	5.0161196	-26.6302386
434	H	H ₅₁	-18.9912569	17.8368707	-6.7902789	487	H	H ₂₈	12.2145755	15.0566515	-22.0817227
435	H	H ₂₁	-5.8007420	25.9767619	-4.5068744	488	H	H ₂₉	1.6028484	16.7987689	-14.8354337
436	H	H ₅₁	-14.9083503	22.5116954	-0.4791346	489	H	H ₂₇	1.5270291	17.3066466	-24.1687236
437	H	H ₂₁	-17.0066403	15.3101310	-14.5092193	490	H	H ₂₈	11.0480235	11.5125213	-24.7455155
438	H	H ₅₁	-11.8181300	22.5085135	-8.7552734	491	H	H ₂₇	-16.3903126	6.4626073	-23.9868591
439	H	H ₂₁	-10.5921551	24.6572912	3.4139662	492	H	H ₂₈	-8.1520879	13.6882404	-24.6128853
440	H	H ₅₁	-1.1535858	26.7743533	-0.3650045	493	H	H ₂₉	-4.7116228	18.0335094	-13.0205281
441	H	H ₂₁	-22.8486652	13.7537976	-4.3894769	494	H	H ₂₇	-1.4080430	12.8689292	-26.8182831
442	H	H ₂₁	-0.1202380	17.6238465	-20.5500782	495	H	H ₂₈	-10.9764515	16.1718158	-22.1026281
443	H	H ₅₁	6.1836280	10.0093692	-24.0521850	496	H	H ₂₉	-15.6179092	6.5342567	-14.6756964
444	H	H ₂₁	-17.1282619	5.1510237	-20.2947273	497	H	H ₃₀	-11.3706993	10.0148145	-23.1813960
445	H	H ₅₁	-8.0683447	8.6222920	-23.9884594	498	H	H ₃₁	-0.1717722	6.6764059	-22.5152867
446	H	H ₂₁	0.0856912	9.5143345	-25.2686168	499	H	H ₃₀	-15.3825563	21.3193061	-9.0154799
447	H	H ₅₁	-6.1225889	16.3004034	-20.4125488	500	H	H ₃₁	-4.2894145	22.6337790	-5.3594630
448	H	H ₂₄	-10.6318495	22.1399039	-16.0553927	501	H	H ₃₀	-18.5027987	20.2910221	-3.9800470
449	H	H ₂₅	-13.4140019	13.3854747	-22.4195702	502	H	H ₃₁	-16.1767717	12.3499732	-12.1837195
450	H	H ₂₆	-3.8550571	5.5909070	-21.4154647	503	H	H ₃₀	-13.6807103	23.9088402	-3.7907297
451	H	H ₂₄	-22.0050625	19.2325576	3.2232005	504	H	H ₃₀	11.4654442	15.5324921	-19.9367776
452	H	H ₂₅	-19.0119071	21.2333931	-7.3149652	505	H	H ₃₁	0.1433915	16.6068146	-16.6041153
453	H	H ₂₆	-6.5746430	20.2627333	-7.6413976	506	H	H ₃₀	11.5774873	10.0417688	-23.0282112
454	H	H ₂₄	-6.9308164	27.9563356	-4.6602929	507	H	H ₃₀	-6.4220104	13.8136132	-23.0779454
455	H	H ₂₅	-16.9994455	23.8341485	-2.8288125	508	H	H ₃₁	-6.7405599	19.0084461	-12.5920669
456	H	H ₂₆	-16.6009813	12.5448214	-8.2090620	509	H	H ₃₀	-11.5779776	15.4423532	-19.9799211
457	H	H ₂₄	-18.1110591	17.1237374	-15.3601341	510	H	H ₃₁	-15.8077368	4.9741476	-16.3811759
458	H	H ₂₅	-14.3930744	24.5787051	-7.6865364	511	H	H ₃₂	-15.5689459	18.3812194	-18.3534459
459	H	H ₂₆	-13.5385204	17.9430141	2.8463268	512	H	H ₃₃	-15.2033863	14.0688450	-17.9821833
460	H	H ₂₄	-10.8592979	26.9316157	3.4261179	513	H	H ₃₄	-10.4626634	6.6526788	-20.3191314
461	H	H ₂₅	-0.0824975	29.3438884	1.6635688	514	H	H ₃₅	-6.8239844	9.0296328	-20.2381497
462	H	H ₂₄	-24.8518507	14.8099774	-4.0506965	515	H	H ₃₂	-23.6181640	18.9148874	-3.1006574
463	H	H ₂₅	13.4143736	13.1146992	-22.4956453	516	H	H ₃₃	-20.8293529	16.9511703	-6.0403603
464	H	H ₂₆	3.7997047	16.0086775	-15.0884157	517	H	H ₃₄	-12.6369573	17.7558407	-9.8187359
465	H	H ₂₄	0.5264758	18.6079210	-22.5105289	518	H	H ₃₅	-11.0481275	19.5229228	-6.1910357
466	H	H ₂₅	8.8610265	11.6817808	-25.4869698	519	H	H ₃₂	-12.1939387	27.8063795	-0.5691811
467	H	H ₂₄	-17.9108895	5.9447911	-22.2915650	520	H	H ₃₃	-13.7858767	23.8713579	0.5534730
468	H	H ₂₅	-8.8892176	11.6330834	-25.3686120	521	H	H ₃₄	-17.4771041	16.1558412	-2.4447304
469	H	H ₂₆	-4.5729566	16.3017592	-14.5732436	522	H	H ₃₅	-15.2013771	16.5266989	-6.1345193
470	H	H ₂₄	-0.4966953	10.7400333	-27.1084481	523	H	H ₃₂	-14.5616572	22.4853467	-14.1995001
471	H	H ₂₅	-8.7924189	16.7557854	-22.5467532	524	H	H ₃₃	-11.5020548	22.5161015	-10.9301267

525	H	H ₃₄	-10.2999243	21.4957238	-1.9771480	578	C	C ₅₅	10.0351412	8.3766198	-21.6568584
526	H	H ₃₅	-13.6701040	18.8953733	-1.8104375	579	C	C ₅₅	-5.1706851	11.8833788	-21.7748681
527	H	H ₃₂	-6.3166604	29.4539749	-0.7605301	580	C	C ₅₅	-10.0606243	15.0910754	-17.7980933
528	H	H ₃₃	-2.7846881	27.2323685	-1.5045216	581	Cu	Cu ₄₈	-5.7834796	23.5589457	-3.1764553
529	H	H ₃₂	-25.1413951	16.6591729	2.2621583	582	H	H ₃₆	-15.1884406	18.0063853	-20.8841402
530	H	H ₃₅	6.8327921	13.5909950	-17.6203643	583	H	H ₃₇	-17.4354928	13.6523416	-19.6412146
531	H	H ₃₂	2.5935004	13.8722196	-26.6607149	584	H	H ₃₈	-11.2218017	5.4085053	-22.1771362
532	H	H ₃₃	4.3771560	10.3835088	-25.0175817	585	H	H ₃₉	-5.7095668	8.3037061	-18.0295476
533	H	H ₃₄	10.9362834	6.8077727	-19.8700181	586	H	H ₃₆	-22.9037586	21.1434668	-4.2305980
534	H	H ₃₅	11.0428342	10.4066809	-17.6145650	587	H	H ₃₇	-22.4375586	17.9763078	-8.1253435
535	H	H ₃₂	-12.8360761	6.2661979	-26.5539137	588	H	H ₃₈	-12.4809965	18.8072352	-11.9498642
536	H	H ₃₃	-8.8637951	6.9682214	-25.0009351	589	H	H ₃₉	-9.7392003	17.5237686	-5.1675134
537	H	H ₃₄	-3.4232999	12.3204490	-20.0498373	590	H	H ₃₆	-14.3426865	27.9173988	-2.0409932
538	H	H ₃₅	-6.8143991	13.4576895	-17.7208615	591	H	H ₃₇	-16.1167307	24.9528769	1.6103966
539	H	H ₃₂	-2.4436389	16.7386072	-24.9904981	592	H	H ₃₈	-19.8591153	15.9497583	-2.3617070
540	H	H ₃₃	-4.4008401	16.9846229	-21.0705716	593	H	H ₃₉	-13.3806065	14.7005689	-5.8322053
541	H	H ₃₄	-10.9934489	14.3375621	-15.5714371	594	H	H ₃₆	-15.8953180	24.1735868	-12.7444799
542	H	H ₃₅	-10.9490147	10.4533966	-17.5736255	595	H	H ₃₇	-11.0935239	25.2708554	-11.0598027
543	H	H ₄₂	-7.8421779	3.6719115	-20.7164565	596	H	H ₃₈	-9.9775777	23.4095257	-0.6905976
544	H	H ₄₂	-8.6809220	17.7959086	-10.9309299	597	H	H ₃₉	-12.5425641	16.5485780	-1.5432771
545	H	H ₄₂	-18.2245660	12.5469201	-3.8522907	598	H	H ₃₆	-4.9442210	31.1732389	0.5360632
546	H	H ₄₂	-9.7132079	20.2247317	1.7937862	599	H	H ₃₇	-1.6334633	29.3765451	-2.8997320
547	H	H ₄₂	7.9111573	16.4960871	-13.2086675	600	H	H ₃₆	15.3850183	9.5116197	-25.6532755
548	H	H ₄₂	-1.4018294	14.4122101	-17.3036939	601	H	H ₃₉	5.7113624	12.0948562	-15.7864199
549	H	H ₄₂	-13.3751138	12.5412592	-13.0575640	602	H	H ₃₆	5.0086324	14.4517910	-27.4013609
550	N	N ₅₂	-1.2928196	8.2165017	-22.1084992	603	H	H ₃₇	5.0590699	9.5417167	-27.6205712
551	N	N ₅₂	-6.1314907	22.4570609	-4.7052845	604	H	H ₃₉	9.7323518	9.7753534	-15.4616405
552	N	N ₅₂	-15.4779108	14.0082553	-11.4266871	605	H	H ₃₆	-12.6242842	8.7407101	-27.3743630
553	N	N ₅₂	-17.0047566	16.7028905	2.6053739	606	H	H ₃₇	-7.8555524	7.3289932	-27.5951630
554	N	N ₅₂	1.3129316	15.6886572	-17.8543530	607	H	H ₃₈	-2.0273971	13.7875950	-21.2909072
555	N	N ₅₂	-7.8323659	17.8832114	-13.7664813	608	H	H ₃₉	-6.2552761	12.2168347	-15.4555004
556	N	N ₅₂	-14.5927322	5.8336671	-17.6597346	609	H	H ₃₆	-4.8303355	17.1029412	-25.9070272
557	N	N ₅₃	-14.1076272	12.7886468	-19.8758557	610	H	H ₃₇	-5.1636491	19.5846239	-21.2674128
558	N	N ₅₃	-19.2356968	18.6286269	-7.0350835	611	H	H ₃₈	-13.0428501	15.6940201	-15.6634181
559	N	N ₅₃	-15.4752568	22.9833025	-0.9217910	612	H	H ₃₉	-9.8420452	8.9844446	-15.7139321
560	N	N ₅₃	-12.3482093	23.1802207	-8.6695270	613	H	H ₃₆	-15.1763157	19.4910744	-20.3377891
561	N	N ₅₃	-0.9101732	27.5366791	-0.0623270	614	H	H ₃₇	-17.2953023	13.2337974	-18.1258313
562	N	N ₅₃	6.7495908	10.3532551	-24.5988430	615	H	H ₃₈	-10.1000080	6.0267780	-23.0936802
563	N	N ₅₃	-8.1733285	9.2462051	-24.5677042	616	H	H ₃₉	-6.9826829	9.2358708	-18.0349932
564	N	N ₅₃	-6.6996700	16.6291043	-20.9579713	617	H	H ₃₆	-23.8211903	21.2070049	-2.9446075
565	O	O ₅₄	-14.0231925	17.8135558	-16.2890959	618	H	H ₃₇	-22.1408289	16.4538251	-7.8333164
566	O	O ₅₄	-21.9754303	17.1436272	-1.8247777	619	H	H ₃₈	-11.9524169	20.1261527	-11.2839723
567	O	O ₅₄	-10.1560416	25.9699259	-0.7445136	620	H	H ₃₉	-11.3173178	17.5620990	-5.1322338
568	O	O ₅₄	-13.8379029	20.0432339	-13.7153164	621	H	H ₃₆	-13.2876400	29.0881543	-2.1515990
569	O	O ₅₄	-6.9255283	26.9515537	-0.3065163	622	H	H ₃₇	-14.9611731	24.2570122	2.4277299
570	O	O ₅₄	-23.0785769	15.6688512	1.0488555	623	H	H ₃₈	-19.9440299	16.2052031	-3.9104854
571	O	O ₅₄	1.5996715	13.5553900	-24.1680726	624	H	H ₃₉	-13.2782178	16.0652552	-5.0418298
572	O	O ₅₄	-12.7541234	5.3069318	-24.0341075	625	H	H ₃₆	-16.5680141	23.5955172	-14.0531476
573	O	O ₅₄	-1.4486834	14.8126241	-23.6145488	626	H	H ₃₇	-10.0452102	24.1489574	-11.4161009
574	C	C ₅₅	-11.4985111	8.8271072	-20.7749204	627	H	H ₃₈	-11.4493787	23.3440752	-0.1444518
575	C	C ₅₅	-14.8012904	18.7038039	-9.0172749	628	H	H ₃₉	-12.5888856	17.2877827	-2.9361401
576	C	C ₅₅	-17.1604668	18.6577829	-2.3413075	629	H	H ₃₆	-6.5191110	31.2655703	0.6374264
577	C	C ₅₅	-11.4637068	22.4024188	-3.9889884	630	H	H ₃₇	-1.8984766	27.9157126	-3.4382881

631	H	H ₃₆	-27.4135220	16.4055863	2.0291053	684	H	H ₄₀	-7.4863119	29.4103795	2.7002637
632	H	H ₃₆	15.3171990	8.2801482	-26.6433640	685	H	H ₄₁	-4.4301151	30.5017036	-2.3133932
633	H	H ₃₈	10.1933973	17.4481722	-16.4205140	686	H	H ₄₀	-26.7895025	14.6779361	-0.2200306
634	H	H ₃₉	6.9455811	11.5514419	-16.6093455	687	H	H ₄₀	12.8370977	7.1218999	-26.8134173
635	H	H ₃₆	3.8813761	15.5397146	-27.6048609	688	H	H ₄₃	9.4292115	12.6816312	-15.3833033
636	H	H ₃₇	4.1720827	8.7672347	-26.5668043	689	H	H ₄₀	3.4935816	16.9888984	-25.0338151
637	H	H ₃₉	8.9783212	9.9697266	-16.8370467	690	H	H ₄₁	2.4670761	12.1874091	-27.5760238
638	H	H ₃₆	-13.9654165	7.9486944	-27.6378823	691	H	H ₄₃	9.2270327	7.6562610	-18.4614898
639	H	H ₃₇	-7.4325743	6.2140789	-26.5565451	692	H	H ₄₀	-15.5848380	7.8892643	-25.3439846
640	H	H ₃₈	-2.9734530	15.0025628	-20.9660937	693	H	H ₄₁	-11.2222914	5.7757747	-27.6886800
641	H	H ₃₉	-6.8700091	11.4634520	-16.6965598	694	H	H ₄₃	-4.6194259	11.0116560	-18.6079566
642	H	H ₃₆	-3.6367260	16.8499218	-26.9081549	695	H	H ₄₀	-3.1438242	13.9234940	-27.0516480
643	H	H ₃₇	-3.8496455	19.0819883	-20.5591764	696	H	H ₄₁	-2.4587559	18.3988549	-23.7902210
644	H	H ₃₈	-13.7293312	14.5442000	-16.4876459	697	H	H ₄₃	-9.2820398	12.7362844	-15.4545556
645	H	H ₃₉	-8.9823870	9.9505661	-16.6186428	698	H	H ₄₄	-13.0771822	19.3050757	-21.3061502
646	H	H ₄₀	-11.7758463	19.0508073	-19.1323392	699	H	H ₄₅	-18.8006380	15.2175898	-18.7453666
647	H	H ₄₁	-17.3693571	16.6263787	-19.7352878	700	H	H ₄₇	-7.7639827	7.5259007	-16.7897045
648	H	H ₄₃	-8.8893178	6.1641069	-18.6662761	701	H	H ₄₄	-20.9957139	21.5217077	-3.0242762
649	H	H ₄₀	-20.7296517	20.5659831	-1.0105474	702	H	H ₄₅	-23.8429345	16.2627770	-6.4542861
650	H	H ₄₁	-24.0748205	18.9202475	-5.6854085	703	H	H ₄₇	-11.0393784	15.6477120	-6.2787486
651	H	H ₄₃	-10.9860603	16.5563224	-8.7076711	704	H	H ₄₄	-13.3293535	28.3862261	-4.3153461
652	H	H ₄₀	-11.3282977	26.7580363	-4.2357255	705	H	H ₄₅	-14.1074729	26.1629867	2.9732646
653	H	H ₄₁	-14.2979898	27.6513377	0.7324651	706	H	H ₄₇	-13.3218676	14.6194827	-3.3256482
654	H	H ₄₃	-15.8590302	14.6157517	-2.7922393	707	H	H ₄₄	-18.0792144	22.9459763	-12.4474143
655	H	H ₄₀	-17.3085627	20.5247108	-12.2226017	708	H	H ₄₅	-10.5688203	24.1702280	-13.5158257
656	H	H ₄₁	-13.2478872	24.9189630	-13.2787983	709	H	H ₄₇	-10.3895824	17.0908690	-2.7195901
657	H	H ₄₃	-9.8118281	19.2870041	-1.5368533	710	H	H ₄₄	-4.7735743	30.0623413	2.5369702
658	H	H ₄₀	-6.2635391	28.4528965	2.9609909	711	H	H ₄₅	-3.4079336	29.8597405	-4.1562065
659	H	H ₄₁	-5.3875431	29.2888860	-2.6228494	712	H	H ₄₄	-27.1809496	13.5670121	2.3268598
660	H	H ₄₀	-26.1086412	13.3832232	0.3673896	713	H	H ₄₄	13.2930321	9.3451754	-27.0626686
661	H	H ₄₀	11.8963581	7.6798117	-25.6803541	714	H	H ₄₇	7.7899639	11.4145473	-14.5439033
662	H	H ₄₃	8.9236580	13.7123814	-14.2975627	715	H	H ₄₄	5.7782338	15.4438813	-25.4780004
663	H	H ₄₀	4.3030564	16.1554715	-23.9679750	716	H	H ₄₅	2.9873232	9.8987866	-28.5103723
664	H	H ₄₁	3.8500083	12.0012586	-28.3173536	717	H	H ₄₄	-13.4817079	9.7806186	-25.5008893
665	H	H ₄₃	10.1915864	6.6216932	-17.7660150	718	H	H ₄₅	-8.8865565	5.4958670	-28.5361281
666	H	H ₄₀	-14.8449165	8.5734952	-24.1331168	719	H	H ₄₇	-5.0070192	10.3006262	-16.5240226
667	H	H ₄₁	-10.5415597	7.0705800	-28.2913581	720	H	H ₄₄	-4.9825513	15.1272818	-27.5068549
668	H	H ₄₃	-3.3567628	11.6765128	-17.9327600	721	H	H ₄₅	-2.6632105	19.8714889	-22.1808025
669	H	H ₄₀	-4.0497756	13.2940977	-25.9249255	722	H	H ₄₇	-8.4825612	10.8299208	-14.6137412
670	H	H ₄₁	-3.8394236	18.8474671	-24.4083315	723	H	H ₄₄	-12.8808272	17.8398063	-20.7454294
671	H	H ₄₃	-10.3777469	12.5705770	-14.3292707	724	H	H ₄₅	-18.0117173	15.2435894	-17.3805008
672	H	H ₄₀	-12.7958135	20.2532156	-19.2314929	725	H	H ₄₇	-6.9270064	6.4531431	-17.5932149
673	H	H ₄₁	-17.1881920	17.1322813	-18.2505233	726	H	H ₄₄	-22.0153060	22.4231194	-2.2257517
674	H	H ₄₃	-9.3599219	7.6401648	-18.3738856	727	H	H ₄₅	-24.4155151	17.4565114	-7.3041503
675	H	H ₄₀	-22.1915548	20.9412866	-0.5473554	728	H	H ₄₇	-9.6937842	16.1402869	-6.9360575
676	H	H ₄₁	-24.0941621	17.6448235	-4.7554273	729	H	H ₄₄	-13.5520812	26.8782998	-3.9028962
677	H	H ₄₃	-12.2953936	16.6478241	-7.8312757	730	H	H ₄₅	-15.4060307	26.8357828	2.3965023
678	H	H ₄₀	-11.1163257	28.2891285	-3.9239157	731	H	H ₄₇	-14.2774878	13.6227543	-4.0859773
679	H	H ₄₁	-12.9769612	27.1133156	1.3990508	732	H	H ₄₄	-16.9366860	22.6242102	-11.4031887
680	H	H ₄₃	-15.0416379	15.9628589	-2.6829499	733	H	H ₄₅	-11.1304285	25.6062419	-13.1990650
681	H	H ₄₀	-17.6555952	21.0643481	-13.6638665	734	H	H ₄₇	-10.4522054	17.1761023	-1.1457450
682	H	H ₄₁	-12.6595500	23.7368571	-14.1416842	735	H	H ₄₄	-5.9738204	31.0403815	2.8554531
683	H	H ₄₃	-10.4861945	19.3158651	-2.9625262	736	H	H ₄₅	-3.9784724	28.3950165	-4.0597445

737	H	H ₄₄	-28.2471853	14.3246603	1.4409850	790	C	C ₂	-21.7686624	-18.8141093	4.0493022
738	H	H ₄₄	13.0633931	9.6484209	-25.5247140	791	C	C ₃	1.6509985	13.3137224	25.3805945
739	H	H ₄₇	6.9733826	12.6620980	-14.0383911	792	C	C ₃	18.8801922	19.3467681	-9.6641939
740	H	H ₄₄	5.3255076	16.7311363	-26.2717313	793	C	C ₃	1.6543565	-13.3138108	-25.3803326
741	H	H ₄₅	2.3039516	9.9671528	-27.0890029	794	C	C ₃	18.8776042	-19.3477838	9.6672156
742	H	H ₄₇	8.4147502	7.7824035	-16.3639973	795	C	C ₃	-20.5326282	-18.8610596	6.8430392
743	H	H ₄₄	-14.7758078	9.7225490	-26.4093705	796	C	C ₄	-4.4418689	14.5419726	18.8159649
744	H	H ₄₅	-9.1988375	4.8544960	-27.1276498	797	C	C ₄	16.1434478	17.9802601	-1.1571983
745	H	H ₄₇	-4.2159304	11.5014502	-15.8789485	798	C	C ₄	-4.4396358	-14.5417332	-18.8166787
746	H	H ₄₄	-5.5532063	14.9585782	-26.0445725	799	C	C ₄	16.1422998	-17.9811296	1.1597882
747	H	H ₄₅	-3.9716221	20.4037986	-22.8703191	800	C	C ₄	-11.7033353	-19.2853604	8.7376495
748	H	H ₄₇	-9.8743505	10.4255334	-13.9961479	801	C	C ₅	-4.2171349	15.4010401	15.8591273
749	O	O ₅₆	-11.4595822	8.6347156	-19.5272593	802	C	C ₅	13.3812942	18.0937044	0.2172094
750	O	O ₅₆	-14.5996515	17.5496747	-8.5755508	803	C	C ₅	-4.2154190	-15.4008119	-15.8598105
751	O	O ₅₆	-16.2073066	18.1050780	-1.7902766	804	C	C ₅	13.3803507	-18.0944231	-0.2150749
752	O	O ₅₆	-10.6633980	21.5017785	-4.3040686	805	C	C ₅	-9.1656199	-19.3328328	6.9800552
753	O	O ₅₆	9.1274013	7.9024876	-21.0009692	806	C	C ₁	-0.4008177	23.3694285	16.1734964
754	O	O ₅₆	-4.9755660	10.8561001	-21.0940308	807	C	C ₁	10.5707813	26.3576852	-1.1848906
755	O	O ₅₆	-9.1204881	14.7835604	-17.0447493	808	C	C ₁	-0.3994909	-23.3694062	-16.1735653
756	C	C ₁	-10.4999864	11.6039873	23.7644179	809	C	C ₁	10.5691679	-26.3582530	1.1865774
757	C	C ₁	23.8275089	15.5199209	1.0157577	810	C	C ₁	-10.1706807	-26.4752868	1.8679595
758	C	C ₁	-10.4968117	-11.6034225	-23.7660981	811	C	C ₂	1.7787158	22.6482839	18.0850589
759	C	C ₁	23.8268318	-15.5212033	-1.0119411	812	C	C ₂	11.2184173	26.4673717	-4.0991666
760	C	C ₁	-13.3306289	-18.6053141	16.9052186	813	C	C ₂	1.7803920	-22.6483805	-18.0847694
761	C	C ₂	-11.1540916	9.0030965	25.2091762	814	C	C ₂	11.2163358	-26.4679767	4.1009707
762	C	C ₂	25.7697240	13.2975489	0.2616587	815	C	C ₂	-12.9977178	-25.9443759	1.0614351
763	C	C ₂	-11.1505305	-9.0024961	-25.2109635	816	C	C ₃	3.5646090	20.8396238	19.5634923
764	C	C ₂	25.7690534	-13.2989355	-0.2575328	817	C	C ₃	11.8529926	25.3700295	-6.7523980
765	C	C ₂	-14.6190245	-16.5751212	18.7755573	818	C	C ₃	3.5666266	-20.8398153	-19.5629237
766	C	C ₃	-11.6486912	6.0621429	25.4575652	819	C	C ₃	11.8505492	-25.3706675	6.7542973
767	C	C ₃	26.6610912	10.4731921	-0.1673204	820	C	C ₃	-15.4180927	-24.3221236	0.6658164
768	C	C ₃	-11.6449403	-6.0615150	-25.4594370	821	C	C ₄	2.4060852	11.9504573	20.9376733
769	C	C ₃	26.6604948	-10.4746275	0.1715939	822	C	C ₄	14.9110227	17.0390713	-8.6209402
770	C	C ₃	-15.0159538	-13.8960948	20.0486630	823	C	C ₄	2.4088012	-11.9505856	-20.9372955
771	C	C ₄	-14.7779962	0.4780680	18.9382768	824	C	C ₄	14.9087287	-17.0398729	8.6233234
772	C	C ₄	23.4820713	3.0353762	4.0810122	825	C	C ₄	-17.3181110	-16.3315429	4.5113830
773	C	C ₄	-14.7749825	-0.4772730	-18.9406426	826	C	C ₅	0.1027566	9.9834824	20.1643037
774	C	C ₄	23.4825674	-3.0366398	-4.0772520	827	C	C ₅	15.6915987	14.6245919	-6.7951761
775	C	C ₄	-8.7077192	-7.3780648	21.1427490	828	C	C ₅	0.1054551	-9.9834891	-20.1642803
776	C	C ₅	-15.6886756	1.0257936	16.0821261	829	C	C ₅	15.6897295	-14.6254372	6.7976939
777	C	C ₅	21.4192958	2.7093203	6.3003855	830	C	C ₅	-15.7956954	-14.5939966	6.6174687
778	C	C ₅	-15.6861570	-1.0249501	-16.0846344	831	C	C ₁	-7.0091750	13.4911407	24.1067503
779	C	C ₅	21.4201585	-2.7104745	-6.2969467	832	C	C ₁	22.0970260	17.9244276	-1.6466039
780	C	C ₅	-5.7341516	-7.3197232	20.4783479	833	C	C ₁	-7.0060343	-13.4907627	-24.1078778
781	C	C ₁	7.2370623	13.9004955	23.7610401	834	C	C ₁	22.0958034	-17.9256158	1.6501369
782	C	C ₁	14.6187088	20.3229106	-13.5446838	835	C	C ₁	-15.0904300	-19.9839045	13.6087216
783	C	C ₁	7.2401214	-13.9008854	-23.7598786	836	C	C ₂	-6.6739297	16.3263945	23.1711719
784	C	C ₁	14.6154466	-20.3236968	13.5470223	837	C	C ₂	20.7143773	20.4518848	-0.7941881
785	C	C ₁	-21.8562559	-18.1955483	1.1882648	838	C	C ₂	-6.6711071	-16.3260357	-23.1722387
786	C	C ₂	4.6603390	13.7877614	25.1479839	839	C	C ₂	20.7131470	-20.4530000	0.7975081
787	C	C ₂	17.1073532	20.1842271	-12.0073965	840	C	C ₂	-14.0428254	-22.4128832	12.1843105
788	C	C ₂	4.6636242	-13.7880126	-25.1472354	841	C	C ₃	-5.5611013	18.4495265	21.3297236
789	C	C ₂	17.1043455	-20.1851476	12.0101355	842	C	C ₃	18.2744153	22.1850537	-0.3702306

843	C	C ₃	-5.5586770	-18.4492275	-21.3306130	896	C	C ₃	9.1764163	18.2247406	-20.2245072
844	C	C ₃	18.2731622	-22.1860370	0.3731559	897	C	C ₃	15.3537601	-11.0178860	-21.6390092
845	C	C ₃	-12.7153310	-23.8190595	9.8610723	898	C	C ₃	9.1721941	-18.2252334	20.2259712
846	C	C ₄	1.9023647	17.8666710	16.1754980	899	C	C ₃	-24.5265179	-13.7128201	-5.9822088
847	C	C ₄	10.2293140	21.4314866	-4.5316805	900	C	C ₄	-21.9537807	5.3270522	8.1768145
848	C	C ₄	1.9040001	-17.8667739	-16.1751904	901	C	C ₄	17.1729690	3.9215897	16.3375841
849	C	C ₄	10.2274339	-21.4320359	4.5333119	902	C	C ₄	4.7810691	10.3732182	-21.1363209
850	C	C ₄	-12.1322236	-20.8721572	1.2829117	903	C	C ₄	17.1753752	-3.9225144	-16.3348311
851	C	C ₅	4.0007171	15.6627850	15.8019761	904	C	C ₄	4.7771274	-10.3734751	21.1370843
852	C	C ₅	9.1851246	19.5374378	-6.7046791	905	C	C ₄	-21.9527601	-5.3258707	-8.1803309
853	C	C ₅	4.0024019	-15.6630023	-15.8013243	906	C	C ₅	-21.1761665	2.9003118	6.4954684
854	C	C ₅	9.1830053	-19.5379330	6.7061557	907	C	C ₅	15.7056937	1.2922321	15.8333291
855	C	C ₅	-13.1861151	-18.3614133	-0.1260570	908	C	C ₅	5.4706264	7.5153103	-20.3131863
856	C	C ₁	0.2241396	25.4126751	12.7630176	909	C	C ₅	15.7081655	-1.2930773	-15.8308139
857	C	C ₁	7.0473617	27.5492210	0.3521832	910	C	C ₅	5.4669654	-7.5156039	20.3140576
858	C	C ₁	0.2248197	-25.4126871	-12.7629819	911	C	C ₅	-21.1752845	-2.8991730	-6.4988547
859	C	C ₁	7.0459332	-27.5495997	-0.3510574	912	C	C ₁	-28.2419588	1.5195996	1.2598304
860	C	C ₁	-7.2718086	-27.4832482	-0.7353746	913	C	C ₁	14.9729577	-2.3802561	23.9091901
861	C	C ₂	-2.0204672	26.7208734	11.1011744	914	C	C ₁	-28.2418361	-1.5180802	-1.2643506
862	C	C ₂	6.5591370	28.0543043	3.3551701	915	C	C ₁	14.9769161	2.3794508	-23.9067951
863	C	C ₂	-2.0201308	-26.7207648	-11.1014968	916	C	C ₁	13.2648535	-5.9198053	24.3002914
864	C	C ₂	6.5581672	-28.0546577	-3.3541172	917	C	C ₂	14.6386954	8.4893935	-23.3695376
865	C	C ₂	-4.5391311	-28.6480536	0.0935210	918	C	C ₂	-28.5118266	4.4130852	0.3113453
866	C	C ₃	-3.7542899	27.0401219	8.8402938	919	C	C ₂	13.8733020	0.1107618	25.2985374
867	C	C ₃	5.4495402	27.5379668	5.9478163	920	C	C ₂	-28.5120184	-4.4115503	-0.3159146
868	C	C ₃	-3.7543252	-27.0399203	-8.8408922	921	C	C ₂	13.8773472	-0.1115094	-25.2963098
869	C	C ₃	5.4490112	-27.5382593	-5.9469483	922	C	C ₂	14.6345003	-8.4901808	23.3718794
870	C	C ₃	-1.6957781	-28.6413272	0.4608627	923	C	C ₃	14.9607163	10.9371368	-21.8102721
871	C	C ₄	4.3825234	23.3653155	3.7541770	924	C	C ₃	-27.7016492	7.1935122	-0.0618491
872	C	C ₄	-2.4198416	23.9419839	0.4050666	925	C	C ₃	12.7412162	2.7965966	25.4749378
873	C	C ₄	-1.9617637	22.6541978	7.8852501	926	C	C ₃	-27.7020491	-7.1920215	0.0574134
874	C	C ₄	-2.4210700	-23.9418544	-0.4054495	927	C	C ₃	12.7451392	-2.7972820	-25.4728994
875	C	C ₄	-1.9617134	-22.6540925	-7.8855626	928	C	C ₃	14.9566267	-10.9379421	21.8126696
876	C	C ₄	4.3818653	-23.3655502	-3.7534815	929	C	C ₄	-20.7690676	11.5620335	3.9213613
877	C	C ₅	4.1838389	21.3179067	5.9689697	930	C	C ₄	12.0326867	8.9942102	18.8342878
878	C	C ₅	-0.1294534	22.5092372	-0.9506487	931	C	C ₄	-20.7690598	-11.5609170	-3.9246805
879	C	C ₅	-4.0535312	21.2798879	6.1904334	932	C	C ₄	12.0352244	-8.9948570	-18.8323654
880	C	C ₅	-0.1308138	-22.5092295	0.9506239	933	C	C ₄	8.7333675	-15.0980676	16.6189201
881	C	C ₅	-4.0536901	-21.2796696	-6.1910833	934	C	C ₅	-18.8107811	10.7601587	6.1391935
882	C	C ₅	4.1836495	-21.3181327	-5.9682948	935	C	C ₅	13.0642178	9.0709505	15.9486783
883	C	C ₁	10.0966097	11.1354814	24.1257653	936	C	C ₅	-18.8103786	-10.7591464	-6.1422060
884	C	C ₁	13.9064408	18.1889720	-16.8453435	937	C	C ₅	13.0662848	-9.0716539	-15.9465842
885	C	C ₁	10.0998798	-11.1360238	-24.1241539	938	C	C ₅	5.7436419	-14.5992250	16.1613553
886	C	C ₁	13.9027695	-18.1897194	16.8475651	939	C	C ₁	-23.7889412	8.3008641	12.9426502
887	C	C ₁	-24.0032202	-15.2211805	-0.3925638	940	C	C ₁	21.7211702	7.6925587	16.4725762
888	C	C ₂	-24.6859078	14.9643790	3.3517724	941	C	C ₁	-23.7873189	-8.2995838	-12.9464601
889	C	C ₂	13.0051371	11.5312139	23.2907401	942	C	C ₁	21.7233961	-7.6937284	-16.4690936
890	C	C ₂	11.6813648	18.7856093	-18.8469510	943	C	C ₁	2.0635202	-14.6836943	24.1342343
891	C	C ₂	13.0082446	-11.5319140	-23.2886560	944	C	C ₂	-25.6920483	6.5872360	11.4295842
892	C	C ₂	11.6773371	-18.7862381	18.8488227	945	C	C ₂	21.6331199	5.3937905	18.3582096
893	C	C ₂	-24.6861759	-14.9630501	-3.3557282	946	C	C ₂	-25.6905765	-6.5858529	-11.4337016
894	C	C ₃	-24.5267339	13.7141392	5.9782853	947	C	C ₂	21.6357692	-5.3949557	-18.3547394
895	C	C ₃	15.3508813	11.0170596	21.6414689	948	C	C ₂	4.0544751	-12.9442569	25.4973783

949	C	C ₃	-26.7264655	4.8687945	9.2124893	1002	C	C ₃	24.4513913	12.0776099	9.1370760
950	C	C ₃	20.5105495	3.0415066	19.8228508	1003	C	C ₃	-18.2464542	-10.2546275	-19.7265019
951	C	C ₃	-26.7252480	-4.8673569	-9.2167659	1004	C	C ₃	24.4522086	-12.0789258	-9.1331598
952	C	C ₃	20.5135616	-3.0426097	-19.8195706	1005	C	C ₃	-6.2062764	-17.4404757	22.0122091
953	C	C ₃	6.2114395	-10.8960162	25.7987195	1006	C	C ₄	-10.2038559	6.2674974	20.9302600
954	C	C ₄	11.9218365	8.4224902	-18.9957571	1007	C	C ₄	22.0445676	9.7465802	0.7192450
955	C	C ₄	-23.4106636	5.0467396	0.6152791	1008	C	C ₄	-10.2008454	-6.2669483	-20.9318946
956	C	C ₄	11.4890154	1.5429056	20.9649456	1009	C	C ₄	22.0441595	-9.7477673	-0.7157102
957	C	C ₄	-23.4108290	-5.0454804	-0.6190243	1010	C	C ₄	-11.8436916	-12.7449670	16.6963699
958	C	C ₄	11.4922985	-1.5435234	-20.9631087	1011	C	C ₅	-9.0814931	3.4804104	20.2847196
959	C	C ₄	11.9183421	-8.4231315	18.9976655	1012	C	C ₅	21.3418880	7.0828718	-0.6428118
960	C	C ₅	12.2339643	9.5211941	-16.1878322	1013	C	C ₅	-9.0784251	-3.4799220	-20.2861728
961	C	C ₅	-21.3316551	6.8480803	-0.6582578	1014	C	C ₅	21.3414013	-7.0840193	0.6462239
962	C	C ₅	9.0979483	3.2525858	20.2241677	1015	C	C ₅	-12.2632428	-9.7513971	16.1424829
963	C	C ₅	-21.3321271	-6.8469320	0.6548400	1016	N	N ₆	-10.0246964	13.2688231	20.4374371
964	C	C ₅	9.1010101	-3.2530754	-20.2227112	1017	N	N ₆	20.5057868	16.3483315	2.5475158
965	C	C ₅	12.2308594	-9.5218528	16.1897936	1018	N	N ₆	-10.0221412	-13.2682839	-20.4390410
966	C	C ₁	-14.5084660	-2.1767588	24.1933076	1019	N	N ₆	20.5053179	-16.3494355	-2.5442289
967	C	C ₁	28.2223645	1.8527156	0.7844953	1020	N	N ₆	-10.4838185	-19.2941318	14.5626600
968	C	C ₁	-14.5044713	2.1775392	-24.1956294	1021	N	N ₇	-11.5150941	11.2974306	24.5692219
969	C	C ₁	28.2223850	-1.8542354	-0.7799697	1022	N	N ₇	25.0669706	15.2792706	1.4375667
970	C	C ₁	-13.7179948	-6.1160475	23.9783356	1023	N	N ₇	-11.5117609	-11.2968115	-24.5710630
971	C	C ₂	-17.0784657	-0.9849724	23.2890158	1024	N	N ₇	25.0663776	-15.2806185	-1.4335586
972	C	C ₂	28.5604874	2.3885874	3.6899194	1025	N	N ₇	-13.5552104	-18.6629724	18.2160842
973	C	C ₂	-17.0746769	0.9858917	-23.2917522	1026	N	N ₈	-10.5490602	8.1411160	25.9871056
974	C	C ₂	28.5609539	-2.3901246	-3.6853443	1027	N	N ₈	26.2577996	12.7567966	-0.8262851
975	C	C ₂	-11.4863840	-7.4072510	25.4601264	1028	N	N ₈	-10.5453380	-8.1405466	-25.9888051
976	C	C ₃	-18.9391688	0.6765479	21.6079905	1029	N	N ₈	26.2569771	-12.7582094	0.8304887
977	C	C ₃	27.8120319	3.2833408	6.4626421	1030	N	N ₈	-15.7121165	-15.8565306	18.8305583
978	C	C ₃	-18.9357486	-0.6755290	-21.6110220	1031	N	N ₉	-14.1958347	0.6565279	21.2847520
979	C	C ₃	27.8128933	-3.2848381	-6.4581847	1032	N	N ₉	25.1674241	3.8801602	2.5570007
980	C	C ₃	-8.8773128	-8.8489041	25.8639768	1033	N	N ₉	-14.1924574	-0.6557648	-21.2870208
981	C	C ₄	-16.1081810	7.6483173	16.2444726	1034	N	N ₉	25.1676265	-3.8815138	-2.5529752
982	C	C ₄	20.7946746	9.0249649	8.2452814	1035	N	N ₉	-10.9753343	-8.0517033	21.6726909
983	C	C ₄	-16.1059867	-7.6474497	-16.2470567	1036	N	N ₁₀	-14.0784396	0.9935441	17.9121141
984	C	C ₄	20.7955082	-9.0260824	-8.2419606	1037	N	N ₁₀	22.1807610	3.3740405	4.0820282
985	C	C ₄	-4.6899158	-13.7587038	19.2498286	1038	N	N ₁₀	-14.0756193	-0.9927866	-17.9143680
986	C	C ₅	-13.3102868	8.9132713	15.8907062	1039	N	N ₁₀	22.1812397	-3.3752343	-4.0784752
987	C	C ₅	18.9079551	10.5577329	6.3362511	1040	N	N ₁₀	-8.1057676	-7.5111636	19.9477411
988	C	C ₅	-13.3082156	-8.9125548	-15.8928391	1041	N	N ₁₁	-16.7101498	1.7216445	15.6186232
989	C	C ₅	18.9084061	-10.5587506	-6.3332220	1042	N	N ₁₁	21.4322141	3.1087749	7.5584473
990	C	C ₅	-5.6006272	-14.4692121	16.3829044	1043	N	N ₁₁	-16.7077411	-1.7207461	-15.6212941
991	C	C ₁	-22.0292206	7.1089792	16.4255691	1044	N	N ₁₁	21.4332617	-3.1099280	-7.5550170
992	C	C ₁	23.9889907	7.6842266	13.0806865	1045	N	N ₁₁	-4.7256892	-8.0193968	20.9640572
993	C	C ₁	-22.0269670	-7.1077930	-16.4291014	1046	N	N ₆	9.0851951	13.8562988	20.5287611
994	C	C ₁	23.9906740	-7.6855182	-13.0768416	1047	N	N ₆	10.9424726	19.7415723	-13.6565073
995	C	C ₁	-1.9640782	-14.1581016	24.5217051	1048	N	N ₆	9.0877332	-13.8567886	-20.5273011
996	C	C ₂	-20.6043666	8.9993350	18.2377616	1049	N	N ₆	10.9392239	-19.7421627	13.6582691
997	C	C ₂	24.5455012	10.1568294	11.5109122	1050	N	N ₆	-20.0276271	-17.0711357	-1.8542651
998	C	C ₂	-20.6019311	-8.9982264	-18.2410600	1051	N	N ₇	6.7392679	14.7889491	24.5371876
999	C	C ₂	24.5467996	-10.1581505	-11.5069804	1052	N	N ₇	15.3995054	21.2945043	-13.2515604
1000	C	C ₂	-3.9453327	-16.2119253	23.6590728	1053	N	N ₇	6.7424057	-14.7893112	-24.5361116
1001	C	C ₃	-18.2490592	10.2556089	19.7235831	1054	N	N ₇	15.3962317	-21.2953328	13.2540249

1055	N	N ₇	-22.1393643	-19.3134276	1.7448163	1108	N	N ₆	-6.2479671	-9.8729847	-23.5707410
1056	N	N ₈	3.9542820	12.8859713	25.9132376	1109	N	N ₆	21.7899788	-14.4406962	2.9590745
1057	N	N ₈	18.2459923	19.4095394	-11.9805688	1110	N	N ₆	-15.5425443	-16.2762256	13.6237534
1058	N	N ₈	3.9577377	-12.8861842	-25.9126042	1111	N	N ₇	-6.6057900	14.4927069	24.7137723
1059	N	N ₈	18.2430290	-19.4105214	11.9834917	1112	N	N ₇	22.2662645	19.0942622	-2.0169655
1060	N	N ₈	-22.2014300	-18.2469007	5.2275814	1113	N	N ₇	-6.6026100	-14.4923515	-24.7148300
1061	N	N ₉	-4.2175907	14.0094494	21.1772340	1114	N	N ₇	22.2649126	-19.0954602	2.0205300
1062	N	N ₉	18.1248256	18.0958790	-2.5608535	1115	N	N ₇	-15.6630194	-21.0351822	13.2904661
1063	N	N ₉	-4.2149546	-14.0092220	-21.1779122	1116	N	N ₈	-7.3407771	17.2651876	22.4350418
1064	N	N ₉	18.1234445	-18.0968534	2.5637507	1117	N	N ₈	20.2816102	21.0675340	0.3466739
1065	N	N ₉	-13.9091599	-19.3350065	9.7581132	1118	N	N ₈	-7.3381089	-17.2647920	-22.4362206
1066	N	N ₁₀	-3.7716195	13.9568475	17.7661389	1119	N	N ₈	20.2805265	-21.0686252	-0.3434275
1067	N	N ₁₀	14.9982935	17.2556034	-1.3964046	1120	N	N ₈	-12.9432254	-23.2245356	12.1818994
1068	N	N ₁₀	-3.7695302	-13.9566436	-17.7667483	1121	N	N ₉	0.1488171	19.3979151	16.9021052
1069	N	N ₁₀	14.9971300	-17.2564109	1.3988087	1122	N	N ₉	11.5012729	22.8211557	-2.9829531
1070	N	N ₁₀	-11.2282591	-18.3637438	7.8328480	1123	N	N ₉	0.1504816	-19.3979230	-16.9020819
1071	N	N ₁₁	-3.9112480	16.6658452	15.4250781	1124	N	N ₉	11.4995655	-22.8217745	2.9847942
1072	N	N ₁₁	12.6720827	19.2399898	0.4716698	1125	N	N ₉	-11.6509001	-22.7771749	2.7274983
1073	N	N ₁₁	-3.9096760	-16.6656344	-15.4257066	1126	N	N ₁₀	1.7754909	16.6772086	15.6676640
1074	N	N ₁₁	12.6711265	-19.2406707	-0.4696464	1127	N	N ₁₀	10.0340801	20.1473774	-4.4897451
1075	N	N ₁₁	-8.7621842	-20.3892422	6.2035654	1128	N	N ₁₀	1.7771075	-16.6773040	-15.6673804
1076	N	N ₆	-2.9610014	22.1368386	13.7368605	1129	N	N ₁₀	10.0322733	-20.1479167	4.4913483
1077	N	N ₆	9.9523526	24.1909999	1.8040999	1130	N	N ₁₀	-11.8101216	-19.6253376	1.4575667
1078	N	N ₆	-2.9600017	-22.1366789	-13.7373364	1131	N	N ₁₁	4.8887838	15.2192127	16.6462381
1079	N	N ₆	9.9513338	-24.1915362	-1.8025023	1132	N	N ₁₁	9.5268235	19.4552581	-7.9595562
1080	N	N ₆	-6.9922776	-25.0610668	3.2495342	1133	N	N ₁₁	4.8906308	-15.2194754	-16.6454579
1081	N	N ₇	-0.2870456	23.7660206	17.4482364	1134	N	N ₁₁	9.5244989	-19.4557710	7.9610833
1082	N	N ₇	11.5435830	27.0735685	-1.7648469	1135	N	N ₁₁	-14.4158212	-18.0182131	-0.3872728
1083	N	N ₇	-0.2855355	-23.7660051	-17.4482828	1136	N	N ₆	2.8462307	22.7481343	12.7962406
1084	N	N ₇	11.5418367	-27.0741897	1.7666955	1137	N	N ₆	6.1561281	25.3933819	-2.5691640
1085	N	N ₇	-11.2573334	-27.1577069	2.2535502	1138	N	N ₆	2.8470535	-22.7482879	-12.7957822
1086	N	N ₈	3.0735183	22.6990311	18.1968204	1139	N	N ₆	6.1543532	-25.3937133	2.5701506
1087	N	N ₈	10.6589482	26.7342318	-5.2425742	1140	N	N ₆	-9.0023607	-24.5567774	-2.2901094
1088	N	N ₈	3.0752173	-22.6991962	-18.1963304	1141	N	N ₇	0.0452609	26.6244815	12.4741773
1089	N	N ₈	10.6566730	-26.7348055	5.2442820	1142	N	N ₇	6.7122472	28.6099774	0.9407421
1090	N	N ₈	-13.7328694	-25.8307002	-0.0054339	1143	N	N ₇	0.0458298	-26.6244850	-12.4741638
1091	N	N ₉	3.8831028	13.7898852	21.3459582	1144	N	N ₇	6.7108652	-28.6103398	-0.9396601
1092	N	N ₉	14.2507326	19.1185195	-9.6066714	1145	N	N ₇	-6.7577914	-28.5965925	-1.0184859
1093	N	N ₉	3.8857794	-13.7900944	-21.3453347	1146	N	N ₈	-3.2762514	26.7075224	11.1788206
1094	N	N ₉	14.2481660	-19.1192862	9.6089529	1147	N	N ₈	7.2552628	27.8764647	4.3881141
1095	N	N ₉	-18.1346132	-17.9769143	2.9758539	1148	N	N ₈	-3.2758976	-26.7073452	-11.1793504
1096	N	N ₁₀	1.9149331	11.6349110	19.6883015	1149	N	N ₈	7.2544604	-27.8768554	-4.3869502
1097	N	N ₁₀	14.1366441	16.3516373	-7.7101476	1150	N	N ₈	-3.9796576	-28.8392755	1.2042076
1098	N	N ₁₀	1.9174569	-11.6350152	-19.6879888	1151	N	N ₉	4.1679814	25.1374523	2.1380794
1099	N	N ₁₀	14.1345357	-16.3523980	7.7124115	1152	N	N ₉	-3.9522213	25.2007689	1.7709185
1100	N	N ₁₀	-16.0525671	-15.7884838	4.4391676	1153	N	N ₉	-0.2147850	23.9759925	8.8848547
1101	N	N ₁₁	-1.2148677	10.0539535	20.7309421	1154	N	N ₉	-3.9532977	-25.2005563	-1.7715510
1102	N	N ₁₁	16.8236801	14.6405016	-5.9117995	1155	N	N ₉	-0.2146499	-23.9759814	-8.8848861
1103	N	N ₁₁	-1.2120931	-10.0538882	-20.7311369	1156	N	N ₉	4.1669724	-25.1376760	-2.1374154
1104	N	N ₁₁	16.8219470	-14.6414077	5.9144979	1157	N	N ₁₀	3.7513539	22.2216148	3.7287599
1105	N	N ₁₁	-15.6103747	-14.9971335	7.9832345	1158	N	N ₁₀	-1.9579312	22.7485412	0.6684969
1106	N	N ₆	-6.2512064	9.8733204	23.5697438	1159	N	N ₁₀	-1.7925522	21.6462338	7.0713331
1107	N	N ₆	21.7912242	14.4395232	-2.9555827	1160	N	N ₁₀	-1.9590402	-22.7484347	-0.6688170

1161	N	N ₁₀	-1.7925808	-21.6461361	-7.0716276	1214	N	N ₈	15.7350203	8.8317682	-22.7558807
1162	N	N ₁₀	3.7507604	-22.2218161	-3.7281623	1215	N	N ₈	-28.5865429	5.0556831	-0.8187812
1163	N	N ₁₁	3.8193688	21.4284997	7.2458841	1216	N	N ₈	12.8517104	0.4312051	26.0397460
1164	N	N ₁₁	1.1263527	22.8817390	-1.1951780	1217	N	N ₈	-28.5869453	-5.0541458	0.8142095
1165	N	N ₁₁	-4.9448583	21.7595226	5.3237769	1218	N	N ₈	12.8558631	-0.4318962	-26.0376909
1166	N	N ₁₁	1.1249360	-22.8817984	1.1953519	1219	N	N ₈	15.7308943	-8.8326144	22.7583975
1167	N	N ₁₁	-4.9451716	-21.7592555	-5.3245745	1220	N	N ₉	-22.6200590	11.8122512	2.3461436
1168	N	N ₁₁	3.8193823	-21.4287044	-7.2452774	1221	N	N ₉	11.5770257	8.5665632	21.1964000
1169	N	N ₆	6.9246336	9.2465693	23.5658782	1222	N	N ₉	-22.6203223	-11.8110337	-2.3497671
1170	N	N ₆	15.2920838	15.7750773	-14.3561704	1223	N	N ₉	11.5799603	-8.5671869	-21.1945421
1171	N	N ₆	6.9279186	-9.2469413	-23.5647732	1224	N	N ₉	11.0398948	-15.2144509	17.4167145
1172	N	N ₆	15.2889359	-15.7759002	14.3586192	1225	N	N ₁₀	-19.9395047	10.6234855	3.9485351
1173	N	N ₆	-22.2173546	-13.7395014	2.5328773	1226	N	N ₁₀	11.7789847	8.2249073	17.8784687
1174	N	N ₇	11.2124286	10.9830101	24.8486475	1227	N	N ₁₀	-19.9394445	-10.6224134	-3.9517224
1175	N	N ₇	13.9878887	18.3883479	-18.1661177	1228	N	N ₁₀	11.7814110	-8.2255409	-17.8765844
1176	N	N ₇	11.2158151	-10.9836140	-24.8468492	1229	N	N ₁₀	8.1576013	-14.0849553	16.1586136
1177	N	N ₇	13.9839874	-18.3891022	18.1683669	1230	N	N ₁₁	-19.1589959	10.4753746	7.4681220
1178	N	N ₇	-25.2003909	-15.0926100	-0.9766100	1231	N	N ₁₁	14.4143705	9.0805788	15.5673565
1179	N	N ₈	-24.3801696	15.5654596	4.4959219	1232	N	N ₁₁	-19.1583664	-10.4743433	-7.4711917
1180	N	N ₈	13.7404559	12.4382149	22.6578916	1233	N	N ₁₁	14.4163752	-9.0813552	-15.5650444
1181	N	N ₈	10.6403384	19.6027905	-18.9579373	1234	N	N ₁₁	4.7415415	-14.7111573	17.1368923
1182	N	N ₈	13.7434168	-12.4389537	-22.6556948	1235	N	N ₆	-20.4412595	9.9776680	13.0429245
1183	N	N ₈	10.6362426	-19.6033631	18.9596418	1236	N	N ₆	19.8865691	9.8140571	13.9901990
1184	N	N ₈	-24.3802841	-15.5641482	-4.4998231	1237	N	N ₆	-20.4397091	-9.9765671	-13.0462032
1185	N	N ₉	-22.7280868	7.4027666	9.1401892	1238	N	N ₆	19.8882778	-9.8151280	-13.9870099
1186	N	N ₉	18.0773833	6.0355004	17.0789645	1239	N	N ₆	0.5509639	-15.8213467	20.9021113
1187	N	N ₉	4.6510416	12.7146918	-21.7166805	1240	N	N ₇	-25.0544418	8.5476731	12.6476864
1188	N	N ₉	18.0797946	-6.0364751	-17.0760587	1241	N	N ₇	22.0659144	7.6687691	17.7492856
1189	N	N ₉	4.6468827	-12.7149424	21.7174276	1242	N	N ₇	-25.0528763	-8.5463249	-12.6516978
1190	N	N ₉	-22.7270256	-7.4015442	-9.1438249	1243	N	N ₇	22.0683451	-7.6699566	-17.7457515
1191	N	N ₁₀	-20.9484441	5.1553143	7.3525633	1244	N	N ₇	2.9841211	-15.0318333	25.0178087
1192	N	N ₁₀	15.9920504	3.6982854	15.8130275	1245	N	N ₈	-26.1963532	5.4041191	11.5517721
1193	N	N ₁₀	4.9566391	9.8544635	-19.9448313	1246	N	N ₈	22.1633653	4.2182954	18.4360467
1194	N	N ₁₀	15.9943898	-3.6991462	-15.8104658	1247	N	N ₈	-26.1947882	-5.4027092	-11.5559683
1195	N	N ₁₀	4.9529115	-9.8547292	19.9456196	1248	N	N ₈	22.1660958	-4.2194884	-18.4324961
1196	N	N ₁₀	-20.9475469	-5.1541878	-7.3559131	1249	N	N ₈	4.0284184	-11.9169579	26.2803125
1197	N	N ₁₁	-22.0089706	2.1681563	5.7060892	1250	N	N ₉	-25.0602295	4.1074256	2.1516031
1198	N	N ₁₁	15.5559539	0.2713373	16.7210652	1251	N	N ₉	13.7630191	0.7870420	21.4353833
1199	N	N ₁₁	6.4531457	6.7391276	-20.8469680	1252	N	N ₉	-25.0601124	-4.1060767	-2.1556177
1200	N	N ₁₁	15.5586065	-0.2721746	-16.7185732	1253	N	N ₉	13.7664033	-0.7877830	-21.4331773
1201	N	N ₁₁	6.4494411	-6.7394755	20.8480052	1254	N	N ₉	11.2935292	-8.1520198	21.3428258
1202	N	N ₁₁	-22.0081767	-2.1669711	-5.7096182	1255	N	N ₁₀	-22.1744300	5.1756842	0.9234714
1203	N	N ₆	10.4450867	3.5290425	-23.7607205	1256	N	N ₁₀	11.1149917	1.9252405	19.8014210
1204	N	N ₆	-26.0201520	-1.0474498	2.8250155	1257	N	N ₁₀	-22.1745607	-5.1744917	-0.9270176
1205	N	N ₆	15.5750352	-4.1174269	20.6540765	1258	N	N ₁₀	11.1180590	-1.9258398	-19.7996344
1206	N	N ₆	-26.0196352	1.0488508	-2.8291870	1259	N	N ₁₀	11.0562926	-8.4421425	18.0508857
1207	N	N ₆	15.5785656	4.1165885	-20.6515813	1260	N	N ₁₁	12.7317255	10.7230085	-15.8493792
1208	N	N ₆	10.4410997	-3.5296052	23.7623968	1261	N	N ₁₁	-21.4682282	8.1560309	-0.9362579
1209	N	N ₇	-29.1366110	2.3608557	1.5132264	1262	N	N ₁₁	8.7368219	4.4142703	20.7957838
1210	N	N ₇	15.5129586	-1.6432455	24.7679957	1263	N	N ₁₁	-21.4688226	-8.1548744	0.9328134
1211	N	N ₇	-29.1364982	-2.3592887	-1.5178867	1264	N	N ₁₁	8.7399086	-4.4147397	-20.7943896
1212	N	N ₇	15.5170154	1.6424091	-24.7655028	1265	N	N ₁₁	12.7286046	-10.7236926	15.8514125
1213	N	N ₇	13.6193776	-6.9197485	24.9686849	1266	N	N ₆	-10.8159329	-2.4970806	23.7439469

1267	N	N ₆	26.0396438	1.9761499	-2.2420139	1320	N	N ₁₀	-11.0140308	-11.8923020	16.1513843
1268	N	N ₆	-10.8120023	2.4976621	-23.7456761	1321	N	N ₁₁	-9.4914758	2.3243975	20.7374912
1269	N	N ₆	26.0391837	-1.9775520	2.2461887	1322	N	N ₁₁	22.1031442	6.0300769	-0.7896808
1270	N	N ₆	-15.2272422	-5.1542862	20.7016728	1323	N	N ₁₁	-9.4882805	-2.3238871	-20.7390089
1271	N	N ₇	-15.4161741	-1.5466543	24.9249490	1324	N	N ₁₁	22.1026952	-6.0312664	0.7932206
1272	N	N ₇	29.2080871	2.5057142	1.3830102	1325	N	N ₁₁	-12.6146402	-8.8190741	16.9890924
1273	N	N ₇	-15.4121026	1.5474836	-24.9274158	1326	O	O ₁₂	-11.7038264	8.6474102	24.1930245
1274	N	N ₇	29.2081768	-2.5072865	-1.3783299	1327	O	O ₁₂	25.2295926	12.6215907	1.1058337
1275	N	N ₇	-13.7961792	-7.0358027	24.9292312	1328	O	O ₁₂	-11.7004167	-8.6467801	-24.1949004
1276	N	N ₈	-18.1877982	-1.3972480	22.6747561	1329	O	O ₁₂	25.2290883	-12.6229486	-1.1017924
1277	N	N ₈	28.6514718	1.6770423	4.8139008	1330	O	O ₁₂	-13.5291616	-16.0607477	18.8699194
1278	N	N ₈	-18.1840886	1.3982274	-22.6776726	1331	O	O ₁₃	-12.5954577	6.2399015	26.2142465
1279	N	N ₈	28.6521524	-1.6785828	-4.8093209	1332	O	O ₁₃	27.7541660	10.6939176	0.3396283
1280	N	N ₈	-10.4681547	-7.0217410	26.2298639	1333	O	O ₁₃	-12.5915940	-6.2392226	-26.2162700
1281	N	N ₉	-18.0244723	6.3660266	17.0241653	1334	O	O ₁₃	27.7536382	-10.6954117	-0.3351808
1282	N	N ₉	22.6066532	7.7119801	9.2029792	1335	O	O ₁₃	-15.1624554	-14.3950506	21.1577671
1283	N	N ₉	-18.0220904	-6.3650564	-17.0270534	1336	O	O ₁₄	-15.9817082	0.6855971	18.9853421
1284	N	N ₉	22.6077115	-7.7131973	-9.1993557	1337	O	O ₁₄	24.0936100	3.0688593	5.1388999
1285	N	N ₉	-4.5859765	-13.0088740	21.5631194	1338	O	O ₁₄	-15.9787069	-0.6847376	-18.9878987
1286	N	N ₁₀	-14.9727593	7.1347180	15.7387550	1339	O	O ₁₄	24.0942713	-3.0701562	-5.1350402
1287	N	N ₁₀	19.8707923	8.5735632	7.3784410	1340	O	O ₁₄	-8.1157157	-7.7653110	22.1396332
1288	N	N ₁₀	-14.9706139	-7.1339130	-15.7411489	1341	O	O ₁₅	-15.4934805	-0.1245173	15.7697503
1289	N	N ₁₀	19.8715200	-8.5746319	-7.3752628	1342	O	O ₁₅	21.2240877	1.5590202	5.9879766
1290	N	N ₁₀	-4.9012739	-12.9736189	18.1785274	1343	O	O ₁₅	-15.4909489	0.1253500	-15.7722255
1291	N	N ₁₁	-12.6141209	9.6687960	16.7069703	1344	O	O ₁₅	21.2249633	-1.5601635	-5.9845709
1292	N	N ₁₁	19.1455369	11.5876514	5.5587094	1345	O	O ₁₅	-5.7341185	-6.1120550	20.4575447
1293	N	N ₁₁	-12.6119624	-9.6681168	-16.7089922	1346	O	O ₁₂	4.1366443	14.0416397	24.0881128
1294	N	N ₁₁	19.1458001	-11.5886815	-5.5556446	1347	O	O ₁₂	16.4273387	20.0843772	-11.0125945
1295	N	N ₁₁	-6.5343174	-15.2945203	15.9720024	1348	O	O ₁₂	4.1397447	-14.0418614	-24.0874562
1296	N	N ₆	-21.7167887	4.2368444	14.0213967	1349	O	O ₁₂	16.4244892	-20.0852620	11.0152298
1297	N	N ₆	22.2028280	4.3790661	13.1919420	1350	O	O ₁₂	-20.5649294	-18.8681954	3.9486112
1298	N	N ₆	-21.7147625	-4.2356746	-14.0248810	1351	O	O ₁₃	1.4622788	14.2613464	26.1383727
1299	N	N ₆	22.2047137	-4.3802612	-13.1883848	1352	O	O ₁₃	19.4820817	20.4157872	-9.6116091
1300	N	N ₆	-0.4901919	-10.7611546	23.8773237	1353	O	O ₁₃	1.4656967	-14.2614248	-26.1381407
1301	N	N ₇	-22.2798141	7.3851431	17.6109376	1354	O	O ₁₃	19.4794415	-20.4168359	9.6147311
1302	N	N ₇	25.0853941	8.2089233	12.8223277	1355	O	O ₁₃	-20.9458556	-19.9855330	7.1125516
1303	N	N ₇	-22.2773882	-7.3839439	-17.6145070	1356	O	O ₁₄	-4.6663214	15.7429528	18.8340265
1304	N	N ₇	25.0870031	-8.2102732	-12.8183114	1357	O	O ₁₄	16.0946401	19.1009297	-0.6726591
1305	N	N ₇	-2.8100132	-14.7564207	25.2076864	1358	O	O ₁₄	-4.6641476	-15.7427028	-18.8347673
1306	N	N ₈	-20.1944262	10.2305737	18.3239692	1359	O	O ₁₄	16.0935024	-19.1017961	0.6752382
1307	N	N ₈	24.2332262	11.4167678	11.4304707	1360	O	O ₁₄	-11.4300857	-20.4720042	8.6363102
1308	N	N ₈	-20.1920420	-10.2294862	-18.3272080	1361	O	O ₁₅	-5.2842089	14.9032541	15.5789422
1309	N	N ₈	24.2344380	-11.4180724	-11.4265869	1362	O	O ₁₅	13.7488269	17.3903343	1.1310684
1310	N	N ₈	-4.0429078	-17.3513926	23.0397788	1363	O	O ₁₅	-5.2825129	-14.9029696	-15.5797894
1311	N	N ₉	-11.4986523	8.2595448	21.3874595	1364	O	O ₁₅	13.7480696	-17.3910739	-1.1288684
1312	N	N ₉	22.7895095	11.5770040	2.1150935	1365	O	O ₁₅	-8.4662291	-18.9430705	7.8877331
1313	N	N ₉	-11.4956768	-8.2589271	-21.3892946	1366	O	O ₁₂	1.3004511	21.5644770	18.1671644
1314	N	N ₉	22.7892195	-11.5782313	-2.1114384	1367	O	O ₁₂	11.6868523	25.3806711	-4.0003250
1315	N	N ₉	-11.2940129	-14.9559265	17.5107979	1368	O	O ₁₂	1.3021955	-21.5645477	-18.1669521
1316	N	N ₁₀	-10.0281013	5.7102190	19.7593907	1369	O	O ₁₂	11.6848511	-25.3813003	4.0021986
1317	N	N ₁₀	21.0392580	8.9455456	0.9643446	1370	O	O ₁₂	-12.9879908	-24.9982232	1.7789422
1318	N	N ₁₀	-10.0252457	-5.7096787	-19.7610005	1371	O	O ₁₃	3.5645394	21.3357480	20.6666706
1319	N	N ₁₀	21.0389281	-8.9466785	-0.9609714	1372	O	O ₁₃	12.7216786	26.1213902	-7.1318493

1373	O	O ₁₃	3.5666962	-21.3359395	-20.6661020	1426	O	O ₁₅	-4.3984516	-20.4527486	-7.0093407
1374	O	O ₁₃	12.7191307	-26.1220757	7.1338920	1427	O	O ₁₅	5.1759002	-20.6814983	-5.6813576
1375	O	O ₁₃	-16.2867787	-25.0734843	1.0452676	1428	O	O ₁₂	-24.3606044	13.7875100	3.2749891
1376	O	O ₁₄	1.7293194	11.8518182	21.9498435	1429	O	O ₁₂	12.9498479	10.4337076	22.7530005
1377	O	O ₁₄	16.1277501	17.0990825	-8.5304484	1430	O	O ₁₂	11.4113052	17.5925052	-18.8293854
1378	O	O ₁₄	1.7321919	-11.8519125	-21.9495598	1431	O	O ₁₂	12.9529272	-10.4344041	-22.7509289
1379	O	O ₁₄	16.1254666	-17.0999520	8.5330408	1432	O	O ₁₂	11.4073417	-17.5931199	18.8312167
1380	O	O ₁₄	-17.8582612	-16.5904282	5.5760173	1433	O	O ₁₂	-24.3608177	-13.7861988	-3.2788918
1381	O	O ₁₅	0.8184555	9.0265066	20.2740647	1434	O	O ₁₃	-25.7012091	13.7412672	6.3087672
1382	O	O ₁₅	15.5680326	13.8416353	-7.6961561	1435	O	O ₁₃	16.2161903	10.9533099	22.4996660
1383	O	O ₁₅	0.8212068	-9.0265510	-20.2739320	1436	O	O ₁₃	9.4855770	18.5061324	-21.3710520
1384	O	O ₁₅	15.5660523	-13.8424735	7.6986521	1437	O	O ₁₃	16.2192092	-10.9541827	-22.4970687
1385	O	O ₁₅	-16.3877464	-13.6006937	6.2966886	1438	O	O ₁₃	9.4811641	-18.5066429	21.3725715
1386	O	O ₁₂	-5.6100817	15.9066283	22.6815936	1439	O	O ₁₃	-25.7009316	-13.7398839	-6.3128838
1387	O	O ₁₂	19.8262774	20.0837967	-1.5837940	1440	O	O ₁₄	-22.9753302	4.6281419	8.0564041
1388	O	O ₁₂	-5.6073017	-15.9063261	-22.6824938	1441	O	O ₁₄	17.6836477	3.0725416	17.0891456
1389	O	O ₁₂	19.8249392	-20.0848634	1.5869674	1442	O	O ₁₄	5.2918988	9.8243625	-22.1284534
1390	O	O ₁₂	-14.2183950	-21.7321449	11.1579413	1443	O	O ₁₄	17.6862232	-3.0734945	-17.0863069
1391	O	O ₁₃	-5.2488383	19.1840299	22.2681212	1444	O	O ₁₄	5.2878330	-9.8246484	22.1293074
1392	O	O ₁₃	18.8112746	23.1690743	-0.8811926	1445	O	O ₁₄	-22.9742826	-4.6269062	-8.0600796
1393	O	O ₁₃	-5.2463035	-19.1837473	-22.2689626	1446	O	O ₁₅	-20.6362118	2.3580871	7.4084940
1394	O	O ₁₃	18.8098850	-23.1700866	0.8842051	1447	O	O ₁₅	16.2946238	1.0817489	14.8194013
1395	O	O ₁₃	-13.5644616	-24.7112921	9.8388999	1448	O	O ₁₅	4.3417268	7.1461718	-20.4054198
1396	O	O ₁₄	2.7969711	18.1597147	16.9293052	1449	O	O ₁₅	16.2969370	-1.0826260	-14.8167908
1397	O	O ₁₄	10.3823176	22.0323908	-5.5660513	1450	O	O ₁₅	4.3380755	-7.1464056	20.4061163
1398	O	O ₁₄	2.7987079	-18.1598652	-16.9288576	1451	O	O ₁₅	-20.6351514	-2.3569762	-7.4118008
1399	O	O ₁₄	10.3802385	-22.0329491	5.5677118	1452	O	O ₁₂	-27.6334894	4.6776758	1.1002860
1400	O	O ₁₄	-13.1797522	-21.2101288	0.7900834	1453	O	O ₁₂	14.0686011	0.6908615	24.2548679
1401	O	O ₁₅	4.3359057	16.0276793	14.6583653	1454	O	O ₁₂	-27.6335722	-4.6761885	-1.1047126
1402	O	O ₁₅	7.9878946	19.6490239	-6.3768108	1455	O	O ₁₂	14.0724426	-0.6916191	-24.2526122
1403	O	O ₁₅	4.3373872	-16.0279120	-14.6576747	1456	O	O ₁₂	13.5609348	-8.8121286	22.9161177
1404	O	O ₁₅	7.9858140	-19.6494546	6.3780950	1457	O	O ₁₃	15.2178221	11.6715145	-22.7416134
1405	O	O ₁₅	-12.3239105	-18.3745189	-1.0259328	1458	O	O ₁₃	-28.7329652	7.7003899	0.3283615
1406	O	O ₁₂	-1.4933702	26.1870858	10.1516565	1459	O	O ₁₃	13.5154446	3.2278984	26.3040001
1407	O	O ₁₂	5.5636250	27.3828900	3.2051853	1460	O	O ₁₃	-28.7333247	-7.6988426	-0.3329690
1408	O	O ₁₂	-1.4931565	-26.1870048	-10.1518995	1461	O	O ₁₃	13.5194824	-3.2286246	-26.3018425
1409	O	O ₁₂	5.5626626	-27.3831901	-3.2042899	1462	O	O ₁₃	15.2135507	-11.6723326	22.7440463
1410	O	O ₁₂	-4.0705742	-27.8217474	-0.6561570	1463	O	O ₁₄	-21.2961836	11.9638414	4.9625097
1411	O	O ₁₃	-3.5492926	28.2136769	8.7736111	1464	O	O ₁₄	13.1258025	9.5623225	18.9093184
1412	O	O ₁₃	5.1177202	28.6742506	6.0976677	1465	O	O ₁₄	-21.2960237	-11.9626965	-4.9659132
1413	O	O ₁₃	-3.5494035	-28.2134862	-8.7741772	1466	O	O ₁₄	13.1283218	-9.5630295	-18.9072135
1414	O	O ₁₃	5.1171544	-28.6745255	-6.0968510	1467	O	O ₁₄	8.1672155	-15.8210727	17.4435572
1415	O	O ₁₃	-1.5688874	-29.7173749	-0.0388589	1468	O	O ₁₅	-18.0624778	11.6913856	5.8535938
1416	O	O ₁₄	4.5743998	23.9859250	4.7930338	1469	O	O ₁₅	12.3095039	10.0003072	15.6740554
1417	O	O ₁₄	-1.7203251	24.8245317	-0.0776071	1470	O	O ₁₅	-18.0621656	-11.6904132	-5.8564885
1418	O	O ₁₄	-2.8531347	23.4803840	7.7300792	1471	O	O ₁₅	12.3114723	-10.0009694	-15.6720858
1419	O	O ₁₄	-1.7216667	-24.8244399	0.0773361	1472	O	O ₁₅	5.7502077	-15.3086747	15.1586856
1420	O	O ₁₄	-2.8531510	-23.4802299	-7.7305393	1473	O	O ₁₂	-25.1291377	6.9297202	10.4079342
1421	O	O ₁₄	4.5738777	-23.9861709	-4.7923026	1474	O	O ₁₂	20.4293916	5.5479848	18.4303924
1422	O	O ₁₅	5.1761040	20.6812194	5.6821891	1475	O	O ₁₂	-25.1278409	-6.9283679	-10.4119580
1423	O	O ₁₅	-0.7768043	21.9739328	-1.8261965	1476	O	O ₁₂	20.4320525	-5.5490848	-18.4271178
1424	O	O ₁₅	-4.3984717	20.4529856	7.0086345	1477	O	O ₁₂	4.6954636	-12.9330410	24.4644385
1425	O	O ₁₅	-0.7782768	-21.9738909	1.8260714	1478	O	O ₁₃	-27.8065444	5.4180476	9.1125492

1479	O	O ₁₃	20.8846001	3.3832606	20.9280764	1532	O	O ₁₅	-7.9463008	-3.8839019	-20.2412696
1480	O	O ₁₃	-27.8053707	-5.4165517	-9.1169997	1533	O	O ₁₅	20.6776517	-7.6256201	1.4906468
1481	O	O ₁₃	20.8877691	-3.3843836	-20.9247373	1534	O	O ₁₅	-12.7316327	-9.9603026	15.0544017
1482	O	O ₁₃	6.9173344	-11.5552028	26.5372470	1535	C	C ₁₆	-10.5747049	12.6156390	22.6863751
1483	O	O ₁₄	12.7579710	9.3186368	-19.1101325	1536	C	C ₁₆	22.7961659	16.2065470	1.8257275
1484	O	O ₁₄	-24.0580038	5.9983786	0.1786842	1537	C	C ₁₆	-10.5717487	-12.6150686	-22.6880762
1485	O	O ₁₄	11.3002632	2.2488310	21.9555649	1538	C	C ₁₆	22.7955782	-16.2077743	-1.8220741
1486	O	O ₁₄	-24.0582977	-5.9970837	-0.1825382	1539	C	C ₁₆	-12.2244612	-19.3139306	16.2229769
1487	O	O ₁₄	11.3036576	-2.2494394	-21.9537543	1540	C	C ₁₇	-13.6005375	2.5275413	22.6075192
1488	O	O ₁₄	12.7544096	-9.3193234	19.1121759	1541	C	C ₁₇	25.7238585	6.0896080	1.9139452
1489	O	O ₁₅	12.7902197	8.4978354	-15.8550842	1542	C	C ₁₇	-13.5970553	-2.5268082	-22.6097044
1490	O	O ₁₅	-21.1754492	6.0341025	-1.5416865	1543	C	C ₁₇	25.7238319	-6.0909934	-1.9098193
1491	O	O ₁₅	8.3854413	2.2751516	20.2902556	1544	C	C ₁₇	-12.1270221	-10.0861816	21.2994668
1492	O	O ₁₅	-21.1760105	-6.0329629	1.5382953	1545	C	C ₁₆	8.2359190	14.2693613	22.7325243
1493	O	O ₁₅	8.3885721	-2.2756024	-20.2889160	1546	C	C ₁₆	13.1872819	20.5646886	-13.8348133
1494	O	O ₁₅	12.7872264	-8.4985243	15.8571360	1547	C	C ₁₆	8.2387957	-14.2698041	-22.7312080
1495	O	O ₁₂	-16.3691826	-0.1017757	22.8350490	1548	C	C ₁₆	13.1839634	-20.5653988	13.8369282
1496	O	O ₁₂	27.6886378	3.2240255	3.5134829	1549	C	C ₁₆	-21.4234456	-18.1437969	-0.2265208
1497	O	O ₁₂	-16.3655208	0.1026550	-22.8376609	1550	C	C ₁₇	-2.1648613	14.1026994	22.4570970
1498	O	O ₁₂	27.6890304	-3.2255164	-3.5090436	1551	C	C ₁₇	18.1770807	18.8077349	-4.8740647
1499	O	O ₁₂	-11.3236610	-8.0342562	24.4259163	1552	C	C ₁₇	-2.1620254	-14.1025843	-22.4574359
1500	O	O ₁₃	-19.4011996	1.2538529	22.5650091	1553	C	C ₁₇	18.1752902	-18.8087142	4.8769821
1501	O	O ₁₃	28.7750186	4.0078372	6.5645782	1554	C	C ₁₇	-16.0139568	-19.4435538	8.5671094
1502	O	O ₁₃	-19.3976530	-1.2528096	-22.5681118	1555	C	C ₁₆	-1.6793086	23.2801194	15.4318548
1503	O	O ₁₃	28.7758576	-4.0093854	-6.5599716	1556	C	C ₁₆	10.5901753	25.8983567	0.2226584
1504	O	O ₁₃	-9.3784011	-9.7091692	26.5506300	1557	C	C ₁₆	-1.6780969	-23.2800285	-15.4321267
1505	O	O ₁₄	-16.0659307	8.5225629	17.0868400	1558	C	C ₁₆	10.5888092	-25.8989271	-0.2209598
1506	O	O ₁₄	21.3640519	10.0789301	8.0436917	1559	C	C ₁₆	-8.9117126	-26.3917134	2.6429190
1507	O	O ₁₄	-16.0636557	-8.5216977	-17.0894165	1560	C	C ₁₇	3.4928115	16.1185331	20.8319835
1508	O	O ₁₄	21.3647921	-10.0800783	-8.0402790	1561	C	C ₁₇	13.6651079	21.1603637	-8.4547068
1509	O	O ₁₄	-5.3015784	-14.8002402	19.3792277	1562	C	C ₁₇	3.4952730	-16.1187215	-20.8314213
1510	O	O ₁₅	-13.6647938	9.3657149	14.8078560	1563	C	C ₁₇	13.6626122	-21.1610990	8.4568953
1511	O	O ₁₅	18.0945570	10.6669725	7.2469662	1564	C	C ₁₇	-17.1586472	-20.1334937	2.4903086
1512	O	O ₁₅	-13.6629263	-9.3649795	-14.8100445	1565	C	C ₁₆	-6.7359615	12.0721978	24.4113997
1513	O	O ₁₅	18.0951519	-10.6679472	-7.2440630	1566	C	C ₁₆	22.4288862	16.6833048	-2.3748423
1514	O	O ₁₅	-4.4326726	-14.6826685	16.0775143	1567	C	C ₁₆	-6.7326970	-12.0718356	-24.4124773
1515	O	O ₁₂	-19.6739530	8.2110535	18.2622282	1568	C	C ₁₆	22.4276062	-16.6845111	2.3784302
1516	O	O ₁₂	24.2169812	9.5454473	10.5079389	1569	C	C ₁₆	-15.6955315	-18.6624688	13.8704766
1517	O	O ₁₂	-19.6714640	-8.2099950	-18.2653772	1570	C	C ₁₇	-1.5235249	19.0143155	18.5855594
1518	O	O ₁₂	24.2181485	-9.5467497	-10.5040660	1571	C	C ₁₇	13.8305812	22.6305651	-2.4209137
1519	O	O ₁₂	-4.5471187	-15.3270945	23.0737663	1572	C	C ₁₇	-1.5215717	-19.0142339	-18.5858012
1520	O	O ₁₃	-18.8640196	10.2147391	20.7742855	1573	C	C ₁₇	13.8289722	-22.6313107	2.4231364
1521	O	O ₁₃	25.6616290	12.2116451	9.1716878	1574	C	C ₁₇	-12.3082549	-23.0780297	5.0199349
1522	O	O ₁₃	-18.8612459	-10.2137234	-20.7773096	1575	C	C ₁₆	1.5286785	24.7424138	12.9965220
1523	O	O ₁₃	25.6624309	-12.2130262	-9.1675777	1576	C	C ₁₆	6.6928506	27.1581649	-1.0359739
1524	O	O ₁₃	-6.8017210	-17.7552173	23.0271995	1577	C	C ₁₆	1.5294281	-24.7424967	-12.9962733
1525	O	O ₁₄	-10.2787806	5.6600469	21.9863821	1578	C	C ₁₆	6.6912265	-27.1585248	1.0370441
1526	O	O ₁₄	23.0726475	9.4192171	0.1483702	1579	C	C ₁₆	-8.2216862	-26.7087891	-1.5741485
1527	O	O ₁₄	-10.2755674	-5.6594930	-21.9880327	1580	C	C ₁₇	2.1445070	26.3746499	1.5961536
1528	O	O ₁₄	23.0721618	-9.4204597	-0.1446696	1581	C	C ₁₇	-3.5847664	25.9512826	4.0557563
1529	O	O ₁₄	-12.7969555	-12.4395936	17.3949678	1582	C	C ₁₇	1.4412746	25.3211236	7.7157074
1530	O	O ₁₅	-7.9493272	3.8843304	20.2399922	1583	C	C ₁₇	-3.5855046	-25.9510886	-4.0563367
1531	O	O ₁₅	20.6783014	7.6245059	-1.4873275	1584	C	C ₁₇	1.4411513	-25.3211998	-7.7154845

1585	C	C ₁₇	2.1433480	-26.3747648	-1.5958130	1638	C	C ₁₈	21.4915761	15.7576139	1.8798432
1586	C	C ₁₆	8.8538034	10.3851258	24.4424703	1639	C	C ₁₈	-10.0317994	-12.3907834	-21.4372465
1587	C	C ₁₆	14.9083804	17.3678089	-16.1175183	1640	C	C ₁₈	21.4910293	-15.7587710	-1.8763980
1588	C	C ₁₆	8.8571554	-10.3856022	-24.4410526	1641	C	C ₁₈	-11.4598448	-18.7062831	15.2469956
1589	C	C ₁₆	14.9048654	-17.3686118	16.1199091	1642	C	C ₁₉	-12.5985347	3.3660036	23.0721500
1590	C	C ₁₆	-23.7625788	-14.7652564	1.0010388	1643	C	C ₁₉	25.4962177	7.1556386	1.0568194
1591	C	C ₁₇	-23.5249984	9.3471693	7.9710905	1644	C	C ₁₉	-12.5950226	-3.3653259	-23.0741660
1592	C	C ₁₇	17.1923863	7.4856388	18.7808505	1645	C	C ₁₉	25.4960039	-7.1570109	-1.0527350
1593	C	C ₁₇	6.3330219	14.3989868	-21.3751098	1646	C	C ₁₉	-12.9012618	-10.8577282	20.4461328
1594	C	C ₁₇	17.1949896	-7.4865637	-18.7780991	1647	C	C ₂₀	-18.5383730	2.3839366	14.2115591
1595	C	C ₁₇	6.3288223	-14.3993279	21.3761262	1648	C	C ₂₀	21.0481439	3.1209273	9.9276667
1596	C	C ₁₇	-23.5242217	-9.3459033	-7.9748582	1649	C	C ₂₀	-18.5362308	-2.3829386	-14.2145302
1597	C	C ₁₆	-27.8126219	0.3850219	2.1166067	1650	C	C ₂₀	21.0495579	-3.1220603	-9.9242944
1598	C	C ₁₆	15.6562159	-3.1878788	22.8668002	1651	C	C ₂₀	-2.5135205	-8.5688875	21.7158749
1599	C	C ₁₆	-27.8123033	-0.3835246	-2.1210641	1652	C	C ₁₈	8.1806987	13.6614137	21.4900283
1600	C	C ₁₆	15.6600468	3.1870358	-22.8642908	1653	C	C ₁₈	12.2437688	19.6632652	-13.3725620
1601	C	C ₁₆	12.1522278	-4.9859747	24.6096245	1654	C	C ₁₈	8.1834044	-13.6618543	-21.4887161
1602	C	C ₁₇	-24.3833478	10.2590625	1.8041486	1655	C	C ₁₈	12.2405707	-19.6639240	13.3745225
1603	C	C ₁₇	12.2242774	6.6853916	22.5593390	1656	C	C ₁₈	-20.4246389	-17.2586278	-0.5943616
1604	C	C ₁₇	-24.3836153	-10.2577500	-1.8080556	1657	C	C ₁₉	-1.0620528	13.4039787	22.9372638
1605	C	C ₁₇	12.2275225	-6.6860496	-22.5573809	1658	C	C ₁₉	18.1381391	18.4216666	-6.2098798
1606	C	C ₁₇	12.1556800	-13.8514959	19.0637476	1659	C	C ₁₉	-1.0590999	-13.4039223	-22.9374294
1607	C	C ₁₆	-22.7543839	9.3434963	13.1565469	1660	C	C ₁₉	18.1361562	-18.4226423	6.2127820
1608	C	C ₁₆	21.2332692	8.8958464	15.7534076	1661	C	C ₁₉	-17.0777198	-18.7333616	8.0203068
1609	C	C ₁₆	-22.7527789	-9.3422715	-13.1601927	1662	C	C ₂₀	-3.8102323	18.5987477	13.9567503
1610	C	C ₁₆	21.2353114	-8.8969892	-15.7500063	1663	C	C ₂₀	11.0844298	20.7360305	1.5410202
1611	C	C ₁₆	1.5170236	-15.5829365	23.0874071	1664	C	C ₂₀	-3.8089980	-18.5985417	-13.9573662
1612	C	C ₁₇	-25.6459968	4.6386007	4.4500623	1665	C	C ₂₀	11.0835554	-20.7366276	-1.5392419
1613	C	C ₁₇	15.9395391	1.7856428	21.0185485	1666	C	C ₂₀	-7.2753604	-21.8556446	4.9620657
1614	C	C ₁₇	-25.6455323	-4.6372196	-4.4541748	1667	C	C ₁₈	-1.8549430	22.3111717	14.4645384
1615	C	C ₁₇	15.9428039	-1.7865010	-21.0159936	1668	C	C ₁₈	9.9947623	24.7028415	0.5714118
1616	C	C ₁₇	9.7025218	-9.3227214	22.7592785	1669	C	C ₁₈	-1.8538253	-22.3110711	-14.4648401
1617	C	C ₁₆	-13.0705345	-2.2570241	24.5455535	1670	C	C ₁₈	9.9935191	-24.7033795	-0.5698102
1618	C	C ₁₆	27.8158249	2.0755628	-0.6237736	1671	C	C ₁₈	-8.1406421	-25.2478293	2.5940565
1619	C	C ₁₆	-13.0664825	2.2577272	-24.5476449	1672	C	C ₁₉	3.6848526	17.1626849	19.9311012
1620	C	C ₁₆	27.8156147	-2.0770597	0.6282284	1673	C	C ₁₉	12.6468058	21.9617181	-7.9451869
1621	C	C ₁₆	-14.7492074	-5.9162900	22.9319782	1674	C	C ₁₉	3.6871256	-17.1628831	-19.9305118
1622	C	C ₁₇	-18.1092365	4.6773576	18.7003596	1675	C	C ₁₉	12.6443480	-21.9623981	7.9472087
1623	C	C ₁₇	24.3277033	6.5041471	8.0860578	1676	C	C ₁₉	-16.3322611	-20.8784362	1.6531298
1624	C	C ₁₇	-18.1064940	-4.6763840	-18.7032542	1677	C	C ₂₀	-3.2840518	9.2249692	21.4800310
1625	C	C ₁₇	24.3286532	-6.5054561	-8.0821633	1678	C	C ₂₀	18.6193810	13.7311094	-4.6959487
1626	C	C ₁₇	-6.2224612	-11.8259001	22.8244306	1679	C	C ₂₀	-3.2811036	-9.2247930	-21.4805541
1627	C	C ₁₆	-22.3285015	5.8235049	15.7353862	1680	C	C ₂₀	18.6178898	-13.7321105	4.6989255
1628	C	C ₁₆	23.7384314	6.2371821	13.3289951	1681	C	C ₂₀	-15.3372803	-14.6958321	10.2993754
1629	C	C ₁₆	-22.3262973	-5.8223034	-15.7389615	1682	C	C ₁₈	-6.4658859	11.1776641	23.3940382
1630	C	C ₁₆	23.7402321	-6.2384600	-13.3251909	1683	C	C ₁₈	21.5569734	15.6119364	-2.3649573
1631	C	C ₁₆	-1.4142610	-12.7990210	24.7843196	1684	C	C ₁₈	-6.4627312	-11.1773165	-23.3950718
1632	C	C ₁₇	-13.7889296	8.6654650	20.9654133	1685	C	C ₁₈	21.5557595	-15.6130958	2.3684057
1633	C	C ₁₇	23.5148104	11.5229931	4.3643676	1686	C	C ₁₈	-15.0936010	-17.5117436	13.3996612
1634	C	C ₁₇	-13.7860339	-8.6647226	-20.9676234	1687	C	C ₁₉	-2.8151201	18.5780032	18.8591219
1635	C	C ₁₇	23.5148901	-11.5242567	-4.3606124	1688	C	C ₁₉	14.7739578	22.0918981	-1.5529853
1636	C	C ₁₇	-9.7293205	-15.5750203	19.1711367	1689	C	C ₁₉	-2.8130986	-18.5778519	-18.8595718
1637	C	C ₁₈	-10.0345627	12.3913236	21.4356384	1690	C	C ₁₉	14.7725151	-22.0926944	1.5553588

1691	C	C ₁₉	-11.9602560	-22.9189417	6.3567262	1744	C	C ₂₀	16.3096737	-9.6408101	-14.1860188
1692	C	C ₂₀	6.9610406	14.3528723	17.5550607	1745	C	C ₂₀	2.5357235	-15.1787239	17.9824886
1693	C	C ₂₀	9.3936268	19.1587726	-10.3606175	1746	C	C ₁₈	-21.4400275	9.1288630	12.7766440
1694	C	C ₂₀	6.9630779	-14.3532469	-17.5539464	1747	C	C ₁₈	20.2833852	8.7883499	14.7513640
1695	C	C ₂₀	9.3909364	-19.1592784	10.3621236	1748	C	C ₁₈	-21.4384722	-9.1277092	-12.7800775
1696	C	C ₂₀	-16.3546787	-17.1126806	-1.5237564	1749	C	C ₁₈	20.2852745	-8.7894415	-14.7481153
1697	C	C ₁₈	1.7368902	23.4420527	12.5553881	1750	C	C ₁₈	1.1527645	-15.0891689	21.8458615
1698	C	C ₁₈	6.4032958	25.8339157	-1.3383136	1751	C	C ₁₉	-25.3923541	4.4289845	5.7976986
1699	C	C ₁₈	1.7376411	-23.4421454	-12.5551147	1752	C	C ₁₉	16.9936803	1.9603284	20.1338729
1700	C	C ₁₈	6.4016909	-25.8342590	1.3393315	1753	C	C ₁₉	-25.3916645	-4.4276181	-5.8017645
1701	C	C ₁₈	-8.1403060	-25.3233472	-1.6272359	1754	C	C ₁₉	16.9968002	-1.9612431	-20.1311506
1702	C	C ₁₉	-3.7735715	25.6445850	5.3980858	1755	C	C ₁₉	8.3946567	-9.4228309	23.2107918
1703	C	C ₁₉	2.7263724	25.3365695	7.1867255	1756	C	C ₂₀	13.7759650	12.4596045	-14.4696593
1704	C	C ₁₉	-3.7740839	-25.6443824	-5.3986875	1757	C	C ₂₀	-21.0679279	10.3171211	-2.0222004
1705	C	C ₁₉	2.7261605	-25.3367155	-7.1862929	1758	C	C ₂₀	7.2923440	6.2685258	21.4922580
1706	C	C ₁₉	1.0469073	-26.4456666	-0.7447253	1759	C	C ₂₀	-21.0688057	-10.3159878	2.0188298
1707	C	C ₂₀	3.7020483	21.1055026	9.6832218	1760	C	C ₂₀	7.2954513	-6.2689179	-21.4910925
1708	C	C ₂₀	3.3126596	23.1667148	-2.2894802	1761	C	C ₂₀	13.7729732	-12.4603457	14.4718645
1709	C	C ₂₀	-7.0138422	22.0790292	4.0292241	1762	C	C ₁₈	-12.1172421	-2.3527355	23.5399798
1710	C	C ₂₀	3.3110469	-23.1668936	2.2900143	1763	C	C ₁₈	26.4950089	1.8718816	-1.0020215
1711	C	C ₂₀	-7.0143872	-22.0786527	-4.0303414	1764	C	C ₁₈	-12.1133398	2.3533876	-23.5419212
1712	C	C ₂₀	3.7024646	-21.1057031	-9.6826215	1765	C	C ₁₈	26.4947437	-1.8733067	1.0062608
1713	C	C ₁₈	8.0828432	9.8725043	23.4107163	1766	C	C ₁₈	-14.3814689	-5.4324657	21.6830633
1714	C	C ₁₈	14.4886003	16.5052719	-15.1167840	1767	C	C ₁₉	-18.0539918	3.3189518	18.9868163
1715	C	C ₁₈	8.0860634	-9.8729380	-23.4094291	1768	C	C ₁₉	24.7441347	5.2843556	7.5673336
1716	C	C ₁₈	14.4852879	-16.5060504	15.1190976	1769	C	C ₁₉	-18.0511271	-3.3179803	-18.9897070
1717	C	C ₁₈	-22.5718779	-14.1293170	1.3164579	1770	C	C ₁₉	24.7450613	-5.2856870	-7.5633727
1718	C	C ₁₉	-23.2060950	10.5715608	7.3814241	1771	C	C ₁₉	-6.6941861	-10.5898543	23.2487444
1719	C	C ₁₉	16.3497874	8.5561416	19.0851483	1772	C	C ₂₀	-11.0981065	11.3485346	17.5223183
1720	C	C ₁₉	6.8567604	15.3757625	-20.5264941	1773	C	C ₂₀	18.8366281	13.6221260	4.3136816
1721	C	C ₁₉	16.3523850	-8.5570208	-19.0825338	1774	C	C ₂₀	-11.0959090	-11.3479378	-17.5240929
1722	C	C ₁₉	6.8526407	-15.3761316	20.5275926	1775	C	C ₂₀	18.8365869	-13.6231393	-4.3106675
1723	C	C ₁₉	-23.2054785	-10.5703126	-7.3851370	1776	C	C ₂₀	-7.7412272	-16.8834454	14.6291324
1724	C	C ₂₀	-23.0337128	0.3348894	4.4812588	1777	C	C ₁₈	-21.4923368	5.3391030	14.7429379
1725	C	C ₂₀	15.2922968	-1.9405392	17.6953641	1778	C	C ₁₈	22.5444824	5.6476725	12.9472286
1726	C	C ₂₀	7.7414582	4.8283600	-21.6218046	1779	C	C ₁₈	-21.4902600	-5.3379468	-14.7463781
1727	C	C ₂₀	15.2952323	1.9397152	-17.6929094	1780	C	C ₁₈	22.5462519	-5.6488853	-12.9436208
1728	C	C ₂₀	7.7377414	-4.8287765	21.6230440	1781	C	C ₁₈	-1.0562931	-11.9637883	23.7388457
1729	C	C ₂₀	-23.0330159	-0.3336490	-4.4849527	1782	C	C ₁₉	-14.7388100	9.0942794	20.0442621
1730	C	C ₁₈	-26.4820285	-0.0266695	2.1087415	1783	C	C ₁₉	23.1405731	11.5626860	5.7034184
1731	C	C ₁₈	15.0446905	-3.3882347	21.6315224	1784	C	C ₁₉	-14.7360880	-9.0934864	-20.0466213
1732	C	C ₁₈	-26.4816940	0.0280949	-2.1129842	1785	C	C ₁₉	23.1408730	-11.5639320	-5.6997086
1733	C	C ₁₈	15.0483382	3.3874241	-21.6291075	1786	C	C ₁₉	-8.4052560	-15.8939011	19.4537005
1734	C	C ₁₈	11.4333428	-4.3945661	23.5735401	1787	C	C ₂₀	-9.3159267	0.0743721	21.6080557
1735	C	C ₁₉	12.9370106	12.7226383	-19.3074245	1788	C	C ₂₀	23.0889283	4.1213335	-1.9015441
1736	C	C ₁₉	-24.8160015	9.2322315	0.9697869	1789	C	C ₂₀	-9.3124666	-0.0738715	-21.6095437
1737	C	C ₁₉	11.8793503	5.4300667	23.0521979	1790	C	C ₂₀	23.0884119	-4.1225761	1.9052422
1738	C	C ₁₉	-24.8163406	-9.2308958	-0.9737627	1791	C	C ₂₀	-13.7760818	-6.8586995	17.8010648
1739	C	C ₁₉	11.8827476	-5.4307059	-23.0502961	1792	C	C ₂₁	-10.6362990	14.4363536	20.6498235
1740	C	C ₁₉	12.9332336	-12.7233349	19.3094986	1793	C	C ₂₁	20.8213254	17.4288389	3.2653125
1741	C	C ₂₀	-18.8468717	10.3865825	9.8543280	1794	C	C ₂₁	-10.6337726	-14.4357821	-20.6515220
1742	C	C ₂₀	16.3079173	9.6399333	14.1886257	1795	C	C ₂₁	20.8209164	-17.4299596	-3.2619767
1743	C	C ₂₀	-18.8458542	-10.3855676	-9.8573497	1796	C	C ₂₁	-10.1878316	-20.5543888	14.8889073

1797	C	C ₂₂	-12.8751093	4.3835492	23.9849017	1850	C	C ₂₃	8.7924115	-19.4344246	9.1139719
1798	C	C ₂₂	26.2640208	8.3175176	1.1311186	1851	C	C ₂₃	-15.0306009	-17.6010724	-1.5333991
1799	C	C ₂₂	-12.8715046	-4.3828570	-23.9869599	1852	C	C ₂₁	3.8059106	23.3689643	13.4921396
1800	C	C ₂₂	26.2637574	-8.3189309	-1.1269131	1853	C	C ₂₁	6.1790134	26.3029590	-3.5504064
1801	C	C ₂₂	-13.3925783	-12.1008768	20.8438739	1854	C	C ₂₁	3.8068103	-23.3691693	-13.4915294
1802	C	C ₂₃	-17.6307753	1.3745897	14.7068456	1855	C	C ₂₁	6.1770226	-26.3032911	3.5513937
1803	C	C ₂₃	21.1653403	2.4127514	8.6736353	1856	C	C ₂₁	-9.9848239	-25.1843010	-2.9471262
1804	C	C ₂₃	-17.6284890	-1.3736405	-14.7096715	1857	C	C ₂₂	-3.4970925	26.5802010	6.3882541
1805	C	C ₂₃	21.1665948	-2.4138900	-8.6702481	1858	C	C ₂₂	3.2957722	26.5207443	6.7330958
1806	C	C ₂₃	-3.5382552	-7.5939549	21.4204958	1859	C	C ₂₂	-3.4975014	-26.5800114	-6.3888221
1807	C	C ₂₁	10.0807095	14.7215715	20.7807258	1860	C	C ₂₂	3.2954220	-26.5209211	-6.7325712
1808	C	C ₂₁	10.5326414	20.7789691	-14.4042336	1861	C	C ₂₂	0.2010260	-27.5485704	-0.7631443
1809	C	C ₂₁	10.0832490	-14.7221139	-20.7791118	1862	C	C ₂₃	4.3495494	20.9574825	8.4284736
1810	C	C ₂₁	10.5292135	-20.7795353	14.4059174	1863	C	C ₂₃	1.9397618	22.8055554	-2.3060361
1811	C	C ₂₁	-20.6131622	-17.8159583	-2.8059057	1864	C	C ₂₃	-6.2884545	21.5275633	5.1179200
1812	C	C ₂₂	-0.1869668	13.9960908	23.8569161	1865	C	C ₂₃	1.9381655	-22.8056585	2.3063395
1813	C	C ₂₂	18.3985065	19.3474497	-7.2283376	1866	C	C ₂₃	-6.2887997	-21.5272255	-5.1189238
1814	C	C ₂₂	-0.1839032	-13.9960818	-23.8569401	1867	C	C ₂₃	4.3497774	-20.9577173	-8.4277730
1815	C	C ₂₂	18.3963143	-19.3484399	7.2312847	1868	C	C ₂₁	6.4723272	9.1258564	24.8201219
1816	C	C ₂₂	-18.2131033	-19.4019480	7.5448818	1869	C	C ₂₁	16.6064414	15.9076637	-14.5733724
1817	C	C ₂₃	-4.4609655	17.4894815	14.4632994	1870	C	C ₂₁	6.4758057	-9.1262041	-24.8190890
1818	C	C ₂₃	12.0050754	19.7060735	1.5867757	1871	C	C ₂₁	16.6032502	-15.9085584	14.5760385
1819	C	C ₂₃	-4.4595845	-17.4892425	-14.4640080	1872	C	C ₂₁	-23.0795682	-14.0049885	3.5220104
1820	C	C ₂₃	12.0042746	-19.7067205	-1.5848473	1873	C	C ₂₂	-24.1917829	11.3834855	6.8292662
1821	C	C ₂₃	-7.5454504	-21.0169120	6.0270052	1874	C	C ₂₂	16.2521023	9.0496829	20.3822801
1822	C	C ₂₁	-3.9695293	22.9744113	13.9953334	1875	C	C ₂₂	7.9401607	16.1589501	-20.9118876
1823	C	C ₂₁	10.5541527	24.9090276	2.7568384	1876	C	C ₂₂	16.2548772	-9.0505576	-20.3796771
1824	C	C ₂₁	-3.9685207	-22.9741987	-13.9959633	1877	C	C ₂₂	7.9359427	-16.1593776	20.9131610
1825	C	C ₂₁	10.5532568	-24.9095946	-2.7551540	1878	C	C ₂₂	-24.1913001	-11.3821833	-6.8331423
1826	C	C ₂₁	-6.5857067	-26.0754918	4.0183690	1879	C	C ₂₃	-22.2302202	0.8240944	5.5432885
1827	C	C ₂₂	3.3530312	18.4701778	20.2819571	1880	C	C ₂₃	15.7250867	-1.0880327	16.6471533
1828	C	C ₂₂	12.9200790	23.2519857	-7.4943225	1881	C	C ₂₃	6.5052014	5.4447724	-21.2985151
1829	C	C ₂₂	3.3552839	-18.4703578	-20.2814225	1882	C	C ₂₃	15.7278128	1.0871864	-16.6446348
1830	C	C ₂₂	12.9176306	-23.2526799	7.4963857	1883	C	C ₂₃	6.5014962	-5.4451222	21.2995554
1831	C	C ₂₂	-16.2737492	-22.2662262	1.7687075	1884	C	C ₂₃	-22.2293771	-0.8228983	-5.5468472
1832	C	C ₂₃	-1.9208939	9.0017316	21.1501031	1885	C	C ₂₁	10.1231024	3.2135028	-25.0100841
1833	C	C ₂₃	17.6890268	13.6350844	-5.7646274	1886	C	C ₂₁	-26.8790962	-1.7100149	3.5914200
1834	C	C ₂₃	-1.9179968	-9.0016273	-21.1504166	1887	C	C ₂₁	16.7559470	-4.6853999	20.8708785
1835	C	C ₂₃	17.6873634	-13.6360354	5.7674548	1888	C	C ₂₁	-26.8784304	1.7114601	-3.5957172
1836	C	C ₂₃	-15.7698537	-14.1991931	9.0411557	1889	C	C ₂₁	16.7595440	4.6844969	-20.8681882
1837	C	C ₂₁	-6.2903616	9.4184409	24.8293894	1890	C	C ₂₁	10.1189231	-3.2140480	25.0117083
1838	C	C ₂₁	22.9527019	14.3144423	-3.6116928	1891	C	C ₂₂	13.4088376	12.4291247	-20.5872427
1839	C	C ₂₁	-6.2868926	-9.4181031	-24.8303932	1892	C	C ₂₂	-26.1010818	8.6997560	1.0781335
1840	C	C ₂₁	22.9513561	-14.3156774	3.6153677	1893	C	C ₂₂	12.6925838	4.7589106	23.9659227
1841	C	C ₂₁	-16.6649871	-16.1626183	14.3465058	1894	C	C ₂₂	-26.1013724	-8.6983519	-1.0823106
1842	C	C ₂₂	-3.3715219	18.7281887	20.1256864	1895	C	C ₂₂	12.6961664	-4.7595928	-23.9638950
1843	C	C ₂₂	16.1110726	22.4714800	-1.6190342	1896	C	C ₂₂	13.4048663	-12.4298466	20.5893922
1844	C	C ₂₂	-3.3693105	-18.7280081	-20.1262219	1897	C	C ₂₃	-18.4888963	10.8705654	8.5882835
1845	C	C ₂₂	16.1096095	-22.4723472	1.6216157	1898	C	C ₂₃	14.9772935	9.8381074	14.5828555
1846	C	C ₂₂	-12.7411475	-23.4620179	7.3724038	1899	C	C ₂₃	-18.4881111	-10.8695697	-8.5912488
1847	C	C ₂₃	6.2356593	15.0171584	16.5429601	1900	C	C ₂₃	14.9790984	-9.8389147	-14.5804497
1848	C	C ₂₃	8.7949256	19.4339516	-9.1125651	1901	C	C ₂₃	3.5085405	-15.2717260	16.9773855
1849	C	C ₂₃	6.2374976	-15.0174938	-16.5419629	1902	C	C ₂₁	-20.7503430	11.0968634	13.6987218

1903	C	C ₂₁	20.4363875	11.0039757	14.2351290	1956	C	C ₂₅	27.2886216	-8.3923839	-2.0828973
1904	C	C ₂₁	-20.7487527	-11.0957471	-13.7020426	1957	C	C ₂₅	-13.0998935	-12.5615017	22.1368672
1905	C	C ₂₁	20.4380717	-11.0050755	-14.2318562	1958	C	C ₂₆	-17.7283610	0.0936219	14.1775480
1906	C	C ₂₁	0.3101579	-17.1020971	21.1847626	1959	C	C ₂₆	20.9505824	1.0400075	8.6774358
1907	C	C ₂₂	-26.2187514	4.9779957	6.7726841	1960	C	C ₂₆	-17.7260963	-0.0926681	-14.1803856
1908	C	C ₂₂	18.1583458	2.6087149	20.5314770	1961	C	C ₂₆	20.9519178	-1.0411351	-8.6740800
1909	C	C ₂₂	-26.2179310	-4.9765845	-6.7768846	1962	C	C ₂₆	-3.2259185	-6.2498942	21.5832965
1910	C	C ₂₂	18.1614905	-2.6096918	-20.5285706	1963	C	C ₂₄	10.2237778	15.3810766	21.9920946
1911	C	C ₂₂	8.0562056	-10.3140693	24.2237516	1964	C	C ₂₄	11.3980919	21.7348237	-14.9142919
1912	C	C ₂₃	13.6458370	11.0972529	-14.9329179	1965	C	C ₂₄	10.2264644	-15.3816271	-21.9904557
1913	C	C ₂₃	-21.1980951	8.8782883	-2.0412118	1966	C	C ₂₄	11.3945298	-21.7354372	14.9161182
1914	C	C ₂₃	7.5525927	4.8679225	21.2511579	1967	C	C ₂₄	-21.6217357	-18.7297450	-2.5401922
1915	C	C ₂₃	-21.1989056	-8.8771474	2.0378163	1968	C	C ₂₅	-0.4309669	15.2952419	24.2806794
1916	C	C ₂₃	7.5557281	-4.8683291	-21.2499475	1969	C	C ₂₅	18.6913132	20.6609270	-6.8878302
1917	C	C ₂₃	13.6428428	-11.0979872	14.9351031	1970	C	C ₂₅	-0.4279028	-15.2952198	-24.2807423
1918	C	C ₂₁	-10.4191389	-2.5698226	25.0122392	1971	C	C ₂₅	18.6891038	-20.6619326	6.8908219
1919	C	C ₂₁	26.9343854	2.2829386	-3.1782964	1972	C	C ₂₅	-18.2619456	-20.7871349	7.6208869
1920	C	C ₂₁	-10.4149972	2.5703828	-25.0139053	1973	C	C ₂₆	-5.7101933	17.2375206	13.8937832
1921	C	C ₂₁	26.9337564	-2.2843883	3.1826113	1974	C	C ₂₆	12.1806430	19.1385837	2.8499275
1922	C	C ₂₁	-16.5188256	-5.3444293	20.9604396	1975	C	C ₂₆	-5.7088974	-17.2372142	-13.8946923
1923	C	C ₂₂	-18.3664260	2.8444973	20.2545057	1976	C	C ₂₆	12.1800698	-19.1392405	-2.8479694
1924	C	C ₂₂	26.0519909	5.1024033	7.1358750	1977	C	C ₂₆	-6.4719279	-20.8165726	6.8963825
1925	C	C ₂₂	-18.3633293	-2.8435094	-20.2574443	1978	C	C ₂₄	-3.8980053	23.9904513	14.9249971
1926	C	C ₂₂	26.0528582	-5.1038044	-7.1317086	1979	C	C ₂₄	11.1625725	26.1248619	2.5259384
1927	C	C ₂₂	-7.6897710	-10.4996899	24.2133374	1980	C	C ₂₄	-3.8969021	-23.9902409	-14.9256255
1928	C	C ₂₃	-11.9178667	10.8313995	16.5412460	1981	C	C ₂₄	11.1615740	-26.1254633	-2.5241469
1929	C	C ₂₃	18.4851623	12.7608073	5.3317941	1982	C	C ₂₄	-7.2656787	-27.2702911	4.1270905
1930	C	C ₂₃	-11.9158026	-10.8307592	-16.5431485	1983	C	C ₂₅	2.8161347	18.7288865	21.5443363
1931	C	C ₂₃	18.4853357	-12.7618020	-5.3288346	1984	C	C ₂₅	14.2279284	23.7372229	-7.5478947
1932	C	C ₂₃	-6.5700562	-16.2630674	15.0104824	1985	C	C ₂₅	2.8185760	-18.7290372	-21.5438903
1933	C	C ₂₁	-22.8262110	3.5532630	14.3324562	1986	C	C ₂₅	14.2254379	-23.7379892	7.5501769
1934	C	C ₂₁	23.1234462	3.6399809	13.8252454	1987	C	C ₂₅	-17.0448718	-22.9092249	2.7386106
1935	C	C ₂₁	-22.8241029	-3.5520352	-14.3361084	1988	C	C ₂₆	-1.4296973	7.7021711	21.2980634
1936	C	C ₂₁	23.1254603	-3.6412260	-13.8215380	1989	C	C ₂₆	17.7606334	12.5009273	-6.5773957
1937	C	C ₂₁	-0.3015926	-10.3481069	25.1377528	1990	C	C ₂₆	-1.4267020	-7.7020923	-21.2983031
1938	C	C ₂₂	-16.0759386	9.2426865	20.4184848	1991	C	C ₂₆	17.7589030	-12.5018828	6.5802381
1939	C	C ₂₂	24.1067250	11.6020451	6.7108807	1992	C	C ₂₆	-16.3326306	-12.9206625	9.0153554
1940	C	C ₂₂	-16.0731636	-9.2418212	-20.4210606	1993	C	C ₂₄	-6.5539480	10.2261605	25.9118534
1941	C	C ₂₂	24.1071779	-11.6033409	-6.7070294	1994	C	C ₂₄	23.8896879	15.3200285	-3.6786457
1942	C	C ₂₂	-8.0344971	-16.3262233	20.7286968	1995	C	C ₂₄	-6.5503412	-10.2258070	-25.9129079
1943	C	C ₂₃	-8.7465371	1.2723527	21.2368501	1996	C	C ₂₄	23.8882794	-15.3213129	3.6824646
1944	C	C ₂₃	22.3114251	5.2581640	-1.9174514	1997	C	C ₂₄	-17.3384862	-17.2456494	14.8632841
1945	C	C ₂₃	-8.7432036	-1.2718820	-21.2382511	1998	C	C ₂₅	-2.6103201	19.3410672	21.1118008
1946	C	C ₂₃	22.3108340	-5.2593647	1.9210244	1999	C	C ₂₅	16.4820554	23.4170674	-2.5654589
1947	C	C ₂₃	-13.5678189	-7.8282094	16.8451187	2000	C	C ₂₅	-2.6079796	-19.3409268	-21.1122184
1948	C	C ₂₄	-11.2219892	14.7754820	21.8517113	2001	C	C ₂₅	16.4803841	-23.4179543	2.5680983
1949	C	C ₂₄	22.0901299	17.9686843	3.3011766	2002	C	C ₂₅	-13.8732830	-24.1838751	7.0193296
1950	C	C ₂₄	-11.2192783	-14.7748774	-21.8535126	2003	C	C ₂₆	6.9872650	15.4423731	15.4555119
1951	C	C ₂₄	22.0896843	-17.9698726	-3.2976419	2004	C	C ₂₆	7.4285454	19.6785313	-9.1506180
1952	C	C ₂₄	-10.8711148	-21.2663358	15.8526660	2005	C	C ₂₆	6.9889090	-15.4427486	-15.4543961
1953	C	C ₂₅	-14.1927323	4.5430520	24.4410812	2006	C	C ₂₆	7.4260177	-19.6789313	9.1518094
1954	C	C ₂₅	27.2887379	8.3909154	2.0872677	2007	C	C ₂₆	-14.4156189	-17.6247898	-2.7781869
1955	C	C ₂₅	-14.1890541	-4.5422876	-24.4433576	2008	C	C ₂₄	3.7050528	24.6449525	13.9690982

2009	C	C ₂₄	6.4490523	27.6286501	-3.3621798	2062	C	C ₂₅	-27.3280740	5.7223647	6.3689842
2010	C	C ₂₄	3.7059658	-24.6451518	-13.9685055	2063	C	C ₂₅	18.2591053	3.0566800	21.8493728
2011	C	C ₂₄	6.4470251	-27.6289969	3.3632112	2064	C	C ₂₅	-27.3273663	-5.7208940	-6.3733612
2012	C	C ₂₄	-10.1540252	-26.5396314	-2.9631985	2065	C	C ₂₅	18.2624420	-3.0576635	-21.8464440
2013	C	C ₂₅	-3.0318077	27.8480751	6.0176447	2066	C	C ₂₅	9.0646636	-11.0880719	24.7995883
2014	C	C ₂₅	2.5605484	27.7093003	6.8233040	2067	C	C ₂₆	14.5046339	10.1570681	-14.3513943
2015	C	C ₂₅	-3.0323466	-27.8479125	-6.0181270	2068	C	C ₂₆	-20.9930574	8.2507436	-3.2756360
2016	C	C ₂₅	2.5601461	-27.7094376	-6.8228970	2069	C	C ₂₆	6.4887172	3.9880202	21.4826720
2017	C	C ₂₅	0.4710874	-28.6004031	-1.6474864	2070	C	C ₂₆	-20.9940243	-8.2496137	3.2722728
2018	C	C ₂₆	5.5890402	20.3050654	8.4363273	2071	C	C ₂₆	6.4919415	-3.9883694	-21.4816331
2019	C	C ₂₆	1.4225795	22.3654223	-3.5311191	2072	C	C ₂₆	14.5017889	-10.1578489	14.3537188
2020	C	C ₂₆	-7.0107879	20.7231895	6.0085770	2073	C	C ₂₄	-11.2715812	-2.4756622	26.0918841
2021	C	C ₂₆	1.4208097	-22.3654997	3.5313521	2074	C	C ₂₄	28.2682220	2.5185332	-2.9203513
2022	C	C ₂₆	-7.0109358	-20.7228118	-6.0097019	2075	C	C ₂₄	-11.2672742	2.4762682	-26.0936863
2023	C	C ₂₆	5.5892942	-20.3053656	-8.4354353	2076	C	C ₂₄	28.2676233	-2.5200550	2.9248818
2024	C	C ₂₄	7.1521945	9.6074066	25.9265652	2077	C	C ₂₄	-17.0004262	-5.8305254	22.1574895
2025	C	C ₂₄	17.1400761	16.7458177	-15.5382828	2078	C	C ₂₅	-18.7048188	3.7647553	21.2362648
2026	C	C ₂₄	7.1558264	-9.6077917	-25.9254188	2079	C	C ₂₅	26.9239021	6.1794168	7.2070143
2027	C	C ₂₄	17.1366882	-16.7467405	15.5410302	2080	C	C ₂₅	-18.7016234	-3.7637485	-21.2392615
2028	C	C ₂₄	-24.2930527	-14.6433130	3.3262451	2081	C	C ₂₅	26.9247239	-6.1808664	-7.2026986
2029	C	C ₂₅	-25.5256410	10.9719644	6.8612246	2082	C	C ₂₅	-8.2233842	-11.6761393	24.7197551
2030	C	C ₂₅	17.0067653	8.4679319	21.4028746	2083	C	C ₂₆	-12.0283699	11.5816080	15.3553024
2031	C	C ₂₅	8.5193403	15.9691761	-22.1681125	2084	C	C ₂₆	17.4180342	13.1649584	6.1560286
2032	C	C ₂₅	17.0097405	-8.4688479	-21.4001471	2085	C	C ₂₆	-12.0265348	-11.5809603	-15.3572313
2033	C	C ₂₅	8.5149317	-15.9696337	22.1694720	2086	C	C ₂₆	17.4183096	-13.1658962	-6.1532367
2034	C	C ₂₅	-25.5251368	-10.9705909	-6.8653114	2087	C	C ₂₆	-5.3923187	-16.6997274	14.3750702
2035	C	C ₂₆	-21.6512269	-0.1211827	6.3983668	2088	C	C ₂₄	-23.7209299	3.9296840	15.3177502
2036	C	C ₂₆	16.3042503	-1.6929617	15.5252897	2089	C	C ₂₄	24.3564269	4.1157737	14.2331670
2037	C	C ₂₆	5.3470141	4.6697157	-21.4320444	2090	C	C ₂₄	-23.7186847	-3.9284080	-15.3215460
2038	C	C ₂₆	16.3068264	1.6920845	-15.5226800	2091	C	C ₂₄	24.3584857	-4.1170839	-14.2292700
2039	C	C ₂₆	5.3433293	-4.6700037	21.4329025	2092	C	C ₂₄	-0.6400521	-11.0868300	26.2570168
2040	C	C ₂₆	-21.6501932	0.1223479	-6.4018344	2093	C	C ₂₅	-16.4241568	8.9706849	21.7381757
2041	C	C ₂₄	10.7510946	3.7396464	-26.1144725	2094	C	C ₂₅	25.4471167	11.6215859	6.3369937
2042	C	C ₂₄	-28.2129447	-1.3912774	3.6919179	2095	C	C ₂₅	-16.4211618	-8.9698013	-21.7408051
2043	C	C ₂₄	17.4618262	-4.5512309	22.0433036	2096	C	C ₂₅	25.4475084	-11.6229559	-6.3329150
2044	C	C ₂₄	-28.2122804	1.3927962	-3.6964393	2097	C	C ₂₅	-9.0268327	-16.4480703	21.6968124
2045	C	C ₂₄	17.4656047	4.5502920	-22.0405117	2098	C	C ₂₆	-7.3541188	1.3500711	21.2732188
2046	C	C ₂₄	10.7467095	-3.7402233	26.1161851	2099	C	C ₂₆	21.6348475	5.5462649	-3.1029504
2047	C	C ₂₅	-26.9762776	9.2290689	2.0211342	2100	C	C ₂₆	-7.3507925	-1.3496743	-21.2744028
2048	C	C ₂₅	13.8572439	5.3732548	24.4148559	2101	C	C ₂₆	21.6340466	-5.5474286	3.1064121
2049	C	C ₂₅	-26.9764506	-9.2276183	-2.0254480	2102	C	C ₂₆	-14.2834494	-7.7070905	15.6537351
2050	C	C ₂₅	13.8608657	-5.3740017	-24.4126307	2103	C	C ₂₇	-11.1667855	13.8530708	22.8993617
2051	C	C ₂₅	13.1152137	-13.3013867	21.6343369	2104	C	C ₂₇	23.0921862	17.3569569	2.5441211
2052	C	C ₂₆	-17.3827442	11.7420689	8.4868299	2105	C	C ₂₇	-11.1638617	-13.8524692	-22.9011540
2053	C	C ₂₆	14.2095911	10.8090879	13.9037239	2106	C	C ₂₇	23.0916597	-17.3581983	-2.5404306
2054	C	C ₂₆	-17.3820198	-11.7411331	-8.4896160	2107	C	C ₂₇	-11.9284734	-20.6383532	16.5153061
2055	C	C ₂₆	14.2112356	-10.8098534	-13.9014440	2108	C	C ₂₈	-15.1947370	3.6817256	23.9953855
2056	C	C ₂₆	3.1702794	-15.9176267	15.7683464	2109	C	C ₂₈	27.5358945	7.3077549	2.9300192
2057	C	C ₂₄	-22.0321703	11.4268191	14.0756133	2110	C	C ₂₈	-15.1910898	-3.6809073	-23.9978226
2058	C	C ₂₄	21.3504934	11.2258411	15.2397051	2111	C	C ₂₈	27.5359655	-7.3092369	-2.9256090
2059	C	C ₂₄	-22.0305317	-11.4256333	-14.0791429	2112	C	C ₂₈	-12.3451745	-11.7728268	23.0045839
2060	C	C ₂₄	21.3523291	-11.2269904	-15.2362840	2113	C	C ₂₉	-18.6847680	-0.1419905	13.1877554
2061	C	C ₂₄	0.6776730	-17.7006736	22.3682481	2114	C	C ₂₉	20.6186375	0.4257895	9.8867598

2115	C	C ₂₉	-18.6826476	0.1429955	-13.1907452	2168	C	C ₂₇	-9.2334216	-27.3350581	-2.2709857
2116	C	C ₂₉	20.6201947	-0.4269004	-9.8834504	2169	C	C ₂₈	1.5621499	28.5375773	2.5002283
2117	C	C ₂₉	-1.9376335	-5.9167776	22.0067018	2170	C	C ₂₈	-2.8397485	28.1619752	4.6822817
2118	C	C ₂₇	9.2802338	15.1546267	22.9822287	2171	C	C ₂₈	1.2787061	27.7029708	7.3481348
2119	C	C ₂₇	12.7481775	21.6278161	-14.6181235	2172	C	C ₂₈	-2.8405120	-28.1618223	-4.6827368
2120	C	C ₂₇	9.2830976	-15.1551273	-22.9807356	2173	C	C ₂₈	1.2783907	-27.7030393	-7.3479317
2121	C	C ₂₇	12.7446786	-21.6285017	14.6201629	2174	C	C ₂₈	1.5610136	-28.5376617	-2.4999762
2122	C	C ₂₇	-22.0285069	-18.9000115	-1.2258609	2175	C	C ₂₉	6.1094546	19.8714185	9.6539363
2123	C	C ₂₈	-1.5207689	16.0007636	23.8016766	2176	C	C ₂₉	2.2652699	22.3323439	-4.6402715
2124	C	C ₂₈	18.7237508	21.0557080	-5.5619544	2177	C	C ₂₉	-8.3739062	20.5372053	5.7877594
2125	C	C ₂₈	-1.5178133	-16.0006816	-23.8019212	2178	C	C ₂₉	2.2633228	-22.3324670	4.6406414
2126	C	C ₂₈	18.7217317	-21.0567159	5.5649545	2179	C	C ₂₉	-8.3740821	-20.5367558	-5.7890939
2127	C	C ₂₈	-17.2046783	-21.5022151	8.1554139	2180	C	C ₂₉	6.1099309	-19.8717479	-9.6529546
2128	C	C ₂₉	-6.2013376	18.0551948	12.8852343	2181	C	C ₂₇	8.3787130	10.2272492	25.7417750
2129	C	C ₂₉	11.4453178	19.5958416	3.9349073	2182	C	C ₂₇	16.2780398	17.4727918	-16.3451964
2130	C	C ₂₉	-6.2002395	-18.0548614	-12.8862257	2183	C	C ₂₇	8.3822853	-10.2277000	-25.7404336
2131	C	C ₂₉	11.4449004	-19.5964574	-3.9330752	2184	C	C ₂₇	16.2744806	-17.4736678	16.3478036
2132	C	C ₂₉	-5.2454273	-21.4182025	6.6499628	2185	C	C ₂₇	-24.6573265	-15.0098320	2.0395174
2133	C	C ₂₇	-2.7301197	24.1632640	15.6695770	2186	C	C ₂₈	-25.8575644	9.7619810	7.4648064
2134	C	C ₂₇	11.1887170	26.6485695	1.2324011	2187	C	C ₂₈	17.8656384	7.4127931	21.1069378
2135	C	C ₂₇	-2.7289140	-24.1631178	-15.6700105	2188	C	C ₂₈	7.9923533	15.0115895	-23.0305843
2136	C	C ₂₇	11.1874850	-26.6491719	-1.2306081	2189	C	C ₂₈	17.8686154	-7.4137541	-21.1040796
2137	C	C ₂₇	-8.4595980	-27.4507524	3.4269402	2190	C	C ₂₈	7.9878610	-15.0120189	23.0318608
2138	C	C ₂₈	2.6370986	17.6950616	22.4584367	2191	C	C ₂₈	-25.8568938	-9.7605877	-7.4689580
2139	C	C ₂₈	15.2494828	22.9509774	-8.0719722	2192	C	C ₂₉	-21.8627066	-1.4664167	6.1610356
2140	C	C ₂₈	2.6397435	-17.6952038	-22.4580128	2193	C	C ₂₉	16.4050738	-3.0707093	15.4767933
2141	C	C ₂₈	15.2469506	-22.9517993	8.0744220	2194	C	C ₂₉	5.4576222	3.3541110	-21.8415042
2142	C	C ₂₈	-17.8875235	-22.1755672	3.5681357	2195	C	C ₂₉	16.4077188	3.0698271	-15.4741698
2143	C	C ₂₉	-2.2593549	6.7045582	21.8066617	2196	C	C ₂₉	5.4539443	-3.3544033	21.8423704
2144	C	C ₂₉	18.7560931	11.5520222	-6.3518591	2197	C	C ₂₉	-21.8616427	1.4675941	-6.1645423
2145	C	C ₂₉	-2.2562278	-6.7044365	-21.8070247	2198	C	C ₂₇	-28.6878408	-0.3234181	2.9380028
2146	C	C ₂₉	18.7544549	-11.5530323	6.3548676	2199	C	C ₂₇	16.8989441	-3.7883446	23.0608573
2147	C	C ₂₉	-16.4986270	-12.2155683	10.2059530	2200	C	C ₂₇	-28.6873584	0.3249619	-2.9425969
2148	C	C ₂₇	-6.7946363	11.5906303	25.7121942	2201	C	C ₂₇	16.9028443	3.7874342	-23.0581457
2149	C	C ₂₇	23.6391689	16.5401383	-3.0397769	2202	C	C ₂₇	11.7845070	-4.6427047	25.9094453
2150	C	C ₂₇	-6.7911431	-11.5902647	-25.7132818	2203	C	C ₂₈	-26.5729006	10.2952329	2.8222398
2151	C	C ₂₇	23.6377924	-16.5414106	3.0435636	2204	C	C ₂₈	14.1826434	6.6535722	23.9720383
2152	C	C ₂₇	-16.8472617	-18.5365127	14.6353748	2205	C	C ₂₈	-26.5730047	-10.2938042	-2.8264873
2153	C	C ₂₈	-1.3219803	19.7791332	20.8442606	2206	C	C ₂₈	14.1861279	-6.6543367	-23.9697600
2154	C	C ₂₈	15.5451846	23.9584458	-3.4329284	2207	C	C ₂₈	12.3864596	-14.4631449	21.3885240
2155	C	C ₂₈	-1.3196980	-19.7790623	-20.8444711	2208	C	C ₂₉	-16.6866205	12.0461080	9.6484851
2156	C	C ₂₈	15.5433506	-23.9592819	3.4354152	2209	C	C ₂₉	14.8083030	11.4936316	12.8551921
2157	C	C ₂₈	-14.2245374	-24.3466296	5.6876275	2210	C	C ₂₉	-16.6857244	-12.0452095	-9.6511603
2158	C	C ₂₉	-15.0788907	17.1917461	3.9133014	2211	C	C ₂₉	14.8097462	-11.4944275	-12.8528264
2159	C	C ₂₉	8.3536525	15.2150002	15.3936172	2212	C	C ₂₉	1.8754592	-16.3975601	15.6284344
2160	C	C ₂₉	6.7259262	19.6462466	-10.3455418	2213	C	C ₂₇	-23.0602110	10.5302779	13.8182593
2161	C	C ₂₉	8.3553041	-15.2154495	-15.3922810	2214	C	C ₂₇	21.7765791	10.1523959	16.0098027
2162	C	C ₂₉	6.7232127	-19.6466065	10.3466069	2215	C	C ₂₇	-23.0585644	-10.5290374	-13.8219498
2163	C	C ₂₉	-15.0791949	-17.1909341	-3.9157196	2216	C	C ₂₇	21.7785987	-10.1535677	-16.0063159
2164	C	C ₂₇	2.5371635	25.3677278	13.6989065	2217	C	C ₂₇	1.2794721	-16.9293603	23.3530316
2165	C	C ₂₇	6.6962150	28.0808313	-2.0607100	2218	C	C ₂₈	-27.5947316	5.9401309	5.0227528
2166	C	C ₂₇	2.5379900	-25.3678638	-13.6985037	2219	C	C ₂₈	17.2114683	2.8882317	22.7465614
2167	C	C ₂₇	6.6943765	-28.0811908	2.0617775	2220	C	C ₂₈	-27.5942494	-5.9386458	-5.0271728

2221	C	C ₂₈	17.2149565	-2.8891586	-22.7438017	2274	C	C ₃₁	-5.4334957	19.1355695	12.4652161
2222	C	C ₂₈	10.3790327	-10.9980252	24.3577818	2275	C	C ₃₁	10.5441988	20.6370637	3.7424376
2223	C	C ₂₉	15.4122378	10.5508666	-13.3858387	2276	C	C ₃₁	-5.4325298	-19.1352786	-12.4660780
2224	C	C ₂₉	-20.6806366	9.0030673	-4.3925602	2277	C	C ₃₁	10.5436900	-20.6376321	-3.7407438
2225	C	C ₂₉	5.2687140	4.4736531	21.9149616	2278	C	C ₃₁	-5.1119789	-22.2337822	5.5318273
2226	C	C ₂₉	-20.6818223	-9.0019544	4.3892485	2279	C	C ₃₀	2.9851958	16.3863569	22.0902168
2227	C	C ₂₉	5.2719825	-4.4739364	-21.9141194	2280	C	C ₃₀	14.9534311	21.6575883	-8.5291049
2228	C	C ₂₉	15.4095245	-10.5516962	13.3883083	2281	C	C ₃₀	2.9878627	-16.3865175	-22.0897393
2229	C	C ₂₇	-12.6314479	-2.3092691	25.8574004	2282	C	C ₃₀	14.9509018	-21.6583923	8.5314956
2230	C	C ₂₇	28.7235820	2.4191024	-1.6109119	2283	C	C ₃₀	-17.9395278	-20.7798719	3.4310397
2231	C	C ₂₇	-12.6271750	2.3099490	-25.8594247	2284	C	C ₃₁	-3.5737078	7.0432665	22.1164483
2232	C	C ₂₇	28.7231883	-2.4206473	1.6155068	2285	C	C ₃₁	19.6278994	11.7606537	-5.2866771
2233	C	C ₂₇	-16.0960953	-6.1307529	23.1693966	2286	C	C ₃₁	-3.5705380	-7.0430737	-22.1170237
2234	C	C ₂₈	-18.7340437	5.1144483	20.9597464	2287	C	C ₃₁	19.6264132	-11.7617092	5.2898165
2235	C	C ₂₈	26.5042135	7.3971885	7.6968016	2288	C	C ₃₁	-16.0562902	-12.8104709	11.3843602
2236	C	C ₂₈	-18.7309597	-5.1134418	-20.9627371	2289	C	C ₃₀	-0.7688204	19.6184818	19.5816111
2237	C	C ₂₈	26.5050499	-7.3986153	-7.6925546	2290	C	C ₃₀	14.2145704	23.5693535	-3.3685157
2238	C	C ₂₈	-7.7744288	-12.9025173	24.2799557	2291	C	C ₃₀	-0.7667362	-19.6184408	-19.5817321
2239	C	C ₂₉	-11.3516448	12.7871299	15.2655768	2292	C	C ₃₀	14.2127621	-23.5701178	3.3707880
2240	C	C ₂₉	16.8259779	14.3953708	5.9218206	2293	C	C ₃₀	-13.4469049	-23.7949974	4.6791295
2241	C	C ₂₉	-11.3498862	-12.7865199	-15.2673895	2294	C	C ₃₁	-16.3834703	16.7399689	3.7725180
2242	C	C ₂₉	16.8261499	-14.3962771	-5.9191213	2295	C	C ₃₁	8.9521533	14.5557128	16.4580302
2243	C	C ₂₉	-5.4768582	-17.7312677	13.4541641	2296	C	C ₃₁	7.4319818	19.3703239	-11.5079448
2244	C	C ₂₇	-23.4834690	5.0956075	16.0273737	2297	C	C ₃₁	8.9540071	-14.5561947	-16.4565959
2245	C	C ₂₇	24.6720519	5.4442196	13.9987590	2298	C	C ₃₁	7.4290957	-19.3707236	11.5091335
2246	C	C ₂₇	-23.4811697	-5.0943438	-16.0311339	2299	C	C ₃₁	-16.3837677	-16.7390874	-3.7751408
2247	C	C ₂₇	24.6739979	-5.4455465	-13.9948131	2300	C	C ₃₀	2.4079778	27.4229492	2.4685035
2248	C	C ₂₇	-1.1931286	-12.3454800	26.0860271	2301	C	C ₃₀	-3.1259876	27.2118152	3.6953151
2249	C	C ₂₈	-15.4905507	8.5197164	22.6497968	2302	C	C ₃₀	0.7190658	26.5042496	7.8049790
2250	C	C ₂₈	25.8246024	11.5559137	5.0106300	2303	C	C ₃₀	-3.1268539	-27.2116469	-3.6958166
2251	C	C ₂₈	-15.4873780	-8.5188840	-22.6522710	2304	C	C ₃₀	0.7188943	-26.5042883	-7.8048638
2252	C	C ₂₈	25.8247815	-11.5573039	-5.0064916	2305	C	C ₃₀	2.4069036	-27.4230789	-2.4681171
2253	C	C ₂₈	-10.3378834	-16.1079933	21.4293430	2306	C	C ₃₁	5.3676249	20.0376057	10.8031667
2254	C	C ₂₉	-6.6026714	0.2491571	21.6498085	2307	C	C ₃₁	3.5926123	22.6705619	-4.4904551
2255	C	C ₂₉	21.7422634	4.6977606	-4.1924549	2308	C	C ₃₁	-8.9593950	21.0934498	4.6712953
2256	C	C ₂₉	-6.5992142	-0.2488013	-21.6508689	2309	C	C ₃₁	3.5906738	-22.6707558	4.4910338
2257	C	C ₂₉	21.7413394	-4.6989290	4.1959274	2310	C	C ₃₁	-8.9597842	-21.0929658	-4.6727411
2258	C	C ₂₉	-15.1422723	-6.6377230	15.4603939	2311	C	C ₃₁	5.3682732	-20.0378944	-10.8023080
2259	C	C ₃₀	-14.9018933	2.6754625	23.0903010	2312	C	C ₃₀	-24.8523605	8.9663762	8.0197732
2260	C	C ₃₀	26.7648429	6.1609851	2.8411616	2313	C	C ₃₀	17.9535643	6.9384382	19.7959660
2261	C	C ₃₀	-14.8983374	-2.6746595	-23.0926935	2314	C	C ₃₀	6.8991918	14.2418540	-22.6257222
2262	C	C ₃₀	26.7649598	-6.1624258	-2.8368733	2315	C	C ₃₀	17.9563616	-6.9394051	-19.7930869
2263	C	C ₃₀	-11.8668767	-10.5400058	22.5936283	2316	C	C ₃₀	6.8948043	-14.2422248	22.6268246
2264	C	C ₃₁	-19.4882648	0.8947602	12.7772375	2317	C	C ₃₀	-24.8515616	-8.9650385	-8.0237546
2265	C	C ₃₁	20.5177176	1.1967452	11.0200818	2318	C	C ₃₁	-22.6466747	-1.8274964	5.0867584
2266	C	C ₃₁	-19.4862685	-0.8937102	-12.7803662	2319	C	C ₃₁	15.9332315	-3.8008258	16.5460749
2267	C	C ₃₁	20.5194172	-1.1978490	-11.0167984	2320	C	C ₃₁	6.7134067	2.8543505	-22.1103972
2268	C	C ₃₁	-1.0332620	-6.9238918	22.2450658	2321	C	C ₃₁	15.9360877	3.7999683	-16.5435232
2269	C	C ₃₀	-2.3958479	15.4061864	22.9044764	2322	C	C ₃₁	6.7097107	-2.8547114	22.1114707
2270	C	C ₃₀	18.4829044	20.1331965	-4.5543672	2323	C	C ₃₁	-22.6457620	1.8287148	-5.0903835
2271	C	C ₃₀	-2.3930082	-15.4060580	-22.9048577	2324	C	C ₃₀	-25.2910828	10.8196970	2.6953580
2272	C	C ₃₀	18.4810929	-20.1341909	4.5573258	2325	C	C ₃₀	13.3564030	7.3119372	23.0675426
2273	C	C ₃₀	-16.0888245	-20.8368994	8.6417047	2326	C	C ₃₀	-25.2912285	-10.8183348	-2.6994150

2327	C	C ₃₀	13.3596957	-7.3126560	-23.0654038	2380	C	C ₃₅	-14.7062186	1.8395258	16.8855574
2328	C	C ₃₀	11.9311013	-14.7447991	20.1049594	2381	C	C ₃₅	21.4942306	3.8337875	5.2989539
2329	C	C ₃₁	-17.1487021	11.5309092	10.8519622	2382	C	C ₃₅	-14.7036089	-1.8387337	-16.8879168
2330	C	C ₃₁	16.1421713	11.2345990	12.5705685	2383	C	C ₃₅	21.4948718	-3.8349426	-5.2955212
2331	C	C ₃₁	-17.1475867	-11.5299855	-10.8547136	2384	C	C ₃₅	-6.7914394	-8.1554403	19.8026239
2332	C	C ₃₁	16.1435764	-11.2354685	-12.5679787	2385	C	C ₃₂	5.9128244	14.4484012	25.7020936
2333	C	C ₃₁	1.0034980	-16.2742970	16.7016522	2386	C	C ₃₂	16.8569707	21.1393651	-13.1637909
2334	C	C ₃₀	-26.7488150	5.3919270	4.0593437	2387	C	C ₃₂	5.9161717	-14.4487191	-25.7011485
2335	C	C ₃₀	16.0468010	2.2463918	22.3271991	2388	C	C ₃₂	16.8537269	-21.1402720	13.1664891
2336	C	C ₃₀	-26.7484482	-5.3904872	-4.0636295	2389	C	C ₃₂	-22.7706116	-19.4011426	3.0676242
2337	C	C ₃₀	16.0502508	-2.2472547	-22.3246333	2390	C	C ₃₃	2.6855102	12.2152471	25.5803811
2338	C	C ₃₀	10.6979645	-10.1075942	23.3332456	2391	C	C ₃₃	18.6948307	18.4978499	-10.9138881
2339	C	C ₃₁	15.4577913	11.8896277	-13.0295593	2392	C	C ₃₃	2.6889507	-12.2153918	-25.5799501
2340	C	C ₃₁	-20.5960201	10.3800706	-4.2584164	2393	C	C ₃₃	18.6920870	-18.4988557	10.9168808
2341	C	C ₃₁	5.1385976	5.8372762	22.1268413	2394	C	C ₃₃	-21.3816731	-17.7080950	6.3267326
2342	C	C ₃₁	-20.5972625	-10.3789619	4.2551163	2395	C	C ₃₄	-4.8909375	13.5916330	19.9445407
2343	C	C ₃₁	5.1418268	-5.8375533	-22.1260155	2396	C	C ₃₄	17.4708062	17.2880016	-1.5278448
2344	C	C ₃₁	15.4550668	-11.8904594	13.0320338	2397	C	C ₃₄	-4.8884772	-13.5913704	-19.9453208
2345	C	C ₃₀	-18.4573944	5.5776302	19.6843924	2398	C	C ₃₄	17.4696348	-17.2889420	1.5306434
2346	C	C ₃₀	25.2093739	7.5611741	8.1594749	2399	C	C ₃₄	-12.5818086	-18.7250466	9.8746739
2347	C	C ₃₀	-18.4545474	-5.5766367	-19.6873493	2400	C	C ₃₅	-3.1501342	14.7897572	16.7260040
2348	C	C ₃₀	25.2102666	-7.5625310	-8.1554369	2401	C	C ₃₅	13.6774505	17.8830194	-1.2427630
2349	C	C ₃₀	-6.7560707	-12.9852319	23.3452336	2402	C	C ₃₅	-3.1482483	-14.7895875	-16.7265098
2350	C	C ₃₁	-10.6034554	13.2190685	16.3348958	2403	C	C ₃₅	13.6762861	-17.8837551	1.2449516
2351	C	C ₃₁	17.3010592	15.1867845	4.9031180	2404	C	C ₃₅	-10.5287134	-18.8085406	6.6184943
2352	C	C ₃₁	-10.6015507	-13.2184993	-16.3365859	2405	C	C ₃₂	1.0142266	23.9637967	18.0884733
2353	C	C ₃₁	17.3010290	-15.1877165	-4.9003423	2406	C	C ₃₂	11.4103162	27.6145965	-3.1183099
2354	C	C ₃₁	-6.7000963	-18.3027736	13.1955693	2407	C	C ₃₂	1.0158303	-23.9638510	-18.0883124
2355	C	C ₃₀	-14.1631732	8.3613848	22.2681519	2408	C	C ₃₂	11.4083307	-27.6152112	3.1201412
2356	C	C ₃₀	24.8584501	11.5037644	4.0123901	2409	C	C ₃₂	-12.4251964	-27.3162878	1.3856353
2357	C	C ₃₀	-14.1600535	-8.3606240	-22.2704123	2410	C	C ₃₃	3.9681455	21.5371241	18.2770403
2358	C	C ₃₀	24.8584734	-11.5051026	-4.0084067	2411	C	C ₃₃	10.4508018	25.7740782	-6.3341731
2359	C	C ₃₀	-10.6988912	-15.6657466	20.1617689	2412	C	C ₃₃	3.9699130	-21.5373375	-18.2764054
2360	C	C ₃₁	-7.2924336	-0.9149285	21.9868166	2413	C	C ₃₃	10.4483997	-25.7746407	6.3358476
2361	C	C ₃₁	22.5457867	3.5670953	-4.0496857	2414	C	C ₃₃	-14.4192565	-24.6076131	-0.4410391
2362	C	C ₃₁	-7.2888610	0.9153203	-21.9879812	2415	C	C ₃₄	3.8830931	12.3776906	20.9770549
2363	C	C ₃₁	22.5449476	-3.5683081	4.0532934	2416	C	C ₃₄	14.1433574	17.6747814	-9.7923432
2364	C	C ₃₁	-15.2561964	-5.7097568	16.4949670	2417	C	C ₃₄	3.8857891	-12.3778999	-20.9764315
2365	C	C ₃₂	-11.3492920	10.4102848	25.7373138	2418	C	C ₃₄	14.1408375	-17.6755420	9.7946054
2366	C	C ₃₂	26.1113393	14.7477451	0.5399401	2419	C	C ₃₄	-18.0272380	-16.5331762	3.1615257
2367	C	C ₃₂	-11.3457246	-10.4096745	-25.7391292	2420	C	C ₃₅	0.4737221	11.3254051	19.5262589
2368	C	C ₃₂	26.1106307	-14.7491494	-0.5357638	2421	C	C ₃₅	14.7644251	15.8030686	-6.4837308
2369	C	C ₃₂	-14.7654735	-18.0826846	18.8304830	2422	C	C ₃₅	0.4762383	-11.3254308	-19.5261825
2370	C	C ₃₃	-10.3018125	6.7575158	25.5659633	2423	C	C ₃₅	14.7625283	-15.8038625	6.4860916
2371	C	C ₃₃	25.9779985	11.3636506	-1.1919395	2424	C	C ₃₅	-15.2393369	-15.6634758	5.6729303
2372	C	C ₃₃	-10.2980816	-6.7569621	-25.5676095	2425	C	C ₃₂	-7.1653020	15.8416754	24.5228400
2373	C	C ₃₃	25.9771987	-11.3650484	1.1960985	2426	C	C ₃₂	22.1848917	20.2548787	-1.1138751
2374	C	C ₃₃	-15.6795437	-14.3907205	18.7741554	2427	C	C ₃₂	-7.1622298	-15.8412887	-24.5239940
2375	C	C ₃₄	-14.0396067	-0.1866054	20.0989756	2428	C	C ₃₂	22.1836234	-20.2560721	1.1174254
2376	C	C ₃₄	24.2011511	2.7990054	2.7538786	2429	C	C ₃₂	-15.0221557	-22.3602499	13.3425625
2377	C	C ₃₄	-14.0363716	0.1873607	-20.1012229	2430	C	C ₃₃	-6.9209874	17.8102500	21.1394991
2378	C	C ₃₄	24.2014477	-2.8003078	-2.7500032	2431	C	C ₃₃	18.8859286	21.3258361	0.7169419
2379	C	C ₃₄	-10.1651927	-6.9246549	21.2092482	2432	C	C ₃₃	-6.9185584	-17.8098770	-21.1406107

2433	C	C ₃₃	18.8848916	-21.3268525	-0.7139171	2486	C	C ₃₅	5.9911501	8.8310648	-19.7664293
2434	C	C ₃₃	-11.9671533	-23.3595001	11.0952463	2487	C	C ₃₅	15.1746299	-2.6126546	-16.3553647
2435	C	C ₃₄	0.9296955	18.9518740	15.7275666	2488	C	C ₃₅	5.9875065	-8.8313868	19.7673866
2436	C	C ₃₄	10.1739218	22.2145576	-3.2247214	2489	C	C ₃₅	-21.1623440	-4.3717307	-6.1348476
2437	C	C ₃₄	0.9311937	-18.9519250	-15.7274123	2490	C	C ₃₂	-29.5984752	3.3948461	0.5819458
2438	C	C ₃₄	10.1722146	-22.2151047	3.2263488	2491	C	C ₃₂	14.7971643	-0.9553309	25.8469465
2439	C	C ₃₄	-11.1042365	-21.9411080	1.6364367	2492	C	C ₃₂	-29.5985642	-3.3932533	-0.5866859
2440	C	C ₃₅	2.5562118	15.5708411	16.2548716	2493	C	C ₃₂	14.8013553	0.9545345	-25.8445764
2441	C	C ₃₅	10.3074366	19.3507764	-5.7018046	2494	C	C ₃₂	14.7970753	-7.7434303	24.6783148
2442	C	C ₃₅	2.5579734	-15.5709773	-16.2544705	2495	C	C ₃₃	15.7024101	9.6427698	-21.5298818
2443	C	C ₃₅	10.3054813	-19.3513309	5.7034541	2496	C	C ₃₃	-27.6430345	6.1343490	-1.1476086
2444	C	C ₃₅	-12.8641520	-18.5992673	1.3367926	2497	C	C ₃₃	11.9408514	1.5194786	25.6552535
2445	C	C ₃₂	-1.2853108	27.2386573	12.3224976	2498	C	C ₃₃	-27.6435516	-6.1328608	1.1431778
2446	C	C ₃₂	7.1578553	28.9640656	2.2996687	2499	C	C ₃₃	11.9448769	-1.5201222	-25.6533360
2447	C	C ₃₂	-1.2847962	-27.2385875	-12.3227073	2500	C	C ₃₃	15.6984476	-9.6436145	21.5323952
2448	C	C ₃₂	7.1566664	-28.9644510	-2.2985214	2501	C	C ₃₄	-21.2016365	12.1289116	2.5723101
2449	C	C ₃₂	-5.8729841	-29.3417319	-0.1060588	2502	C	C ₃₄	11.0143207	9.1347128	19.9619210
2450	C	C ₃₃	-4.1025153	26.2133319	10.0644729	2503	C	C ₃₄	-21.2018735	-12.1277696	-2.5757114
2451	C	C ₃₃	6.7899296	27.0027206	5.4784090	2504	C	C ₃₄	11.0170241	-9.1353041	-19.9601653
2452	C	C ₃₃	-4.1023111	-26.2131105	-10.0651335	2505	C	C ₃₄	10.1843737	-15.3657335	16.2298932
2453	C	C ₃₃	6.7893490	-27.0030859	-5.4773222	2506	C	C ₃₅	-19.6305664	9.8932173	5.1893883
2454	C	C ₃₃	-2.6881064	-28.2083858	1.5244901	2507	C	C ₃₅	12.7908318	7.8827689	16.8647827
2455	C	C ₃₄	4.8999214	23.8908232	2.4095363	2508	C	C ₃₅	-19.6302606	-9.8921621	-5.1925249
2456	C	C ₃₄	-3.9033638	24.1836054	0.7095562	2509	C	C ₃₅	12.7931150	-7.8834581	-16.8627299
2457	C	C ₃₄	-0.9956284	22.7437457	9.0728859	2510	C	C ₃₅	6.8367368	-13.6519865	16.6447269
2458	C	C ₃₄	-3.9045501	-24.1833959	-0.7101779	2511	C	C ₃₂	-26.0597462	7.4767522	12.6061792
2459	C	C ₃₄	-0.9953969	-22.7436916	-9.0730483	2512	C	C ₃₂	22.6904697	6.4859482	18.3576355
2460	C	C ₃₄	4.8990177	-23.8910868	-2.4087521	2513	C	C ₃₂	-26.0581266	-7.4753505	-12.6103487
2461	C	C ₃₅	3.1331083	21.7496320	4.9739815	2514	C	C ₃₂	22.6930577	-6.4871701	-18.3539969
2462	C	C ₃₅	-0.5167151	22.5183790	0.5089256	2515	C	C ₃₂	3.3646951	-14.1444554	26.1254887
2463	C	C ₃₅	-2.6155426	21.5977779	5.8564778	2516	C	C ₃₃	-26.0206128	4.4265401	10.4800824
2464	C	C ₃₅	-0.5178404	-22.5183516	-0.5090058	2517	C	C ₃₃	21.3044627	3.0399781	18.5304417
2465	C	C ₃₅	-2.6157635	-21.5976385	-5.8568888	2518	C	C ₃₃	-26.0191744	-4.4251391	-10.4842538
2466	C	C ₃₅	3.1327432	-21.7498018	-4.9734731	2519	C	C ₃₃	21.3072640	-3.0411254	-18.5270254
2467	C	C ₃₂	12.3543815	11.8784227	24.6083724	2520	C	C ₃₃	4.7116721	-10.6870103	25.8860316
2468	C	C ₃₂	13.0802920	19.3526509	-18.8063924	2521	C	C ₃₄	-24.0971754	3.7624703	1.0974053
2469	C	C ₃₂	12.3576855	-11.8790883	-24.6063894	2522	C	C ₃₄	12.4324403	0.3341178	21.0085072
2470	C	C ₃₂	13.0762408	-19.3533540	18.8084830	2523	C	C ₃₄	-24.0972067	-3.7611733	-1.1012659
2471	C	C ₃₂	-25.4345425	-15.7213147	-2.2856003	2524	C	C ₃₄	12.4357881	-0.3347878	-21.0065110
2472	C	C ₃₃	-23.7035932	14.9218875	5.6316616	2525	C	C ₃₄	11.6612675	-7.4160837	20.1258761
2473	C	C ₃₃	14.4660400	12.2066904	21.4002126	2526	C	C ₃₅	11.0238065	9.5686749	-17.1060454
2474	C	C ₃₃	9.2381557	19.1724697	-19.0607284	2527	C	C ₃₅	-21.5172159	6.4853943	0.8059408
2475	C	C ₃₃	14.4688116	-12.2074702	-21.3978888	2528	C	C ₃₅	10.4936626	3.2455023	19.6226975
2476	C	C ₃₃	9.2340713	-19.1729675	19.0622117	2529	C	C ₃₅	-21.5174363	-6.4842370	-0.8093825
2477	C	C ₃₃	-23.7034955	-14.9206130	-5.6354515	2530	C	C ₃₅	10.4966347	-3.2460668	-19.6210181
2478	C	C ₃₄	-21.7488843	6.3147599	9.3360498	2531	C	C ₃₅	11.0205484	-9.5692676	17.1078079
2479	C	C ₃₄	17.9147932	5.1874877	15.8808860	2532	C	C ₃₂	-16.8573666	-1.6259742	24.6538734
2480	C	C ₃₄	3.8344026	11.5789312	-21.2433005	2533	C	C ₃₂	29.7089797	2.1500502	2.7169554
2481	C	C ₃₄	17.9170521	-5.1884524	-15.8780135	2534	C	C ₃₂	-16.8533311	1.6268810	-24.6565716
2482	C	C ₃₄	3.8303738	-11.5791371	21.2439122	2535	C	C ₃₂	29.7093002	-2.1516491	-2.7121972
2483	C	C ₃₄	-21.7477374	-6.3135893	-9.3395339	2536	C	C ₃₂	-12.8560692	-7.1036986	26.0554606
2484	C	C ₃₅	-21.1630905	4.3728690	6.1314614	2537	C	C ₃₃	-18.6333886	-0.8015967	21.4107214
2485	C	C ₃₅	15.1721479	2.6118382	16.3577937	2538	C	C ₃₃	27.7079298	1.8644828	5.9210327

2539	C	C ₃₃	-18.6299074	0.8025991	-21.4137032	2592	C	C ₃₆	5.6005023	15.8073610	26.3477042
2540	C	C ₃₃	27.7087836	-1.8659733	-5.9165985	2593	C	C ₃₆	17.3644946	22.5556635	-12.8512992
2541	C	C ₃₃	-9.0789778	-7.3401709	25.8835618	2594	C	C ₃₆	5.6038660	-15.8076633	-26.3468022
2542	C	C ₃₄	-17.4029816	6.9583380	15.8282522	2595	C	C ₃₆	17.3612290	-22.5565983	12.8540821
2543	C	C ₃₄	21.1882102	8.0701183	9.3674371	2596	C	C ₃₆	-22.9658728	-20.9092282	3.2882619
2544	C	C ₃₄	-17.4008227	-6.9574010	-15.8310417	2597	C	C ₃₇	2.3145066	11.3953550	26.8457735
2545	C	C ₃₄	21.1892746	-8.0712591	-9.3640407	2598	C	C ₃₇	20.0807613	17.9761924	-11.3809515
2546	C	C ₃₄	-3.7888222	-13.1843939	20.3379544	2599	C	C ₃₇	2.3181969	-11.3954800	-26.8454005
2547	C	C ₃₅	-13.6682189	7.5024142	16.3110528	2600	C	C ₃₇	20.0779707	-17.9772722	11.3841630
2548	C	C ₃₅	19.6529425	9.2606146	6.0958520	2601	C	C ₃₇	-22.3967800	-17.2954359	7.4268941
2549	C	C ₃₅	-13.6660070	-7.5016801	-16.3132337	2602	C	C ₃₈	-6.4167478	13.7562304	20.1271299
2550	C	C ₃₅	19.6534206	-9.2616726	-6.0927026	2603	C	C ₃₈	18.3653619	17.2670643	-0.2677454
2551	C	C ₃₅	-5.9878128	-13.2772673	17.2341853	2604	C	C ₃₈	-6.4142642	-13.7558860	-20.1281528
2552	C	C ₃₂	-22.0911287	8.7090353	18.2162495	2605	C	C ₃₈	18.3643934	-17.2680522	0.2706841
2553	C	C ₃₂	25.3131717	9.6551864	12.7168343	2606	C	C ₃₈	-11.9507877	-19.1525291	11.2191438
2554	C	C ₃₂	-22.0886856	-8.7078470	-18.2197841	2607	C	C ₃₉	-2.1871263	13.8208628	16.0103794
2555	C	C ₃₂	25.3146856	-9.6565485	-12.7127815	2608	C	C ₃₉	12.7275242	16.9180002	-1.9807515
2556	C	C ₃₂	-3.2264615	-16.1472285	24.9910777	2609	C	C ₃₉	-2.1853101	-13.8207455	-16.0107275
2557	C	C ₃₃	-18.8052583	10.6976452	18.3759079	2610	C	C ₃₉	12.7263002	-16.9186856	1.9827924
2558	C	C ₃₃	23.5143474	12.0808387	10.3382816	2611	C	C ₃₉	-10.5416239	-17.5605120	5.7126705
2559	C	C ₃₃	-18.8028863	-10.6966328	-18.3789221	2612	C	C ₃₆	0.6465000	24.3841987	19.5502397
2560	C	C ₃₃	23.5153568	-12.0821047	-10.3345130	2613	C	C ₃₆	12.7799974	28.3294100	-3.3667904
2561	C	C ₃₃	-4.7129918	-17.6072005	21.7606420	2614	C	C ₃₆	0.6483139	-24.3842330	-19.5501395
2562	C	C ₃₄	-10.1485122	7.8296685	20.9647776	2615	C	C ₃₆	12.7779328	-28.3300987	3.3688430
2563	C	C ₃₄	21.8168461	11.2580907	1.0480504	2616	C	C ₃₆	-13.4273078	-28.1391421	2.2616522
2564	C	C ₃₄	-10.1455688	-7.8291223	-20.9664033	2617	C	C ₃₇	5.4158670	22.0645457	18.3851144
2565	C	C ₃₄	21.8164124	-11.2592647	-1.0445570	2618	C	C ₃₇	9.7416890	26.5185751	-7.4868360
2566	C	C ₃₄	-11.6712723	-14.2402223	16.2731491	2619	C	C ₃₇	5.4176225	-22.0648381	-18.3842414
2567	C	C ₃₅	-10.2005455	4.2539451	19.6058704	2620	C	C ₃₇	9.7390682	-26.5190991	7.4883945
2568	C	C ₃₅	21.2084031	7.4883074	0.8163991	2621	C	C ₃₇	-15.1576554	-24.9266389	-1.7596522
2569	C	C ₃₅	-10.1976413	-4.2533955	-19.6075077	2622	C	C ₃₈	4.6377536	11.4891436	21.9905658
2570	C	C ₃₅	21.2081270	-7.4894479	-0.8130079	2623	C	C ₃₈	14.7615751	17.1896813	-11.1222789
2571	C	C ₃₅	-11.0107811	-10.4857367	16.5936541	2624	C	C ₃₈	4.6406599	-11.4893926	-21.9898264
2572	C	C ₃₆	-12.6669393	10.5687288	26.5249350	2625	C	C ₃₈	14.7588639	-17.1904756	11.1246424
2573	C	C ₃₆	27.4191117	14.9032483	1.3444434	2626	C	C ₃₈	-19.4001079	-15.8262563	3.2030590
2574	C	C ₃₆	-12.6632585	-10.5680455	-26.5269735	2627	C	C ₃₉	0.2363519	11.2796122	18.0031341
2575	C	C ₃₆	27.4185200	-14.9047231	-1.3400566	2628	C	C ₃₉	13.5899002	15.3423823	-5.5968400
2576	C	C ₃₆	-14.7558352	-18.6254157	20.2751270	2629	C	C ₃₉	0.2386290	-11.2796231	-18.0031069
2577	C	C ₃₇	-9.4853402	6.1265842	26.7096066	2630	C	C ₃₉	13.5881730	-15.3431129	5.5990126
2578	C	C ₃₇	26.6385226	11.1667617	-2.5694597	2631	C	C ₃₉	-13.8273468	-15.2725849	5.1914337
2579	C	C ₃₇	-9.4813922	-6.1260746	-26.7111211	2632	C	C ₃₆	-6.5960468	16.6748749	25.7012515
2580	C	C ₃₇	26.6375136	-11.1681950	2.5737240	2633	C	C ₃₆	22.7835894	21.4312926	-1.9290567
2581	C	C ₃₇	-17.1565315	-13.9538453	18.7577564	2634	C	C ₃₆	-6.5928287	-16.6745204	-25.7023051
2582	C	C ₃₈	-14.6285148	-1.5844246	20.3785970	2635	C	C ₃₆	22.7821294	-21.4325186	1.9327050
2583	C	C ₃₈	24.9396163	1.4451273	2.7781637	2636	C	C ₃₆	-16.1901075	-23.3693437	13.1858943
2584	C	C ₃₈	-14.6251651	1.5852117	-20.3809395	2637	C	C ₃₇	-7.9749980	18.8830164	20.7637544
2585	C	C ₃₈	24.9399829	-1.4464694	-2.7741697	2638	C	C ₃₇	18.9346402	22.1031596	2.0572195
2586	C	C ₃₈	-10.3148914	-5.7438351	22.1901427	2639	C	C ₃₇	-7.9726854	-18.8825869	-20.7650334
2587	C	C ₃₉	-13.5186888	2.4461833	16.1267139	2640	C	C ₃₇	18.9337765	-22.1041782	-2.0541888
2588	C	C ₃₉	20.1636843	4.3984466	4.7842540	2641	C	C ₃₇	-10.9619497	-24.4466058	11.5542858
2589	C	C ₃₉	-13.5162333	-2.4454556	-16.1288799	2642	C	C ₃₈	1.6292351	20.1470771	15.0471339
2590	C	C ₃₉	20.1642191	-4.3995321	-4.7810226	2643	C	C ₃₈	9.0678314	23.2903053	-3.2111496
2591	C	C ₃₉	-6.6481768	-8.3711170	18.2903200	2644	C	C ₃₈	1.6305652	-20.1471648	-15.0468726

2645	C	C ₃₈	9.0660615	-23.2907926	3.2125978	2698	C	C ₃₆	15.9227528	-0.3437411	26.7185117
2646	C	C ₃₈	-10.6974961	-22.8112911	0.4288778	2699	C	C ₃₆	-30.8152559	-4.0316088	-1.3027732
2647	C	C ₃₉	1.8697728	14.2932582	15.7547013	2700	C	C ₃₆	15.9270556	0.3428852	-26.7159677
2648	C	C ₃₉	10.4114594	17.9020443	-5.2079003	2701	C	C ₃₆	14.8880511	-8.7126081	25.8837378
2649	C	C ₃₉	1.8715264	-14.2933588	-15.7544021	2702	C	C ₃₇	17.1468466	9.9059829	-21.1070777
2650	C	C ₃₉	10.4096615	-17.9026047	5.2095682	2703	C	C ₃₇	-28.0430637	6.7044965	-2.5075189
2651	C	C ₃₉	-12.2818382	-17.3522758	2.0146641	2704	C	C ₃₇	10.8964532	1.6651674	26.7608979
2652	C	C ₃₆	-0.9436620	28.7383422	12.2319233	2705	C	C ₃₇	-28.0438223	-6.7029867	2.5030241
2653	C	C ₃₆	6.6894131	30.4264860	2.4256104	2706	C	C ₃₇	10.9006583	-1.6657531	-26.7591571
2654	C	C ₃₆	-0.9432524	-28.7382900	-12.2320826	2707	C	C ₃₇	17.1429328	-9.9069056	21.1098233
2655	C	C ₃₆	6.6881632	-30.4268456	-2.4245411	2708	C	C ₃₈	-21.0747131	13.6672018	2.5341170
2656	C	C ₃₆	-5.7460851	-30.7037596	-0.8151142	2709	C	C ₃₈	10.6922631	10.6156539	20.2568794
2657	C	C ₃₇	-5.5730290	26.3387306	10.4747471	2710	C	C ₃₈	-21.0750442	-13.6660679	-2.5374908
2658	C	C ₃₇	7.8569247	27.0095033	6.5774813	2711	C	C ₃₈	10.6949381	-10.6162295	-20.2551659
2659	C	C ₃₇	-5.5727745	-26.3384303	-10.4756416	2712	C	C ₃₈	10.3795669	-16.8093873	15.7183580
2660	C	C ₃₇	7.8565168	-27.0099263	-6.5762221	2713	C	C ₃₉	-18.7846949	8.6820757	4.7179345
2661	C	C ₃₇	-2.2848270	-28.6473331	2.9355717	2714	C	C ₃₉	12.1434642	6.7299847	16.0544683
2662	C	C ₃₈	6.4094601	24.1880201	2.4722624	2715	C	C ₃₉	-18.7844143	-8.6810658	-4.7209369
2663	C	C ₃₈	-4.6482559	24.7055307	-0.5329000	2716	C	C ₃₉	12.1456687	-6.7306396	-16.0525158
2664	C	C ₃₈	-1.7602582	22.8220726	10.4071109	2717	C	C ₃₉	6.6383689	-12.2506112	16.0111427
2665	C	C ₃₈	-4.6496685	-24.7052800	0.5321530	2718	C	C ₃₆	-27.3805426	8.2333840	12.3589531
2666	C	C ₃₈	-1.7598179	-22.8219763	-10.4074020	2719	C	C ₃₆	23.0287145	6.9538147	19.7876011
2667	C	C ₃₈	6.4085503	-24.1883641	-2.4712413	2720	C	C ₃₆	-27.3790035	-8.2319099	-12.3633417
2668	C	C ₃₉	2.1831573	20.6296488	4.5180671	2721	C	C ₃₆	23.0315047	-6.9550541	-19.7839130
2669	C	C ₃₉	-0.2663063	21.1928166	1.2470439	2722	C	C ₃₆	4.3471026	-15.0005042	26.9502137
2670	C	C ₃₉	-1.9160326	20.5513649	4.9730984	2723	C	C ₃₇	-26.6030384	3.0872746	11.0213707
2671	C	C ₃₉	-0.2672431	-21.1928014	-1.2470919	2724	C	C ₃₇	22.2543932	1.8087037	18.4443377
2672	C	C ₃₉	-1.9163488	-20.5512616	-4.9734060	2725	C	C ₃₇	-26.6014317	-3.0858439	-11.0256256
2673	C	C ₃₉	2.1827733	-20.6297673	-4.5177114	2726	C	C ₃₇	22.2572544	-1.8099022	-18.4407688
2674	C	C ₃₆	13.2814651	11.6263161	25.8286714	2727	C	C ₃₇	4.3439903	-9.6268820	26.9662088
2675	C	C ₃₆	13.6952788	19.5537100	-20.2183219	2728	C	C ₃₈	12.9564530	6.6052127	-20.3948990
2676	C	C ₃₆	13.2849817	-11.6270317	-25.8265400	2729	C	C ₃₈	-24.8551222	3.1090713	-0.0843730
2677	C	C ₃₆	13.6909974	-19.5544465	20.2205129	2730	C	C ₃₈	11.8987874	-0.6988315	22.0313624
2678	C	C ₃₆	-26.9765851	-15.6498803	-2.4564025	2731	C	C ₃₈	-24.8553006	-3.1077333	0.0803906
2679	C	C ₃₇	-23.6028018	15.9762693	6.7451822	2732	C	C ₃₈	11.9023508	0.6981912	-22.0294573
2680	C	C ₃₇	15.2111063	13.5096221	21.0699598	2733	C	C ₃₈	12.9528315	-6.6059103	20.3969765
2681	C	C ₃₇	8.3923507	20.4458067	-19.2189562	2734	C	C ₃₉	-20.1964442	6.3599309	1.6078091
2682	C	C ₃₇	15.2137521	-13.5104407	-21.0675242	2735	C	C ₃₉	10.5360831	3.5206491	18.0976836
2683	C	C ₃₇	8.3881722	-20.4462585	19.2203017	2736	C	C ₃₉	-20.1965298	-6.3588445	-1.6110403
2684	C	C ₃₇	-23.6025795	-15.9749989	-6.7489631	2737	C	C ₃₉	10.5387955	-3.5212161	-18.0959967
2685	C	C ₃₈	-22.0678345	5.5987281	10.6650672	2738	C	C ₃₉	9.6574805	-9.4562306	16.3781226
2686	C	C ₃₈	19.3137371	4.7888133	15.3663741	2739	C	C ₃₆	-17.5406263	-0.7996567	25.7909586
2687	C	C ₃₈	2.7543816	11.2740126	-22.3022122	2740	C	C ₃₆	30.8996834	3.1254566	2.9879018
2688	C	C ₃₈	19.3159391	-4.7898524	-15.3632828	2741	C	C ₃₆	-17.5364515	0.8006004	-25.7937663
2689	C	C ₃₈	2.7502017	-11.2741611	22.3026549	2742	C	C ₃₆	30.8999939	-3.1271193	-2.9829543
2690	C	C ₃₈	-22.0664251	-5.5975405	-10.6686012	2743	C	C ₃₆	-13.3636816	-8.2798889	26.9507333
2691	C	C ₃₉	-19.9657921	4.7414993	5.2344393	2744	C	C ₃₇	-19.8989097	-1.5803705	20.9734990
2692	C	C ₃₉	13.7537594	2.9155296	15.8381742	2745	C	C ₃₇	28.0819416	0.8237117	7.0055200
2693	C	C ₃₉	6.2122483	8.7828912	-18.2423350	2746	C	C ₃₇	-19.8954581	1.5814401	-20.9766787
2694	C	C ₃₉	13.7561385	-2.9162697	-15.8359724	2747	C	C ₃₇	28.0830250	-0.8252237	-7.0010185
2695	C	C ₃₉	6.2088532	-8.7832256	18.2433307	2748	C	C ₃₇	-8.1876409	-6.6713308	26.9593717
2696	C	C ₃₉	-19.9652075	-4.7404249	-5.2376366	2749	C	C ₃₈	-18.3723854	7.9931931	15.2172797
2697	C	C ₃₆	-30.8152538	4.0332682	1.2978324	2750	C	C ₃₈	20.9994301	8.7646068	10.7334543

2751	C	C ₃₈	-18.3703800	-7.9922038	-15.2202251	2804	C	C ₄₁	4.4681884	12.4351178	27.2307934
2752	C	C ₃₈	21.0006803	-8.7657361	-10.7300963	2805	C	C ₄₁	19.1797820	19.3841073	-13.1341424
2753	C	C ₃₈	-2.6307011	-14.1638047	20.6268595	2806	C	C ₄₁	4.4718774	-12.4353570	-27.2300855
2754	C	C ₃₉	-12.6954611	6.4653026	15.7151841	2807	C	C ₄₁	19.1766343	-19.3851391	13.1372119
2755	C	C ₃₉	18.8103822	8.2617912	5.2777213	2808	C	C ₄₁	-23.6491614	-18.0704008	5.5037035
2756	C	C ₃₉	-12.6932979	-6.4646195	-15.7172166	2809	C	C ₄₂	-7.4023256	13.2130572	17.7521338
2757	C	C ₃₉	18.8107860	-8.2628043	-5.2747039	2810	C	C ₄₂	16.9109658	16.0068799	1.5221168
2758	C	C ₃₉	-6.1178388	-11.9925648	16.3918370	2811	C	C ₄₂	-7.4001908	-13.2126573	-17.7533284
2759	C	C ₃₆	-22.6833515	8.5924234	19.6255665	2812	C	C ₄₂	16.9103434	-16.0077889	-1.5194144
2760	C	C ₃₆	26.8292248	9.8100311	12.5492116	2813	C	C ₄₂	-9.5107696	-18.1820479	11.1119734
2761	C	C ₃₆	-22.6806651	-8.5912031	-19.6291973	2814	C	C ₄₃	-3.5308972	12.5347508	17.5442057
2762	C	C ₃₆	26.8307053	-9.8114741	-12.5449201	2815	C	C ₄₃	14.8974407	15.8746252	-1.8571520
2763	C	C ₃₆	-4.1504979	-16.4760867	26.1694282	2816	C	C ₄₃	-3.5287672	-12.5345605	-17.5447735
2764	C	C ₃₇	-18.8735314	12.2283636	18.2677796	2817	C	C ₄₃	14.8962805	-15.8754271	1.8595386
2765	C	C ₃₇	23.2313139	13.5083115	10.8298811	2818	C	C ₄₃	-11.3681168	-16.9120136	7.8826444
2766	C	C ₃₇	-18.8712636	-12.2273484	-18.2707993	2819	C	C ₄₀	-1.3607171	23.6793692	18.4395492
2767	C	C ₃₇	23.2323186	-13.5095630	-10.8261530	2820	C	C ₄₀	12.9392060	27.0814959	-1.3230917
2768	C	C ₃₇	-4.3616478	-19.0547539	21.3856778	2821	C	C ₄₀	-1.3590419	-23.6792961	-18.4397663
2769	C	C ₃₈	-9.1238029	8.2141073	22.0659696	2822	C	C ₄₀	12.9375389	-27.0821927	1.3251667
2770	C	C ₃₈	22.1878495	12.0526833	-0.2331220	2823	C	C ₄₀	-11.5795238	-27.4811533	3.6444333
2771	C	C ₃₈	-9.1207104	-8.2136170	-22.0674267	2824	C	C ₄₁	3.9031531	23.9384404	18.0729205
2772	C	C ₃₈	22.1871613	-12.0538784	0.2366818	2825	C	C ₄₁	9.9563032	28.0109677	-5.5831723
2773	C	C ₃₈	-13.0669153	-14.7336397	15.8049972	2826	C	C ₄₁	3.9047607	-23.9386499	-18.0722987
2774	C	C ₃₉	-10.2427231	4.0425016	18.0771250	2827	C	C ₄₁	9.9538976	-28.0115035	5.5847673
2775	C	C ₃₉	19.9558047	6.8963958	1.4977288	2828	C	C ₄₁	-13.8596926	-26.8636266	-1.0809614
2776	C	C ₃₉	-10.2400501	-4.0419511	-18.0787614	2829	C	C ₄₂	4.2246050	9.1204416	20.9480648
2777	C	C ₃₉	19.9556789	-6.8974701	-1.4945306	2830	C	C ₄₂	14.4263971	14.6010900	-10.8875396
2778	C	C ₃₉	-9.7159024	-9.9062553	15.9845235	2831	C	C ₄₂	4.2274697	-9.1206685	-20.9473909
2779	C	C ₄₀	-12.9139905	11.7612877	24.4774277	2832	C	C ₄₂	14.4238645	-14.6018665	10.8898508
2780	C	C ₄₀	25.6199314	15.4945067	2.7897606	2833	C	C ₄₂	-18.6518208	-13.3590922	3.6736084
2781	C	C ₄₀	-12.9107040	-11.7605933	-24.4794925	2834	C	C ₄₃	2.6144935	11.5203783	18.3935773
2782	C	C ₄₀	25.6195472	-15.4958854	-2.7856581	2835	C	C ₄₃	12.6986779	16.0201428	-7.7444678
2783	C	C ₄₀	-12.7094540	-19.2893395	19.2518743	2836	C	C ₄₃	2.6168162	-11.5205200	-18.3931528
2784	C	C ₄₁	-9.9375389	8.4183891	27.3042396	2837	C	C ₄₃	12.6965817	-16.0208261	7.7465013
2785	C	C ₄₁	27.0354340	13.4422893	-1.8803432	2838	C	C ₄₃	-15.3139595	-15.2514238	3.2794958
2786	C	C ₄₁	-9.9336216	-8.4178543	-27.3058311	2839	C	C ₄₀	-5.5843410	14.5207400	25.7707508
2787	C	C ₄₁	27.0344101	-13.4437447	1.8846756	2840	C	C ₄₀	22.6535252	19.5362731	-3.3645652
2788	C	C ₄₁	-17.1012902	-16.3622745	18.8405760	2841	C	C ₄₀	-5.5809870	-14.5204388	-25.7716494
2789	C	C ₄₂	-14.4201318	-2.6176138	17.9708085	2842	C	C ₄₀	22.6519353	-19.5374923	3.3681936
2790	C	C ₄₂	22.9322357	-0.1166864	3.4411057	2843	C	C ₄₀	-17.0716645	-21.1769717	12.8942813
2791	C	C ₄₂	-14.4171147	2.6183904	-17.9731215	2844	C	C ₄₁	-8.5737928	17.9547897	22.9024483
2792	C	C ₄₂	22.9327956	0.1154531	-3.4374377	2845	C	C ₄₁	21.1957245	21.6633868	1.3584681
2793	C	C ₄₂	-8.5156941	-4.1208279	21.1717688	2846	C	C ₄₁	-8.5710994	-17.9543291	-22.9038167
2794	C	C ₄₃	-12.6437180	0.8415254	17.6401996	2847	C	C ₄₁	21.1947754	-21.6645275	-1.3550734
2795	C	C ₄₃	21.2536652	3.3712268	2.9436238	2848	C	C ₄₁	-12.6245219	-24.1827585	13.2748699
2796	C	C ₄₃	-12.6409301	-0.8408442	-17.6422290	2849	C	C ₄₂	3.0022521	18.9323368	13.1571009
2797	C	C ₄₃	21.2539556	-3.3723707	-2.9402192	2850	C	C ₄₂	6.9466875	21.8557730	-3.8242349
2798	C	C ₄₃	-8.6131652	-7.0867013	18.6370723	2851	C	C ₄₂	3.0033409	-18.9324997	-13.1566124
2799	C	C ₄₀	6.7002913	16.2250236	24.2469417	2852	C	C ₄₂	6.9449000	-21.8561475	3.8253517
2800	C	C ₄₀	14.9603003	22.5900516	-12.7255111	2853	C	C ₄₂	-9.9490565	-20.9732764	-1.3015947
2801	C	C ₄₀	6.7033016	-16.2253836	-24.2458723	2854	C	C ₄₃	0.7605236	16.1377264	14.7513413
2802	C	C ₄₀	14.9570426	-22.5908569	12.7279086	2855	C	C ₄₃	9.8387647	19.2522294	-3.3402142
2803	C	C ₄₀	-21.6611242	-20.6204485	1.2854094	2856	C	C ₄₃	0.7620178	-16.1377675	-14.7512185

2857	C	C ₄₃	9.8371941	-19.2527587	3.3417893	2910	C	C ₄₁	-29.5592044	4.8692506	-1.9316220
2858	C	C ₄₃	-10.5999261	-19.0284983	2.0407104	2911	C	C ₄₁	12.4156494	-0.1692038	27.3314825
2859	C	C ₄₀	1.0440984	27.4975830	11.8755412	2912	C	C ₄₁	-29.5597680	-4.8676606	1.9268921
2860	C	C ₄₀	5.5736434	29.4420268	0.5807239	2913	C	C ₄₁	12.4200393	0.1685346	-27.3294886
2861	C	C ₄₀	1.0445233	-27.4976394	-11.8753729	2914	C	C ₄₁	17.1395589	-8.5180862	23.1271499
2862	C	C ₄₀	5.5721600	-29.4423270	-0.5798293	2915	C	C ₄₂	-18.5436918	13.7754497	3.1819234
2863	C	C ₄₀	-6.6178042	-29.1351125	-2.3633827	2916	C	C ₄₂	9.9637367	11.2536308	17.8279569
2864	C	C ₄₁	-4.1807500	26.9980047	12.3380052	2917	C	C ₄₂	-18.5439272	-13.7744519	-3.1848927
2865	C	C ₄₁	8.6541659	28.3122022	4.7033957	2918	C	C ₄₂	9.9659799	-11.2541667	-17.8263628
2866	C	C ₄₁	-4.1802291	-26.9977799	-12.3386741	2919	C	C ₄₂	8.5773909	-16.7035037	13.8266946
2867	C	C ₄₁	8.6533883	-28.3126674	-4.7020130	2920	C	C ₄₃	-19.1423737	10.1163523	2.8035033
2868	C	C ₄₁	-4.4742813	-29.5408137	2.4327832	2921	C	C ₄₃	10.4776700	7.5696456	17.5940144
2869	C	C ₄₂	7.2909884	21.7846768	3.0134448	2922	C	C ₄₃	-19.1424627	-10.1153225	-2.8065670
2870	C	C ₄₂	-4.2740514	22.6712272	-2.1352795	2923	C	C ₄₃	10.4800877	-7.5702094	-17.5923373
2871	C	C ₄₂	-3.0160843	20.5287284	10.3095169	2924	C	C ₄₃	8.6619785	-13.1954449	15.0824748
2872	C	C ₄₂	-4.2756199	-22.6709980	2.1345998	2925	C	C ₄₀	-25.5618805	9.7848791	12.0487186
2873	C	C ₄₂	-3.0155304	-20.5285666	-10.3099969	2926	C	C ₄₀	21.6266685	8.6277685	18.7663001
2874	C	C ₄₂	7.2902974	-21.7850678	-3.0122851	2927	C	C ₄₀	-25.5604772	-9.7835037	-12.0528111
2875	C	C ₄₃	3.4358456	21.3361546	2.6099944	2928	C	C ₄₀	21.6292105	-8.6289324	-18.7628366
2876	C	C ₄₃	-2.6249308	21.5743692	1.2267664	2929	C	C ₄₀	3.9308132	-16.1399886	24.8671407
2877	C	C ₄₃	-0.8100819	20.5647529	7.0910724	2930	C	C ₄₁	-26.9056779	4.7722820	12.7008502
2878	C	C ₄₃	-2.6258948	-21.5742273	-1.2271900	2931	C	C ₄₁	23.5915602	3.7976842	18.3580379
2879	C	C ₄₃	-0.8100560	-20.5647096	-7.0912009	2932	C	C ₄₁	-26.9038991	-4.7708344	-12.7051575
2880	C	C ₄₃	3.4351179	-21.3363399	-2.6094422	2933	C	C ₄₁	23.5942966	-3.7989536	-18.3542610
2881	C	C ₄₀	11.5701870	9.9448923	25.8363863	2934	C	C ₄₁	3.3093365	-11.7047802	27.5689714
2882	C	C ₄₀	14.8045296	17.6953451	-19.1830446	2935	C	C ₄₂	13.3986843	5.7496247	-17.9462907
2883	C	C ₄₀	11.5737839	-9.9455162	-25.8345267	2936	C	C ₄₂	-22.8607135	2.9695073	-1.7949718
2884	C	C ₄₀	14.8004994	-17.6961426	19.1854206	2937	C	C ₄₂	9.4621395	-0.9682964	21.0756428
2885	C	C ₄₀	-26.3748423	-14.2944329	-0.5705699	2938	C	C ₄₂	-22.8611667	-2.9682770	1.7913103
2886	C	C ₄₁	-24.6306618	16.9886776	4.8495579	2939	C	C ₄₂	9.4655612	0.9677870	-21.0741266
2887	C	C ₄₁	13.9584387	13.8518598	23.0670974	2940	C	C ₄₂	13.3954951	-5.7503456	17.9484361
2888	C	C ₄₁	10.6729132	21.0900539	-18.9763372	2941	C	C ₄₃	-21.2375475	4.2259379	1.5605282
2889	C	C ₄₁	13.9613782	-13.8526108	-23.0648633	2942	C	C ₄₃	11.3298014	1.3139479	18.4725946
2890	C	C ₄₁	10.6687333	-21.0906289	18.9780500	2943	C	C ₄₃	-21.2375338	-4.2247948	-1.5639303
2891	C	C ₄₁	-24.6308017	-16.9873516	-4.8535047	2944	C	C ₄₃	11.3326842	-1.3145583	-18.4707766
2892	C	C ₄₂	-20.1777110	3.7741053	10.5283561	2945	C	C ₄₃	9.9046691	-7.5554862	17.7803089
2893	C	C ₄₂	18.5200532	3.2864450	13.3580243	2946	C	C ₄₀	-15.1852549	-0.6048810	26.0419719
2894	C	C ₄₂	1.6578714	9.2162002	-21.0841930	2947	C	C ₄₀	29.9076164	3.7209009	0.9118516
2895	C	C ₄₂	18.5220160	-3.2874407	-13.3550640	2948	C	C ₄₀	-15.1810474	0.6056984	-26.0444049
2896	C	C ₄₂	1.6539930	-9.2162897	21.0844608	2949	C	C ₄₀	29.9075586	-3.7225100	-0.9070643
2897	C	C ₄₂	-20.1762226	-3.7730201	-10.5315840	2950	C	C ₄₀	-14.7266595	-8.1831039	25.0060884
2898	C	C ₄₃	-19.6113296	5.7733671	7.3733120	2951	C	C ₄₁	-19.2516899	-2.3347287	23.1593812
2899	C	C ₄₃	15.2504018	4.4913485	14.8173722	2952	C	C ₄₁	29.7347650	0.7452400	5.2653796
2900	C	C ₄₃	4.3611883	10.2545929	-18.6581079	2953	C	C ₄₁	-19.2478589	2.3357655	-23.1624692
2901	C	C ₄₃	15.2525373	-4.4921692	-14.8149300	2954	C	C ₄₁	29.7355616	-0.7468390	-5.2606248
2902	C	C ₄₃	4.3576543	-10.2548278	18.6588076	2955	C	C ₄₁	-10.4877696	-6.4025897	27.5943653
2903	C	C ₄₃	-19.6104522	-5.7723116	-7.3764538	2956	C	C ₄₂	-16.8464078	8.9792989	13.3116243
2904	C	C ₄₀	-29.6930266	2.6480759	2.8376821	2957	C	C ₄₂	18.4651396	9.4544516	10.5489667
2905	C	C ₄₀	16.8793612	-1.1180270	24.7098710	2958	C	C ₄₂	-16.8447654	-8.9783930	-13.3143184
2906	C	C ₄₀	-29.6927137	-2.6464779	-2.8424379	2959	C	C ₄₂	18.4663180	-9.4554451	-10.5460105
2907	C	C ₄₀	16.8833868	1.1171177	-24.7071626	2960	C	C ₄₂	-1.6219922	-14.4052311	18.2067862
2908	C	C ₄₀	12.8092156	-7.6084630	25.9764481	2961	C	C ₄₃	-14.8523389	6.0056761	14.8067994
2909	C	C ₄₁	17.1437148	8.5171623	-23.1243966	2962	C	C ₄₃	19.1810578	7.2772373	7.4182311

2963	C	C ₄₃	-14.8502917	-6.0048778	-14.8091725	3016	C	C ₄₆	-7.1454005	13.4655764	18.8877291
2964	C	C ₄₃	19.1818542	-7.2782707	-7.4151521	3017	C	C ₄₆	17.7145943	16.5710506	0.8474154
2965	C	C ₄₃	-4.3318946	-11.6419170	17.9332619	3018	C	C ₄₆	-7.1430960	-13.4651923	-18.8888713
2966	C	C ₄₀	-22.6507925	6.3918855	18.6635087	3019	C	C ₄₆	17.7138377	-16.5720031	-0.8445828
2967	C	C ₄₀	26.3151537	7.4680140	12.4089898	3020	C	C ₄₆	-10.5713809	-18.6706865	11.3479593
2968	C	C ₄₀	-22.6481536	-6.3906660	-18.6671396	3021	C	C ₄₇	-2.8150672	12.4709714	16.2067629
2969	C	C ₄₀	26.3167303	-7.4694306	-12.4047727	3022	C	C ₄₇	13.4074145	15.5833699	-1.8731132
2970	C	C ₄₀	-3.6689526	-14.1245073	26.2541090	3023	C	C ₄₇	-2.8131429	-12.4708210	-16.2072079
2971	C	C ₄₁	-21.1638740	11.3490295	18.3334701	3024	C	C ₄₇	13.4062757	-15.5840925	1.8752663
2972	C	C ₄₁	24.5617470	12.3468505	12.5340540	3025	C	C ₄₇	-10.5937214	-16.4104127	6.6768492
2973	C	C ₄₁	-21.1615554	-11.3478897	-18.3368649	3026	C	C ₄₄	-0.6581159	23.6557830	19.7963872
2974	C	C ₄₁	24.5630847	-12.3481716	-12.5301247	3027	C	C ₄₄	13.7493867	27.5024635	-2.5484917
2975	C	C ₄₁	-3.4020926	-18.5663992	23.5911263	3028	C	C ₄₄	-0.6562139	-23.6557487	-19.7964866
2976	C	C ₄₂	-6.9407772	7.2200075	21.0087515	3029	C	C ₄₄	13.7475011	-27.5032022	2.5506867
2977	C	C ₄₂	20.3400779	11.1571627	-1.8626389	3030	C	C ₄₄	-13.0923220	-27.6955994	3.6702881
2978	C	C ₄₂	-6.9378003	-7.2196343	-21.0098615	3031	C	C ₄₅	5.3313446	23.5142101	18.0972125
2979	C	C ₄₂	20.3391797	-11.1582571	1.8658952	3032	C	C ₄₅	9.3252655	27.8210211	-6.9195812
2980	C	C ₄₂	-13.4017938	-13.1965626	13.7081434	3033	C	C ₄₅	5.3329736	-23.5144969	-18.0963594
2981	C	C ₄₃	-9.6928861	6.3822852	18.4742717	3034	C	C ₄₅	9.3226523	-27.8215227	6.9210733
2982	C	C ₄₃	19.6760984	9.3155533	1.4338885	3035	C	C ₄₅	-14.6566528	-26.2539433	-2.1825208
2983	C	C ₄₃	-9.6902747	-6.3817636	-18.4758244	3036	C	C ₄₆	4.5336467	10.0783524	21.5647159
2984	C	C ₄₃	19.6758194	-9.3166120	-1.4307384	3037	C	C ₄₆	14.6574361	15.7177057	-11.1927336
2985	C	C ₄₃	-9.9859189	-12.1638290	15.1098316	3038	C	C ₄₆	4.5365587	-10.0785970	-21.5639864
2986	C	C ₄₄	-13.6688518	10.8045749	25.3990330	3039	C	C ₄₆	14.6547998	-15.7184941	11.1950788
2987	C	C ₄₄	26.9244859	14.6993077	2.7730419	3040	C	C ₄₆	-19.1918859	-14.3848766	3.4512248
2988	C	C ₄₄	-13.6653691	-10.8038393	-25.4012223	3041	C	C ₄₇	1.5637299	10.8820407	17.4659537
2989	C	C ₄₄	26.9241314	-14.7007565	-2.7687312	3042	C	C ₄₇	12.5261343	15.0223146	-6.5840258
2990	C	C ₄₄	-13.2593513	-18.7159589	20.5569869	3043	C	C ₄₇	1.5659430	-10.8821262	-17.4656956
2991	C	C ₄₅	-8.9323061	7.3227729	27.4873622	3044	C	C ₄₇	12.5242719	-15.0229893	6.5860354
2992	C	C ₄₅	26.8500706	12.5876268	-3.0967306	3045	C	C ₄₇	-14.0907460	-14.5624212	3.9128141
2993	C	C ₄₅	-8.9282996	-7.3222917	-27.4887957	3046	C	C ₄₄	-5.2654897	15.9988766	25.9680781
2994	C	C ₄₅	26.8488998	-12.5890708	3.1010254	3047	C	C ₄₄	22.4453559	21.0469289	-3.3560885
2995	C	C ₄₅	-17.9210561	-15.2121690	18.3409334	3048	C	C ₄₄	-5.2621918	-15.9985932	-25.9689219
2996	C	C ₄₆	-14.5666162	-2.3397951	19.1221557	3049	C	C ₄₄	22.4436848	-21.0481369	3.3596836
2997	C	C ₄₆	23.9473049	0.4163610	3.1098457	3050	C	C ₄₄	-17.1822757	-22.5939283	12.3415688
2998	C	C ₄₆	-14.5634283	2.3405794	-19.1244910	3051	C	C ₄₅	-9.0974587	18.6962000	21.6863629
2999	C	C ₄₆	23.9477783	-0.4176502	-3.1060083	3052	C	C ₄₅	20.3107456	21.9908461	2.5468804
3000	C	C ₄₆	-9.3843864	-4.6969009	21.7529354	3053	C	C ₄₅	-9.0949941	-18.6957092	-21.6878270
3001	C	C ₄₇	-12.4256179	1.4309918	16.2493643	3054	C	C ₄₅	20.3099696	-21.9919387	-2.5436302
3002	C	C ₄₇	19.8709677	3.6184767	3.5407050	3055	C	C ₄₅	-11.2158281	-24.6641516	12.9805552
3003	C	C ₄₇	-12.4230910	-1.4303243	-16.2513478	3056	C	C ₄₆	2.4719228	19.6654864	13.9408098
3004	C	C ₄₇	19.8713396	-3.6195468	-3.5375182	3057	C	C ₄₆	7.7730267	22.6758832	-3.5457480
3005	C	C ₄₇	-7.4484153	-7.2698927	17.6679180	3058	C	C ₄₆	2.4730946	-19.6656192	-13.9404152
3006	C	C ₄₄	5.6136355	16.7555929	25.1501257	3059	C	C ₄₆	7.7712384	-22.6763020	3.5469957
3007	C	C ₄₄	16.1965156	23.1645373	-12.0775963	3060	C	C ₄₆	-10.2451767	-21.9492331	-0.6748742
3008	C	C ₄₄	5.6167580	-16.7558964	-25.1492187	3061	C	C ₄₇	1.1541563	14.6915506	14.5309883
3009	C	C ₄₄	16.1933379	-23.1654102	12.0801978	3062	C	C ₄₇	9.6663560	17.8710789	-3.9382294
3010	C	C ₄₄	-21.8109072	-21.5142779	2.4923477	3063	C	C ₄₇	1.1556885	-14.6916113	-14.5308119
3011	C	C ₄₅	3.5864820	11.2798573	27.5978925	3064	C	C ₄₇	9.6647544	-17.8715982	3.9397720
3012	C	C ₄₅	20.1036608	18.2412268	-12.8390914	3065	C	C ₄₇	-10.8211039	-17.5316560	1.9667496
3013	C	C ₄₅	3.5902947	-11.2800501	-27.5973197	3066	C	C ₄₄	0.3349523	28.7409513	11.4034111
3014	C	C ₄₅	20.1006210	-18.2423089	12.8423120	3067	C	C ₄₄	5.3425970	30.4090909	1.7134944
3015	C	C ₄₅	-23.6915286	-17.1866289	6.7136403	3068	C	C ₄₄	0.3352338	-28.7409700	-11.4033539

3069	C	C ₄₄	5.3412370	-30.4093778	-1.7126421	3122	C	C ₄₆	-19.6693063	13.9533202	2.8808136
3070	C	C ₄₄	-5.6776447	-30.3106101	-2.2855031	3123	C	C ₄₆	10.2434236	11.1828945	18.9707938
3071	C	C ₄₅	-5.5243556	26.4446666	11.9738911	3124	C	C ₄₆	-19.6695964	-13.9522614	-2.8839654
3072	C	C ₄₅	9.0964929	27.4939945	5.8776636	3125	C	C ₄₆	10.2458589	-11.1834461	-18.9691515
3073	C	C ₄₅	-5.5238564	-26.4443701	-11.9747712	3126	C	C ₄₆	9.4231850	-16.9635842	14.6053496
3074	C	C ₄₅	9.0959598	-27.4944853	-5.8761994	3127	C	C ₄₇	-18.1664611	9.1646918	3.4516759
3075	C	C ₄₅	-3.5731897	-29.1174841	3.5520974	3128	C	C ₄₇	10.6827271	6.9650452	16.2263168
3076	C	C ₄₆	7.1446401	22.9344526	2.7596795	3129	C	C ₄₇	-18.1663990	-9.1637141	-3.4545854
3077	C	C ₄₆	-4.5863917	23.6862083	-1.6060652	3130	C	C ₄₇	10.6849496	-6.9656198	-16.2246075
3078	C	C ₄₆	-2.5573584	21.5867100	10.5888999	3131	C	C ₄₇	7.4810763	-12.3040094	14.7841402
3079	C	C ₄₆	-4.5879247	-23.6859617	1.6053326	3132	C	C ₄₄	-26.9347397	9.4553718	11.5230167
3080	C	C ₄₆	-2.5568268	-21.5865738	-10.5893009	3133	C	C ₄₄	21.9128363	7.9789027	20.0954941
3081	C	C ₄₆	7.1438514	-22.9348382	-2.7585286	3134	C	C ₄₄	-26.9334021	-9.4539221	-11.5273314
3082	C	C ₄₇	2.8046248	20.1068426	3.2445337	3135	C	C ₄₄	21.9156237	-7.9800820	-20.0919842
3083	C	C ₄₇	-1.5871584	20.4645159	1.1672919	3136	C	C ₄₄	5.0173410	-15.8946042	25.8814995
3084	C	C ₄₇	-1.2166763	19.6404082	5.9541654	3137	C	C ₄₅	-26.5998994	3.3039033	12.5281338
3085	C	C ₄₇	-1.5880692	-20.4644297	-1.1675504	3138	C	C ₄₅	23.5069831	2.3943255	17.8076767
3086	C	C ₄₇	-1.2167853	-19.6403426	-5.9543612	3139	C	C ₄₅	-26.5980650	-3.3024714	-12.5323963
3087	C	C ₄₇	2.8040643	-20.1069944	-3.2440792	3140	C	C ₄₅	23.5097060	-2.3955916	-17.8039063
3088	C	C ₄₄	13.0406615	10.1339570	26.1206402	3141	C	C ₄₅	3.0881502	-10.2115486	27.5973216
3089	C	C ₄₄	14.2841208	18.1636252	-20.5204864	3142	C	C ₄₆	13.3825172	6.0057382	-19.1086554
3090	C	C ₄₄	13.0443001	-10.1346590	-26.1185504	3143	C	C ₄₆	-23.8823048	2.9206744	-1.1859516
3091	C	C ₄₄	14.2798571	-18.1643937	20.5227727	3144	C	C ₄₆	10.4998964	-1.0124051	21.6570650
3092	C	C ₄₄	-27.3247166	-14.3305476	-1.7432869	3145	C	C ₄₆	-23.8826512	-2.9193876	1.1821175
3093	C	C ₄₅	-23.6124575	17.3070492	5.9279366	3146	C	C ₄₆	10.5034160	1.0118407	-21.6553873
3094	C	C ₄₅	14.3229266	14.5765619	21.7853199	3147	C	C ₄₆	13.3791363	-6.0064577	19.1107948
3095	C	C ₄₅	9.2902316	21.5155665	-18.5201133	3148	C	C ₄₇	-19.8743971	4.8655336	1.5049436
3096	C	C ₄₅	14.3256326	-14.5773327	-21.7830261	3149	C	C ₄₇	10.5068116	2.1123050	17.4949975
3097	C	C ₄₅	9.2861063	-21.5160662	18.5215998	3150	C	C ₄₇	-19.8744159	-4.8644647	-1.5081227
3098	C	C ₄₅	-23.6124397	-17.3057787	-5.9317167	3151	C	C ₄₇	10.5095022	-2.1128700	-17.4933179
3099	C	C ₄₆	-21.0756201	4.5145851	10.7815475	3152	C	C ₄₇	9.3647177	-7.9532298	16.4310113
3100	C	C ₄₆	19.0763184	3.9265011	14.1944248	3153	C	C ₄₄	-16.4572886	0.2081629	26.1989886
3101	C	C ₄₆	1.9995453	10.1201273	-21.7804943	3154	C	C ₄₄	30.5581947	4.3512911	2.1296816
3102	C	C ₄₆	19.0783819	-3.9275278	-14.1913691	3155	C	C ₄₄	-16.4530955	-0.2072769	-26.2016264
3103	C	C ₄₆	1.9955117	-10.1202345	21.7808126	3156	C	C ₄₄	30.5582950	-4.3529347	-2.1247932
3104	C	C ₄₆	-21.0741372	-4.5134512	-10.7849213	3157	C	C ₄₄	-14.1053799	-9.1873364	25.9596570
3105	C	C ₄₇	-18.8662469	5.1479344	6.2079172	3158	C	C ₄₅	-19.8306882	-2.8391235	21.8603334
3106	C	C ₄₇	13.9751073	3.7101376	14.5569827	3159	C	C ₄₅	28.9896487	-0.1482543	6.2264624
3107	C	C ₄₇	4.8913773	9.2544030	-17.6466763	3160	C	C ₄₅	-19.8270341	2.8401889	-21.8634991
3108	C	C ₄₇	13.9772406	-3.7108886	-14.5547511	3161	C	C ₄₅	28.9906573	0.1466935	-6.2218158
3109	C	C ₄₇	4.8880460	-9.2546665	17.6474613	3162	C	C ₄₅	-9.1636636	-5.6792856	27.6218026
3110	C	C ₄₇	-18.8655243	-5.1469199	-6.2109337	3163	C	C ₄₆	-17.6923413	8.6376847	14.0760955
3111	C	C ₄₄	-30.3664120	4.0351931	2.7505191	3164	C	C ₄₆	19.5907581	9.1950027	10.8360233
3112	C	C ₄₄	16.9378813	0.0883814	25.6723151	3165	C	C ₄₆	-17.6905534	-8.6367312	-14.0789372
3113	C	C ₄₄	-30.3661927	-4.0335585	-2.7553851	3166	C	C ₄₆	19.5919970	-9.1960566	-10.8328883
3114	C	C ₄₄	16.9419877	-0.0892940	-25.6695968	3167	C	C ₄₆	-1.9018615	-14.3943727	19.3636246
3115	C	C ₄₄	13.4240325	-9.0127874	26.1635649	3168	C	C ₄₇	-13.3720654	5.8990792	14.5312672
3116	C	C ₄₅	17.9895312	9.4377758	-22.2911413	3169	C	C ₄₇	18.2214299	7.3236701	6.2539978
3117	C	C ₄₅	-29.4061877	6.0833836	-2.8032478	3170	C	C ₄₇	-13.3700586	-5.8983592	-14.5334109
3118	C	C ₄₅	11.4168706	0.7963910	27.9036005	3171	C	C ₄₇	18.2220367	-7.3246514	-6.2510756
3119	C	C ₄₅	-29.4069715	-6.0818011	2.7985385	3172	C	C ₄₇	-4.8522993	-11.2533149	16.5706696
3120	C	C ₄₅	11.4213007	-0.7970067	-27.9017651	3173	C	C ₄₄	-22.5207503	7.1293718	19.9912232
3121	C	C ₄₅	17.9854566	-9.4387426	22.2940153	3174	C	C ₄₄	27.2749414	8.5257487	11.8764498

3175	C	C ₄₄	-22.5179336	-7.1281614	-19.9948208	3228	Cu	Cu ₄₈	9.4632955	-2.5976544	22.2771762
3176	C	C ₄₄	27.2763880	-8.5272176	-11.8720760	3229	Cu	Cu ₄₈	9.1581853	12.9023382	18.7749855
3177	C	C ₄₄	-4.7588636	-15.1439987	26.5645189	3230	Cu	Cu ₄₈	9.5493372	18.3996942	-13.1569182
3178	C	C ₄₅	-20.3212341	12.6001159	18.2230207	3231	Cu	Cu ₄₈	9.1604977	-12.9028295	-18.7735281
3179	C	C ₄₅	23.8623491	13.6400440	12.1791392	3232	Cu	Cu ₄₈	9.5462363	-18.4002074	13.1584438
3180	C	C ₄₅	-20.3189969	-12.5990232	-18.2262700	3233	Cu	Cu ₄₈	-18.7073459	-15.7078383	-2.4782645
3181	C	C ₄₅	23.8635664	-13.6413298	-12.1753084	3234	Cu	Cu ₄₈	3.1679454	20.8202613	12.4786626
3182	C	C ₄₅	-3.5451763	-19.6119591	22.5077042	3235	Cu	Cu ₄₈	6.0074542	23.5163831	-3.1822131
3183	C	C ₄₆	-7.7671513	7.8138841	21.6255274	3236	Cu	Cu ₄₈	3.1688324	-20.8204317	-12.4781563
3184	C	C ₄₆	21.1924150	11.7586437	-1.2901616	3237	Cu	Cu ₄₈	6.0056819	-23.5167060	3.1831730
3185	C	C ₄₆	-7.7641037	-7.8134667	-21.6267683	3238	Cu	Cu ₄₈	-9.1753839	-22.5852196	-2.2262903
3186	C	C ₄₆	21.1915755	-11.7597833	1.2935504	3239	H	H ₄₉	-14.8734740	0.5663201	21.8096084
3187	C	C ₄₆	-13.4279129	-14.0408979	14.5462435	3240	H	H ₄₉	25.9674596	3.8258977	2.8729533
3188	C	C ₄₇	-9.4813773	5.2176265	17.5133131	3241	H	H ₄₉	-14.8700152	-0.5655189	-21.8119955
3189	C	C ₄₇	18.9212945	7.9912632	1.4002363	3242	H	H ₄₉	25.9677070	-3.8272940	-2.8688019
3190	C	C ₄₇	-9.4788494	-5.2171157	-17.5148352	3243	H	H ₄₉	-11.0978607	-8.1965806	22.5134076
3191	C	C ₄₇	18.9210882	-7.9922799	-1.3972156	3244	H	H ₅₀	-16.7937662	2.5139045	15.9466686
3192	C	C ₄₇	-9.4425486	-10.7773902	14.7825037	3245	H	H ₅₀	21.6376081	3.9368108	7.6786634
3193	Cu	Cu ₄₈	-9.4559477	-2.7413037	22.3160263	3246	H	H ₅₀	-16.7913475	-2.5130014	-15.9493545
3194	Cu	Cu ₄₈	24.1768373	1.5842112	-2.8116695	3247	H	H ₅₀	21.6386289	-3.9379750	-7.6751995
3195	Cu	Cu ₄₈	-9.4522286	2.7418121	-22.3175383	3248	H	H ₅₀	-4.8474825	-8.8720053	20.9865666
3196	Cu	Cu ₄₈	24.1763046	-1.5855125	2.8155428	3249	H	H ₄₉	-4.5683285	14.5816297	21.7093455
3197	Cu	Cu ₄₈	-14.7241181	-4.3626900	18.9499869	3250	H	H ₄₉	18.6702780	18.7252622	-2.3610785
3198	Cu	Cu ₄₈	-18.5761140	9.7032215	12.6281819	3251	H	H ₄₉	-4.5656389	-14.5813832	-21.7100812
3199	Cu	Cu ₄₈	18.6403464	9.7215317	12.5189883	3252	H	H ₄₉	18.6688895	-18.7262677	2.3640729
3200	Cu	Cu ₄₈	-18.5746169	-9.7022207	-12.6311630	3253	H	H ₄₉	-14.1039510	-20.0674608	10.1570083
3201	Cu	Cu ₄₈	18.6418291	-9.7225345	-12.5160052	3254	H	H ₅₀	-3.2381027	17.0201768	15.8367573
3202	Cu	Cu ₄₈	-0.0676614	-15.1806782	19.1895265	3255	H	H ₅₀	12.6348003	19.7811876	-0.2020255
3203	Cu	Cu ₄₈	-20.5897439	3.5707064	12.5231078	3256	H	H ₅₀	-3.2364816	-17.0200042	-15.8372668
3204	Cu	Cu ₄₈	20.4584262	3.5315513	12.7474145	3257	H	H ₅₀	12.6337057	-19.7818681	0.2040525
3205	Cu	Cu ₄₈	-20.5879250	-3.5695975	-12.5264103	3258	H	H ₅₀	-9.3979841	-20.7326019	5.7281520
3206	Cu	Cu ₄₈	20.4602791	-3.5326529	-12.7441347	3259	H	H ₄₉	3.9149516	14.0130281	22.1772634
3207	Cu	Cu ₄₈	0.1274356	-9.5824398	22.3981324	3260	H	H ₄₉	14.9115214	19.5451940	-9.9576448
3208	Cu	Cu ₄₈	-9.0736280	12.9884330	18.7316593	3261	H	H ₄₉	3.9177507	-14.0132392	-22.1766347
3209	Cu	Cu ₄₈	18.6156063	15.7920115	2.4447178	3262	H	H ₄₉	14.9088700	-19.5459975	9.9600394
3210	Cu	Cu ₄₈	-9.0713265	-12.9879453	-18.7331092	3263	H	H ₄₉	-18.8273076	-18.3942107	3.2723563
3211	Cu	Cu ₄₈	18.6151502	-15.7930130	-2.4417383	3264	H	H ₅₀	-1.5762260	10.8270209	20.8086556
3212	Cu	Cu ₄₈	-9.5444436	-18.4583381	13.0421827	3265	H	H ₅₀	16.9571165	15.3465773	-5.4449963
3213	Cu	Cu ₄₈	-5.9944498	8.4982783	22.1717579	3266	H	H ₅₀	-1.5734825	-10.8269354	-20.8089126
3214	Cu	Cu ₄₈	20.6717149	12.8109795	-2.8809773	3267	H	H ₅₀	16.9554137	-15.3474889	5.4477065
3215	Cu	Cu ₄₈	-5.9913526	-8.4979556	-22.1727190	3268	H	H ₅₀	-15.3824858	-15.8094136	8.1333014
3216	Cu	Cu ₄₈	20.6705695	-12.8120924	2.8842906	3269	H	H ₄₉	0.4141045	20.0692243	17.3715649
3217	Cu	Cu ₄₈	-14.6796792	-14.5722437	13.1109781	3270	H	H ₄₉	11.6706821	23.6202008	-3.2554515
3218	Cu	Cu ₄₈	5.7535489	8.6184385	22.1722881	3271	H	H ₄₉	0.4158053	-20.0692456	-17.3715042
3219	Cu	Cu ₄₈	14.7805165	14.6524697	-12.8775989	3272	H	H ₄₉	11.6688849	-23.6208295	3.2573246
3220	Cu	Cu ₄₈	5.7566325	-8.6187484	-22.1713655	3273	H	H ₄₉	-12.0855719	-23.4982485	2.5471124
3221	Cu	Cu ₄₈	14.7776679	-14.6532655	12.8799685	3274	H	H ₅₀	4.5664791	15.0100803	17.4137280
3222	Cu	Cu ₄₈	-20.5347759	-12.9610960	3.0535451	3275	H	H ₅₀	10.3737295	19.4002739	-8.0875387
3223	Cu	Cu ₄₈	9.4670038	2.5971450	-22.2756606	3276	H	H ₅₀	4.5684607	-15.0103261	-17.4129965
3224	Cu	Cu ₄₈	-24.1267354	-1.7103978	2.7476402	3277	H	H ₅₀	10.3713896	-19.4008320	8.0891995
3225	Cu	Cu ₄₈	14.6596842	-4.4929164	18.9071864	3278	H	H ₅₀	-14.9405389	-18.0579321	0.2907767
3226	Cu	Cu ₄₈	-24.1262028	1.7116961	-2.7515032	3279	H	H ₄₉	4.5318990	25.8869334	2.3526818
3227	Cu	Cu ₄₈	14.6629547	4.4921274	-18.9048388	3280	H	H ₄₉	-4.0611351	26.0251873	1.5502770

3281	H	H ₄₉	-0.4697587	24.6934742	9.2853755	3334	H	H ₄₉	-11.6904048	8.3517122	22.2192338
3282	H	H ₄₉	-4.0622866	-26.0249685	-1.5509284	3335	H	H ₄₉	23.5817430	11.8456187	1.9218832
3283	H	H ₄₉	-0.4696017	-24.6934489	-9.2854508	3336	H	H ₄₉	-11.6872934	-8.3510833	-22.2211048
3284	H	H ₄₉	4.5308830	-25.8871775	-2.3519548	3337	H	H ₄₉	23.5814128	-11.8468874	-1.9181088
3285	H	H ₅₀	3.0977888	21.8873543	7.3546713	3338	H	H ₄₉	-11.8945850	-15.2808753	18.0312149
3286	H	H ₅₀	1.5125750	23.2420259	-0.5139362	3339	H	H ₅₀	-10.3419529	2.2109293	20.7313856
3287	H	H ₅₀	-4.6094786	22.3318585	4.7733170	3340	H	H ₅₀	22.5398346	5.7949976	-0.0894954
3288	H	H ₅₀	1.5112407	-23.2421068	0.5141760	3341	H	H ₅₀	-10.3387506	-2.2103744	-20.7330323
3289	H	H ₅₀	-4.6099174	-22.3316109	-4.7740530	3342	H	H ₅₀	22.5395108	-5.7962112	0.0931085
3290	H	H ₅₀	3.0977915	-21.8875211	-7.3541749	3343	H	H ₅₀	-12.2009862	-8.8339426	17.7406860
3291	H	H ₄₉	-23.5014283	7.3533065	9.5177794	3344	H	H ₁₈	-9.6375984	11.5623044	21.2844863
3292	H	H ₄₉	18.7935867	5.9692310	17.5540794	3345	H	H ₁₈	21.2858814	14.9848161	1.4021696
3293	H	H ₄₉	4.7081766	12.8756878	-22.5616064	3346	H	H ₁₈	-9.6348170	-11.5617862	-21.2860269
3294	H	H ₄₉	18.7960814	-5.9702433	-17.5510645	3347	H	H ₁₈	21.2853042	-14.9859623	-1.3987573
3295	H	H ₄₉	4.7038806	-12.8759408	22.5623586	3348	H	H ₁₈	-11.6510694	-17.8168185	15.0470297
3296	H	H ₄₉	-23.5002972	-7.3520412	-9.5215464	3349	H	H ₁₉	-11.7246126	3.2469463	22.7755615
3297	H	H ₅₀	-22.5058013	2.6554430	5.1975183	3350	H	H ₁₉	24.8236183	7.0957633	0.4165850
3298	H	H ₅₀	15.2987229	0.5370288	17.4996307	3351	H	H ₁₉	-11.7211441	-3.2463157	-22.7774371
3299	H	H ₅₀	7.2072140	7.1508068	-20.9164616	3352	H	H ₁₉	24.8233067	-7.0970997	-0.4126064
3300	H	H ₅₀	15.3014901	-0.5378516	-17.4971841	3353	H	H ₁₉	-13.1024367	-10.5410208	19.5946022
3301	H	H ₅₀	7.2034789	-7.1511959	20.9176230	3354	H	H ₂₀	-18.4927071	3.2355617	14.5656200
3302	H	H ₅₀	-22.5051048	-2.6542312	-5.2011262	3355	H	H ₂₀	21.2023726	4.0312878	9.9405497
3303	H	H ₄₉	-23.2288284	12.3767372	2.5683821	3356	H	H ₂₀	-18.4905505	-3.2345668	-14.5685802
3304	H	H ₄₉	11.9881486	9.0729521	21.7560234	3357	H	H ₂₀	21.2037497	-4.0324291	-9.9371524
3305	H	H ₄₉	-23.2290837	-12.3754879	-2.5720980	3358	H	H ₂₀	-2.7134188	-9.4658254	21.6250288
3306	H	H ₄₉	11.9911438	-9.0735985	-21.7540960	3359	H	H ₁₈	7.4739455	13.0852295	21.3122045
3307	H	H ₄₉	11.2374448	-15.8997514	17.8962684	3360	H	H ₁₈	12.5300274	18.9635044	-12.8326561
3308	H	H ₅₀	-19.8636278	9.9991840	7.5878057	3361	H	H ₁₈	7.4766550	-13.0856318	-21.3110070
3309	H	H ₅₀	14.9387837	8.5514192	15.9946217	3362	H	H ₁₈	12.5269514	-18.9641786	12.8346620
3310	H	H ₅₀	-19.8629456	-9.9981157	-7.5909832	3363	H	H ₁₈	-20.0042470	-16.7665753	0.0721702
3311	H	H ₅₀	14.9408895	-8.5522246	-15.9922214	3364	H	H ₁₉	-0.9030659	12.5362292	22.6443118
3312	H	H ₅₀	4.9216275	-14.3890760	17.9124052	3365	H	H ₁₉	17.9361073	17.5412782	-6.4293896
3313	H	H ₄₉	-25.8612066	4.3426596	1.9287304	3366	H	H ₁₉	-0.9001144	-12.5361807	-22.6444563
3314	H	H ₄₉	13.9387292	0.8385197	22.2798005	3367	H	H ₁₉	17.9341334	-17.5422435	6.4322625
3315	H	H ₄₉	-25.8611329	-4.3412678	-1.9328721	3368	H	H ₁₉	-17.0346474	-17.8062481	7.9684219
3316	H	H ₄₉	13.9422483	-0.8392717	-22.2775577	3369	H	H ₂₀	-2.9724993	18.7851571	14.3150037
3317	H	H ₄₉	11.9187009	-8.4389046	21.8657303	3370	H	H ₂₀	10.9439312	21.1273442	0.7091439
3318	H	H ₅₀	12.4080694	11.3762469	-16.3028885	3371	H	H ₂₀	-2.9712186	-18.7849973	-14.3154784
3319	H	H ₅₀	-21.7894381	8.6197657	-0.2890187	3372	H	H ₂₀	10.9429092	-21.1279332	-0.7073909
3320	H	H ₅₀	9.3816964	4.9731034	20.8905626	3373	H	H ₂₀	-7.9725031	-22.0007491	4.3638790
3321	H	H ₅₀	-21.7899503	-8.6185922	0.2855242	3374	H	H ₁₈	-1.1461097	21.7310680	14.3077823
3322	H	H ₅₀	9.3847712	-4.9736092	-20.8890553	3375	H	H ₁₈	9.5917807	24.2126354	-0.1074378
3323	H	H ₅₀	12.4048513	-11.3769147	16.3048760	3376	H	H ₁₈	-1.1449896	-21.7310065	-14.3079653
3324	H	H ₄₉	-18.5720263	6.8263705	17.5032752	3377	H	H ₁₈	9.5904616	-24.2131518	0.1089753
3325	H	H ₄₉	23.2217092	8.1921404	9.5668956	3378	H	H ₁₈	-8.4463971	-24.5493031	2.0629140
3326	H	H ₄₉	-18.5695967	-6.8253708	-17.5062511	3379	H	H ₁₉	4.0382283	16.9855372	19.0871034
3327	H	H ₄₉	23.2227933	-8.1933904	-9.5631749	3380	H	H ₁₉	11.7758173	21.6324783	-7.9056509
3328	H	H ₄₉	-4.6535815	-13.6499488	22.1338477	3381	H	H ₁₉	4.0403692	-16.9857544	-19.0864578
3329	H	H ₅₀	-12.5860181	9.3588960	17.5124299	3382	H	H ₁₉	11.7733865	-21.6331124	7.9075389
3330	H	H ₅₀	19.8644507	11.4972654	5.0890509	3383	H	H ₁₉	-15.8145308	-20.4453615	1.0104870
3331	H	H ₅₀	-12.5837182	-9.3582191	-17.5144433	3384	H	H ₂₀	-3.6379779	10.0753238	21.3633777
3332	H	H ₅₀	19.8646492	-11.4983344	-5.0858693	3385	H	H ₂₀	18.5718597	14.4634805	-4.1273078
3333	H	H ₅₀	-7.2814042	-15.1958547	16.3935701	3386	H	H ₂₀	-3.6351003	-10.0751283	-21.3639591

3387	H	H ₂₀	18.5704218	-14.4644801	4.1302831	3440	H	H ₁₈	14.2208067	2.9898796	-21.4806858
3388	H	H ₂₀	-14.9358474	-15.5322295	10.3349529	3441	H	H ₁₈	11.6620143	-4.6161430	22.6997582
3389	H	H ₁₈	-6.4304400	11.4998426	22.5221442	3442	H	H ₁₉	13.1364998	12.1502085	-18.6003268
3390	H	H ₁₈	20.7477833	15.7067455	-1.9160912	3443	H	H ₁₉	-24.2281515	8.8911680	0.3329435
3391	H	H ₁₈	-6.4274530	-11.4994973	-22.5231698	3444	H	H ₁₉	11.0920024	5.0303973	22.7558761
3392	H	H ₁₈	20.7466299	-15.7078633	1.9194217	3445	H	H ₁₉	-24.2285816	-8.8898648	-0.3368200
3393	H	H ₁₈	-14.3197699	-17.5961603	12.8904326	3446	H	H ₁₉	11.0953734	-5.0309940	-22.7541016
3394	H	H ₁₉	-3.3177065	18.1801719	18.1828994	3447	H	H ₁₉	13.1328574	-12.1509151	18.6024289
3395	H	H ₁₉	14.5065594	21.4677964	-0.9149139	3448	H	H ₂₀	-19.5618784	9.7920113	9.9167481
3396	H	H ₁₉	-3.3157716	-18.1799936	-18.1834294	3449	H	H ₂₀	16.8060465	8.9816189	14.6212116
3397	H	H ₁₉	14.5052577	-21.4685768	0.9172357	3450	H	H ₂₀	-19.5608147	-9.7909573	-9.9198884
3398	H	H ₁₉	-11.1903010	-22.4425588	6.5766540	3451	H	H ₂₀	16.8078969	-8.9825237	-14.6185179
3399	H	H ₂₀	6.4927880	14.0368225	18.2954334	3452	H	H ₂₀	2.7524782	-14.7305369	18.7703918
3400	H	H ₂₀	10.3060757	18.9732402	-10.3784722	3453	H	H ₁₈	-21.2372645	8.3492809	12.3122951
3401	H	H ₂₀	6.4949632	-14.0371712	-18.2943983	3454	H	H ₁₈	19.9002249	7.9557701	14.5949016
3402	H	H ₂₀	10.3033877	-18.9737952	10.3801246	3455	H	H ₁₈	-21.2357380	-8.3481378	-12.3156977
3403	H	H ₂₀	-16.7990080	-17.0647433	-0.7067049	3456	H	H ₁₈	19.9021394	-7.9568416	-14.5917118
3404	H	H ₁₈	1.0605553	23.0308339	12.0683976	3457	H	H ₁₈	1.3332069	-14.1970028	21.6562272
3405	H	H ₁₈	6.3862443	25.2189286	-0.6417481	3458	H	H ₁₉	-24.6550612	3.9182356	6.0554129
3406	H	H ₁₈	1.0612424	-23.0308908	-12.0682290	3459	H	H ₁₉	16.9200219	1.6446128	19.2587815
3407	H	H ₁₈	6.3847862	-25.2192733	0.6427769	3460	H	H ₁₉	-24.6543000	-3.9169086	-6.0593622
3408	H	H ₁₈	-7.4469886	-24.9071391	-1.1692279	3461	H	H ₁₉	16.9230159	-1.6455232	-19.2560725
3409	H	H ₁₉	-4.0912980	24.8028322	5.6381106	3462	H	H ₁₉	7.7310944	-8.8904203	22.8272478
3410	H	H ₁₉	3.2137610	24.5446687	7.1371190	3463	H	H ₂₀	13.2135852	13.1066431	-14.8245430
3411	H	H ₁₉	-4.0917279	-24.8026115	-5.6387692	3464	H	H ₂₀	-21.1846773	10.7645773	-1.2178266
3412	H	H ₁₉	3.2135879	-24.5448426	-7.1365992	3465	H	H ₂₀	7.9715006	6.8812376	21.3366699
3413	H	H ₁₉	0.8771633	-25.7471304	-0.1528268	3466	H	H ₂₀	-21.1854510	-10.7634363	1.2144289
3414	H	H ₂₀	2.8961226	21.5627411	9.7070386	3467	H	H ₂₀	7.9745480	-6.8816656	-21.3353993
3415	H	H ₂₀	3.6687847	23.4917519	-1.4978481	3468	H	H ₂₀	13.2105044	-13.1073531	14.8266532
3416	H	H ₂₀	-6.5640190	22.6409010	3.4451735	3469	H	H ₁₈	-12.4159149	-2.3143870	22.6601255
3417	H	H ₂₀	3.6672802	-23.4919498	1.4984384	3470	H	H ₁₈	25.8877849	1.6440203	-0.3355497
3418	H	H ₂₀	-6.5646830	-22.6405476	-3.4462259	3471	H	H ₁₈	-12.4121668	2.3150552	-22.6621147
3419	H	H ₂₀	2.8965144	-21.5628967	-9.7065763	3472	H	H ₁₈	25.8876444	-1.6454145	0.3397013
3420	H	H ₁₈	8.4006289	9.9699127	22.5424047	3473	H	H ₁₈	-13.4755383	-5.2924046	21.5265636
3421	H	H ₁₈	13.5743110	16.4274063	-14.9669072	3474	H	H ₁₉	-17.8148322	2.7189152	18.3180447
3422	H	H ₁₈	8.4037064	-9.9703644	-22.5410617	3475	H	H ₁₉	24.1419387	4.5776475	7.5182372
3423	H	H ₁₈	13.5710254	-16.4281364	14.9690790	3476	H	H ₁₉	-17.8120536	-2.7179560	-18.3209010
3424	H	H ₁₈	-21.9752614	-13.9580782	0.6242388	3477	H	H ₁₉	24.1428891	-4.5789476	-7.5143660
3425	H	H ₁₉	-22.3197899	10.8509232	7.3615985	3478	H	H ₁₉	-6.3310687	-9.8128714	22.8896621
3426	H	H ₁₉	15.8486825	8.9487131	18.4078431	3479	H	H ₂₀	-10.9781301	10.8381693	18.2909866
3427	H	H ₁₉	6.4715707	15.5078801	-19.6909387	3480	H	H ₂₀	19.5076612	13.3442045	3.7321378
3428	H	H ₁₉	15.8511465	-8.9495670	-18.4052994	3481	H	H ₂₀	-10.9757878	-10.8375788	-18.2927434
3429	H	H ₁₉	6.4675881	-15.5082282	19.6919743	3482	H	H ₂₀	19.5075435	-13.3452548	-3.7290107
3430	H	H ₁₉	-22.3191980	-10.8497212	-7.3651777	3483	H	H ₂₀	-8.5322906	-16.5702425	15.0057498
3431	H	H ₂₀	-23.4400226	0.9490078	3.9142542	3484	H	H ₁₈	-20.7147723	5.8171816	14.5659548
3432	H	H ₂₀	14.9213016	-1.5548456	18.4551820	3485	H	H ₁₈	21.9344137	6.1749850	12.4843713
3433	H	H ₂₀	8.5187830	5.3334394	-21.5555374	3486	H	H ₁₈	-20.7127572	-5.8160679	-14.5692662
3434	H	H ₂₀	14.9243362	1.5540427	-18.4527932	3487	H	H ₁₈	21.9360746	-6.1761664	-12.4808533
3435	H	H ₂₀	8.5150448	-5.3338986	21.5569060	3488	H	H ₁₈	-1.2236494	-12.2625904	22.8744396
3436	H	H ₂₀	-23.4394431	-0.9477458	-3.9180115	3489	H	H ₁₉	-14.4817906	9.2786295	19.1678138
3437	H	H ₁₈	-25.8830703	0.4380613	1.5700800	3490	H	H ₁₉	22.2369580	11.5570389	5.9306749
3438	H	H ₁₈	14.2172015	-2.9906456	21.4829678	3491	H	H ₁₉	-14.4792165	-9.2778496	-19.1701370
3439	H	H ₁₈	-25.8828480	-0.4366685	-1.5742244	3492	H	H ₁₉	22.2372803	-11.5582355	-5.9271142

3493	H	H ₁₉	-7.7585448	-15.8127393	18.7878304	3546	H	H ₅₁	4.8228449	25.6962118	5.8970192
3494	H	H ₂₀	-10.2422024	0.0116348	21.5903131	3547	H	H ₅₁	-3.6683381	-25.3570229	-7.8673156
3495	H	H ₂₀	23.5461550	3.9207373	-1.1186268	3548	H	H ₅₁	4.8224062	-25.6964705	-5.8962518
3496	H	H ₂₀	-10.2387511	-0.0110824	-21.5919608	3549	H	H ₅₁	-1.1550894	-26.7742917	0.3648224
3497	H	H ₂₀	23.5457570	-3.9220037	1.1223934	3550	H	H ₂₁	5.6574153	8.7014323	24.9554572
3498	H	H ₂₀	-13.3071522	-6.9303284	18.5993202	3551	H	H ₂₁	17.1917468	15.4157550	-14.0461536
3499	H	H ₂₁	-10.6696742	15.0575666	19.9537592	3552	H	H ₂₁	5.6609470	-8.7017371	-24.9545495
3500	H	H ₂₁	20.1526776	17.8437574	3.7675765	3553	H	H ₂₁	17.1886669	-15.4166795	14.0489032
3501	H	H ₂₁	-10.6672863	-15.0569924	-19.9554681	3554	H	H ₂₁	-22.8501109	-13.7525683	4.3858196
3502	H	H ₂₁	20.1523189	-17.8448416	-3.7643509	3555	H	H ₅₁	-22.9643478	12.6668201	6.0955474
3503	H	H ₂₁	-9.4857397	-20.9791359	14.4437311	3556	H	H ₅₁	14.8236341	10.2739667	19.9917654
3504	H	H ₅₁	-11.1076882	5.1402515	23.8021008	3557	H	H ₅₁	8.1412294	17.0225185	-19.2072795
3505	H	H ₅₁	25.1131291	9.2554270	-0.1040179	3558	H	H ₅₁	14.8262910	-10.2747651	-19.9893881
3506	H	H ₅₁	-11.1041538	-5.1396536	-23.8038806	3559	H	H ₅₁	8.1372442	-17.0229559	19.2085796
3507	H	H ₅₁	25.1126135	-9.2567788	0.1080416	3560	H	H ₅₁	-22.9640510	-12.6655843	-6.0992246
3508	H	H ₅₁	-14.0088130	-12.5193657	19.0620451	3561	H	H ₂₁	9.4386673	2.5926639	-25.1497324
3509	H	H ₂₁	-20.3344112	17.7006927	3.6794259	3562	H	H ₂₁	-26.5648613	-2.4396481	4.0836376
3510	H	H ₂₁	10.7070241	14.8710117	20.1135101	3563	H	H ₂₁	17.1261139	-5.2139050	20.1948215
3511	H	H ₂₁	9.6280794	20.8466617	-14.5964944	3564	H	H ₂₁	-26.5640684	2.4410768	-4.0878862
3512	H	H ₂₁	10.7094508	-14.8715875	-20.1117979	3565	H	H ₂₁	17.1296337	5.2129825	-20.1920739
3513	H	H ₂₁	9.6246229	-20.8471800	14.5980375	3566	H	H ₂₁	9.4345047	-2.5931730	25.1512507
3514	H	H ₂₁	-20.3347660	-17.6995987	-3.6826811	3567	H	H ₅₁	14.1433111	10.7030797	-20.1017417
3515	H	H ₅₁	1.0798298	12.5729527	23.7841203	3568	H	H ₅₁	-25.8003741	7.2779312	-0.2034217
3516	H	H ₅₁	17.9120644	18.1536627	-8.6332055	3569	H	H ₅₁	11.6573486	3.1212600	23.9381120
3517	H	H ₅₁	1.0829618	-12.5730101	-23.7839519	3570	H	H ₅₁	-25.8008033	-7.2765429	0.1992909
3518	H	H ₅₁	17.9097005	-18.1546271	8.6360770	3571	H	H ₅₁	11.6610095	-3.1218873	-23.9362457
3519	H	H ₅₁	-18.9932996	-17.8358489	6.7872391	3572	H	H ₅₁	14.1395083	-10.7038407	20.1040063
3520	H	H ₂₁	-4.7624529	22.8724067	13.5249660	3573	H	H ₂₁	-20.0680005	11.6913814	13.9106860
3521	H	H ₂₁	10.5641635	24.5769416	3.6228573	3574	H	H ₂₁	20.1887771	11.7262554	13.7050485
3522	H	H ₂₁	-4.7615146	-22.8721497	-13.5257329	3575	H	H ₂₁	-20.0663994	-11.6903014	-13.9138998
3523	H	H ₂₁	10.5634206	-24.5775086	-3.6211744	3576	H	H ₂₁	20.1903396	-11.7273416	-13.7018168
3524	H	H ₂₁	-5.8028645	-25.9764491	4.5059415	3577	H	H ₂₁	-0.1244788	-17.6238402	20.5500605
3525	H	H ₅₁	3.7379848	19.2287104	18.5889502	3578	H	H ₅₁	-25.0902103	4.4537419	8.2205469
3526	H	H ₅₁	11.1712280	23.6097409	-6.8592157	3579	H	H ₅₁	18.9068117	2.6360523	18.7754023
3527	H	H ₅₁	3.7399277	-19.2289109	-18.5883556	3580	H	H ₅₁	-25.0891355	-4.4523911	-8.2245685
3528	H	H ₅₁	11.1688596	-23.6103408	6.8609977	3581	H	H ₅₁	18.9096798	-2.6370691	-18.7723788
3529	H	H ₅₁	-14.9096399	-22.5108921	0.4767410	3582	H	H ₅₁	6.1792363	-10.0097003	24.0531661
3530	H	H ₂₁	-6.1291667	8.5110927	24.9827616	3583	H	H ₂₁	-9.5136349	-2.6782014	25.1814324
3531	H	H ₂₁	23.1363055	13.5084241	-4.0469064	3584	H	H ₂₁	26.6419551	2.3547373	-4.0555890
3532	H	H ₂₁	-6.1256262	-8.5107636	-24.9837389	3585	H	H ₂₁	-9.5094583	2.6787126	-25.1829519
3533	H	H ₂₁	23.1349263	-13.5096684	4.0506072	3586	H	H ₂₁	26.6411772	-2.3561723	4.0598630
3534	H	H ₂₁	-17.0097986	-15.3092158	14.5064960	3587	H	H ₂₁	-17.1317873	-5.1501029	20.2919899
3535	H	H ₅₁	-4.8701273	17.6041770	19.7314657	3588	H	H ₅₁	-17.7060618	1.0481895	20.0071135
3536	H	H ₅₁	16.6890516	21.0769120	-0.4418633	3589	H	H ₅₁	25.7745782	3.4186526	6.2347567
3537	H	H ₅₁	-4.8679126	-17.6039149	-19.7322455	3590	H	H ₅₁	-17.7029213	-1.0472363	-20.0099508
3538	H	H ₅₁	16.6878540	-21.0778107	0.4445394	3591	H	H ₅₁	25.7753946	-3.4200410	-6.2306212
3539	H	H ₅₁	-11.8207357	-22.5078769	8.7533772	3592	H	H ₅₁	-8.0726451	-8.6218567	23.9871613
3540	H	H ₂₁	4.5873225	22.8922981	13.6649261	3593	H	H ₂₁	-23.0067079	2.7789077	13.8564605
3541	H	H ₂₁	6.0057978	26.0050388	-4.4158091	3594	H	H ₂₁	22.9212191	2.7531596	14.0025194
3542	H	H ₂₁	4.5882838	-22.8925456	-13.6641877	3595	H	H ₂₁	-23.0046412	-2.7776687	-13.8601502
3543	H	H ₂₁	6.0036917	-26.0053609	4.4167648	3596	H	H ₂₁	22.9233153	-2.7543927	-13.9988513
3544	H	H ₂₁	-10.5929407	-24.6567215	-3.4156602	3597	H	H ₂₁	0.0811335	-9.5143375	25.2686215
3545	H	H ₅₁	-3.6682379	25.3572200	7.8667305	3598	H	H ₅₁	-16.7550103	9.5775193	18.6387233

3599	H	H ₅₁	22.8780880	11.3762758	8.1874671	3652	H	H ₂₄	-18.1144379	-17.1227629	15.3572349
3600	H	H ₅₁	-16.7525425	-9.5766183	-18.6414024	3653	H	H ₂₅	-2.9746519	19.4746201	21.9601179
3601	H	H ₅₁	22.8787913	-11.3775071	-8.1838031	3654	H	H ₂₅	17.3686205	23.7040682	-2.6085526
3602	H	H ₅₁	-6.1267378	-16.3000731	20.4115642	3655	H	H ₂₅	-2.9721792	-19.4744590	-21.9606004
3603	H	H ₂₄	-11.6395618	15.5949838	21.9614261	3656	H	H ₂₅	17.3669243	-23.7050015	2.6113257
3604	H	H ₂₄	22.2721657	18.7189529	3.8129935	3657	H	H ₂₅	-14.3956294	-24.5779300	7.6842289
3605	H	H ₂₄	-11.6368882	-15.5943565	-21.9632957	3658	H	H ₂₆	6.5624530	15.8926010	14.7547986
3606	H	H ₂₄	22.2717623	-18.7201503	-3.8094331	3659	H	H ₂₆	6.9767634	19.8711583	-8.3550319
3607	H	H ₂₄	-10.6356186	-22.1393309	16.0536850	3660	H	H ₂₆	6.5639641	-15.8929539	-14.7537490
3608	H	H ₂₅	-14.3940122	5.2136197	25.0474399	3661	H	H ₂₆	6.9743614	-19.8715342	8.3561519
3609	H	H ₂₅	27.8083732	9.1550196	2.1502566	3662	H	H ₂₆	-13.5390217	-17.9422852	-2.8484963
3610	H	H ₂₅	-14.3902834	-5.2128456	-25.0497424	3663	H	H ₂₄	4.3971300	25.0322130	14.4578022
3611	H	H ₂₅	27.8082229	-9.1565178	-2.1457936	3664	H	H ₂₄	6.4632151	28.2234539	-4.0789577
3612	H	H ₂₅	-13.4183087	-13.3847536	22.4174269	3665	H	H ₂₄	4.3980951	-25.0324502	-14.4570949
3613	H	H ₂₆	-17.1713787	-0.5878662	14.4754961	3666	H	H ₂₄	6.4610420	-28.2238034	4.0800025
3614	H	H ₂₆	21.0264999	0.5445191	7.8950253	3667	H	H ₂₄	-10.8601944	-26.9310321	-3.4278528
3615	H	H ₂₆	-17.1690223	0.5887903	-14.4782466	3668	H	H ₂₅	-2.8499567	28.4819588	6.6703734
3616	H	H ₂₆	21.0277398	-0.5456507	-7.8916577	3669	H	H ₂₅	2.9335820	28.5062384	6.5289026
3617	H	H ₂₆	-3.8587817	-5.5906996	21.4148477	3670	H	H ₂₅	-2.8504200	-28.4818058	-6.6708280
3618	H	H ₂₄	10.9279188	15.9768083	22.1319956	3671	H	H ₂₅	2.9330896	-28.5063974	-6.5284262
3619	H	H ₂₄	11.0778952	22.4433951	-15.4297519	3672	H	H ₂₅	-0.0838075	-29.3438855	-1.6635736
3620	H	H ₂₄	10.9306066	-15.9773970	-22.1302420	3673	H	H ₂₆	6.0560784	20.1753948	7.6443135
3621	H	H ₂₄	11.0742122	-22.4439919	15.4315301	3674	H	H ₂₆	0.5321491	22.1113509	-3.6004365
3622	H	H ₂₄	-22.0055804	-19.2313751	-3.2267151	3675	H	H ₂₆	-6.5874058	20.3318537	6.7364716
3623	H	H ₂₅	0.1433668	15.6881961	24.8933376	3676	H	H ₂₆	0.5303801	-22.1113804	3.6005268
3624	H	H ₂₅	18.8693089	21.2749651	-7.5593270	3677	H	H ₂₆	-6.5874152	-20.3314991	-6.7375272
3625	H	H ₂₅	0.1465102	-15.6882036	-24.8933161	3678	H	H ₂₆	6.0562133	-20.1757199	-7.6433482
3626	H	H ₂₅	18.8669561	-21.2759790	7.5623404	3679	H	H ₂₄	6.7929833	9.5026019	26.7752473
3627	H	H ₂₅	-19.0142250	-21.2323687	7.3119132	3680	H	H ₂₄	18.0594119	16.8055972	-15.6456998
3628	H	H ₂₆	-6.2112716	16.5052557	14.1842125	3681	H	H ₂₄	6.7967615	-9.5029661	-26.7741675
3629	H	H ₂₆	12.7866390	18.4371410	2.9612391	3682	H	H ₂₄	18.0559982	-16.8065681	15.6485864
3630	H	H ₂₆	-6.2098883	-16.5049215	-14.1852071	3683	H	H ₂₄	-24.8532944	-14.8086394	4.0467133
3631	H	H ₂₆	12.7861210	-18.4378292	-2.9591911	3684	H	H ₂₅	-26.1881957	11.5009099	6.4758817
3632	H	H ₂₆	-6.5769572	-20.2623794	7.6403443	3685	H	H ₂₅	16.9314566	8.7800332	22.2770457
3633	H	H ₂₄	-4.6191886	24.5619640	15.0560357	3686	H	H ₂₅	9.2572301	16.4759701	-22.4248929
3634	H	H ₂₄	11.5510431	26.5985815	3.2249317	3687	H	H ₂₅	16.9345465	-8.7809449	-22.2743320
3635	H	H ₂₄	-4.6181008	-24.5617145	-15.0567807	3688	H	H ₂₅	9.2527473	-16.4764679	22.4263738
3636	H	H ₂₄	11.5501242	-26.5992039	-3.2230775	3689	H	H ₂₅	-26.1877848	-11.4995005	-6.4800762
3637	H	H ₂₄	-6.9330616	-27.9559627	4.6591839	3690	H	H ₂₆	-21.1287682	0.1599931	7.1153996
3638	H	H ₂₅	2.5838582	19.5974883	21.7787071	3691	H	H ₂₆	16.6136826	-1.1673231	14.8223553
3639	H	H ₂₅	14.4164799	24.5929642	-7.2388547	3692	H	H ₂₆	4.5151385	5.0418379	-21.2431784
3640	H	H ₂₅	2.5862882	-19.5976280	-21.7782894	3693	H	H ₂₆	16.6161164	1.1664291	-14.8196948
3641	H	H ₂₅	14.4140016	-24.5937402	7.2411644	3694	H	H ₂₆	4.5114658	-5.0420812	21.2439038
3642	H	H ₂₅	-17.0011825	-23.8332328	2.8260853	3695	H	H ₂₆	-21.1276352	-0.1588557	-7.1187854
3643	H	H ₂₆	-0.5487236	7.5048365	21.0649081	3696	H	H ₂₄	10.4910932	3.5102000	-26.9758667
3644	H	H ₂₆	17.1501305	12.3830995	-7.2722586	3697	H	H ₂₄	-28.7844188	-1.8650570	4.2497779
3645	H	H ₂₆	-0.5457500	-7.5048077	-21.0649920	3698	H	H ₂₄	18.2932873	-4.9486236	22.1573565
3646	H	H ₂₆	17.1483004	-12.3840215	7.2750001	3699	H	H ₂₄	-28.7836339	1.8666073	-4.2543952
3647	H	H ₂₆	-16.6029761	-12.5439282	8.2064045	3700	H	H ₂₄	18.2970988	4.9476403	-22.1544342
3648	H	H ₂₄	-6.5696407	9.8706925	26.7689332	3701	H	H ₂₄	10.4865834	-3.5107641	26.9775447
3649	H	H ₂₄	24.6812534	15.1925518	-4.1459351	3702	H	H ₂₅	-27.8333496	8.8779269	2.1171616
3650	H	H ₂₄	-6.5658845	-9.8703385	-26.7699880	3703	H	H ₂₅	14.4193243	4.9354105	25.0143934
3651	H	H ₂₄	24.6797688	-15.1938803	4.1498892	3704	H	H ₂₅	-27.8334837	-8.8764297	-2.1216155

3705	H	H ₂₅	14.4230609	-4.9361871	-25.0120807	3758	H	H ₂₇	-11.5309530	14.0630283	23.7284242
3706	H	H ₂₅	13.4100644	-13.1154228	22.4978036	3759	H	H ₂₇	23.9509992	17.7122555	2.5288635
3707	H	H ₂₆	-17.1293076	12.0917444	7.6650289	3760	H	H ₂₇	-11.5279132	-14.0624091	-23.7302629
3708	H	H ₂₆	13.3301106	10.9748057	14.1505435	3761	H	H ₂₇	23.9504545	-17.7135458	-2.5250197
3709	H	H ₂₆	-17.1287298	-12.0908228	-7.6677708	3762	H	H ₂₇	-12.4232402	-21.1006616	17.1521118
3710	H	H ₂₆	13.3317820	-10.9755244	-14.1484012	3763	H	H ₂₈	-16.0658931	3.7932726	24.3022969
3711	H	H ₂₆	3.7964300	-16.0088834	15.0890325	3764	H	H ₂₈	28.2170234	7.3634383	3.5613009
3712	H	H ₂₄	-22.2091291	12.2363328	14.5011324	3765	H	H ₂₈	-16.0622061	-3.7924081	-24.3048693
3713	H	H ₂₄	21.6832166	12.0811154	15.3993805	3766	H	H ₂₈	28.2171980	-7.3649570	-3.5567808
3714	H	H ₂₄	-22.2074624	-12.2351365	-14.5046958	3767	H	H ₂₈	-12.1552969	-12.0845303	23.8603512
3715	H	H ₂₄	21.6850254	-12.0822826	-15.3959064	3768	H	H ₂₉	-18.7760717	-0.9966817	12.8173221
3716	H	H ₂₄	0.5218737	-18.6079501	22.5106183	3769	H	H ₂₉	20.4737052	-0.4983176	9.9195387
3717	H	H ₂₅	-27.8991695	6.0875539	7.0103892	3770	H	H ₂₉	-18.7739695	0.9976922	-12.8203297
3718	H	H ₂₅	19.0384219	3.4830388	22.1353657	3771	H	H ₂₉	20.4753220	0.4972150	-9.9162554
3719	H	H ₂₅	-27.8983728	-6.0860522	-7.0148588	3772	H	H ₂₉	-1.7013988	-5.0195063	22.1297941
3720	H	H ₂₅	19.0417775	-3.4840635	-22.1323165	3773	H	H ₂₇	9.3456612	15.5851596	23.8036106
3721	H	H ₂₅	8.8563164	-11.6822578	25.4883903	3774	H	H ₂₇	13.3532422	22.2553728	-14.9412127
3722	H	H ₂₆	14.4698804	9.2623940	-14.6196693	3775	H	H ₂₇	9.3486399	-15.5856627	-23.8021129
3723	H	H ₂₆	-21.0732064	7.3223115	-3.3478208	3776	H	H ₂₇	13.3496493	-22.2560905	14.9433463
3724	H	H ₂₆	6.6035789	3.0697931	21.3511956	3777	H	H ₂₇	-22.6990417	-19.5083222	-1.0145586
3725	H	H ₂₆	-21.0741409	-7.3211786	3.3444529	3778	H	H ₂₈	-1.6668070	16.8756127	24.0835069
3726	H	H ₂₆	6.6068366	-3.0701501	-21.3501288	3779	H	H ₂₈	18.9087745	21.9420016	-5.3466250
3727	H	H ₂₆	14.4670413	-9.2631729	14.6219876	3780	H	H ₂₈	-1.6638614	-16.8755243	-24.0837669
3728	H	H ₂₄	-10.9431744	-2.5345091	26.9606624	3781	H	H ₂₈	18.9067395	-21.9430205	5.3496613
3729	H	H ₂₄	28.8541358	2.7283723	-3.6122786	3782	H	H ₂₈	-17.2436870	-22.4314302	8.1893868
3730	H	H ₂₄	-10.9387157	2.5350969	-26.9624091	3783	H	H ₂₉	-7.0297611	17.8845240	12.4957395
3731	H	H ₂₄	28.8534214	-2.7299248	3.6168983	3784	H	H ₂₉	11.5521771	19.2131175	4.7770713
3732	H	H ₂₄	-17.9147776	-5.9438264	22.2886920	3785	H	H ₂₉	-7.0287231	-17.8841473	-12.4968563
3733	H	H ₂₅	-18.9158727	3.4622169	22.0933465	3786	H	H ₂₉	11.5519113	-19.2137401	-4.7752163
3734	H	H ₂₅	27.8053681	6.0738772	6.9197276	3787	H	H ₂₉	-4.5239592	-21.2789547	7.2219892
3735	H	H ₂₅	-18.9125225	-3.4611994	-22.0963730	3788	H	H ₂₇	-2.6583252	24.8419498	16.3011394
3736	H	H ₂₅	27.8061525	-6.0753737	-6.9152738	3789	H	H ₂₇	11.5921330	27.4668937	1.0528369
3737	H	H ₂₅	-8.8939078	-11.6326043	25.3671849	3790	H	H ₂₇	-2.6570512	-24.8418072	-16.3015630
3738	H	H ₂₆	-12.5463474	11.2709971	14.6489867	3791	H	H ₂₇	11.5908249	-27.4675173	-1.0509815
3739	H	H ₂₆	17.1198264	12.6145020	6.8428595	3792	H	H ₂₇	-8.9348309	-28.2479665	3.4838908
3740	H	H ₂₆	-12.5446049	-11.2703227	-14.6509916	3793	H	H ₂₈	2.2822068	17.8658595	23.2986485
3741	H	H ₂₆	17.1202406	-12.6154241	-6.8401136	3794	H	H ₂₈	16.1189409	23.2729676	-8.1100674
3742	H	H ₂₆	-4.5761681	-16.3015146	14.5725197	3795	H	H ₂₈	2.2849698	-17.8659821	-23.2982847
3743	H	H ₂₄	-24.4658390	3.4046823	15.5014078	3796	H	H ₂₈	16.1163824	-23.2738354	8.1126508
3744	H	H ₂₄	24.9627578	3.5500354	14.6533440	3797	H	H ₂₈	-18.4021973	-22.6018397	4.2119359
3745	H	H ₂₄	-24.4635356	-3.4033662	-15.5053230	3798	H	H ₂₉	-1.9485017	5.8385320	21.9297689
3746	H	H ₂₄	24.9649227	-3.5513790	-14.6493454	3799	H	H ₂₉	18.8329550	10.7999441	-6.8906122
3747	H	H ₂₄	-0.5016106	-10.7400058	27.1083648	3800	H	H ₂₉	-1.9453036	-5.8384286	-21.9300723
3748	H	H ₂₅	-17.3084853	9.0856571	22.0065087	3801	H	H ₂₉	18.8312723	-10.8009583	6.8936327
3749	H	H ₂₅	26.1014050	11.6689365	6.9979949	3802	H	H ₂₉	-16.8863413	-11.3721235	10.2140179
3750	H	H ₂₅	-17.3054534	-9.0847258	-22.0092798	3803	H	H ₂₇	-6.9912761	12.1511946	26.4272893
3751	H	H ₂₅	26.1018913	-11.6703409	-6.9938165	3804	H	H ₂₇	24.2654501	17.2269427	-3.0580203
3752	H	H ₂₅	-8.7969388	-16.7553123	22.5453460	3805	H	H ₂₇	-6.9877023	-12.1508186	-26.4284077
3753	H	H ₂₆	-6.9312189	2.1497228	21.0492221	3806	H	H ₂₇	24.2640275	-17.2282483	3.0619053
3754	H	H ₂₆	21.1147254	6.3173575	-3.1609875	3807	H	H ₂₇	-17.2769724	-19.2810961	14.9892178
3755	H	H ₂₆	-6.9279644	-2.1493515	-21.0503224	3808	H	H ₂₈	-0.8204308	20.1767322	21.5210073
3756	H	H ₂₆	21.1138828	-6.3184947	3.1643739	3809	H	H ₂₈	15.8135848	24.5823035	-4.0704078
3757	H	H ₂₆	-14.1861441	-8.3539083	14.9899428	3810	H	H ₂₈	-0.8180669	-20.1766883	-21.5211372

3811	H	H ₂₈	15.8116180	-24.5831548	4.0729420	3864	H	H ₂₉	14.3287235	12.1169830	12.3581597
3812	H	H ₂₈	-14.9944556	-24.8230741	5.4688825	3865	H	H ₂₉	-15.9301651	-12.5874793	-9.6251188
3813	H	H ₂₉	-14.6650466	17.1993682	4.7473263	3866	H	H ₂₉	14.3300550	-12.1177541	-12.3558655
3814	H	H ₂₉	8.8574234	15.4922767	14.6613239	3867	H	H ₂₉	1.5995654	-16.7988545	14.8356867
3815	H	H ₂₉	5.8083120	19.8019253	-10.3714154	3868	H	H ₂₇	-23.9334452	10.7224132	14.0783136
3816	H	H ₂₉	8.8589384	-15.4927536	-14.6599041	3869	H	H ₂₇	22.4069186	10.2731316	16.6844729
3817	H	H ₂₉	5.8055858	-19.8022376	10.3723442	3870	H	H ₂₇	-23.9317691	-10.7211258	-14.0821433
3818	H	H ₂₉	-14.6652131	-17.1985789	-4.7496749	3871	H	H ₂₇	22.4090413	-10.2743376	-16.6808840
3819	H	H ₂₇	2.4478583	26.2466141	13.9905837	3872	H	H ₂₇	1.5222251	-17.3067281	24.1689646
3820	H	H ₂₇	6.8606825	28.9817955	-1.8972937	3873	H	H ₂₈	-28.3349851	6.4329386	4.7626875
3821	H	H ₂₇	2.4486833	-26.2467461	-13.9901906	3874	H	H ₂₈	17.2872438	3.1857575	23.6207462
3822	H	H ₂₇	6.8588126	-28.9821643	1.8983896	3875	H	H ₂₈	-28.3345710	-6.4314121	-4.7672347
3823	H	H ₂₇	-9.3086002	-28.2622690	-2.2819528	3876	H	H ₂₈	17.2908534	-3.1866877	-23.6179787
3824	H	H ₂₈	1.7324342	29.2323907	3.0901488	3877	H	H ₂₈	11.0434452	-11.5131146	24.7472783
3825	H	H ₂₈	-2.5234877	28.9997591	4.4417342	3878	H	H ₂₉	15.9813839	9.9399545	-12.9829941
3826	H	H ₂₈	0.7921915	28.4907283	7.3982315	3879	H	H ₂₉	-20.5316438	8.6032024	-5.2155694
3827	H	H ₂₈	-2.5243320	-28.9996233	-4.4421382	3880	H	H ₂₉	4.5505545	3.9065426	22.0634789
3828	H	H ₂₈	0.7918407	-28.4907702	-7.3981090	3881	H	H ₂₉	-20.5329452	-8.6020965	5.2122758
3829	H	H ₂₈	1.7313532	-29.2324847	-3.0898672	3882	H	H ₂₉	4.5538749	-3.9067885	-22.0627443
3830	H	H ₂₉	6.9473964	19.4650843	9.6873699	3883	H	H ₂₉	15.9787756	-9.9408144	12.9855532
3831	H	H ₂₉	1.9345330	22.0750768	-5.4726185	3884	H	H ₂₇	-13.2264261	-2.2407685	26.5672208
3832	H	H ₂₉	-8.8811214	20.0336976	6.3857358	3885	H	H ₂₇	29.6168279	2.5752286	-1.4101861
3833	H	H ₂₉	1.9324668	-22.0751809	5.4729281	3886	H	H ₂₇	-13.2220577	2.2414806	-26.5693409
3834	H	H ₂₉	-8.8811760	-20.0332200	-6.3871566	3887	H	H ₂₇	29.6164647	-2.5768238	1.4149367
3835	H	H ₂₉	6.9479011	-19.4654579	-9.6862585	3888	H	H ₂₇	-16.3944963	-6.4617242	23.9842287
3836	H	H ₂₇	8.8675721	10.5351847	26.4717078	3889	H	H ₂₈	-18.9413817	5.7264892	21.6344667
3837	H	H ₂₇	16.6113402	18.0223313	-17.0186296	3890	H	H ₂₈	27.0938308	8.1215505	7.7190341
3838	H	H ₂₇	8.8712439	-10.5356636	-26.4702781	3891	H	H ₂₈	-18.9382218	-5.7254696	-21.6375020
3839	H	H ₂₇	16.6076478	-18.0232260	17.0212944	3892	H	H ₂₈	27.0946264	-8.1230084	-7.7146961
3840	H	H ₂₇	-25.4794738	-15.4156861	1.8783785	3893	H	H ₂₈	-8.1567660	-13.6878021	24.6115828
3841	H	H ₂₈	-26.7445892	9.4885680	7.5021193	3894	H	H ₂₉	-11.4062194	13.2970078	14.4923668
3842	H	H ₂₈	18.3811581	7.0301932	21.7783649	3895	H	H ₂₉	16.1184460	14.6812969	6.4495042
3843	H	H ₂₈	8.3638432	14.8896553	-23.8732460	3896	H	H ₂₉	-11.4046145	-13.2963946	-14.4941900
3844	H	H ₂₈	18.3842638	-7.0311828	-21.7754196	3897	H	H ₂₉	16.1186920	-14.6821642	-6.4469237
3845	H	H ₂₈	8.3592212	-14.8901058	23.8745877	3898	H	H ₂₉	-4.7146812	-18.0332553	13.0197709
3846	H	H ₂₈	-26.7438971	-9.4871281	-7.5064062	3899	H	H ₂₇	-24.0752839	5.3805025	16.6806274
3847	H	H ₂₉	-21.4885085	-2.1152022	6.7130988	3900	H	H ₂₇	25.4836374	5.7936754	14.2768992
3848	H	H ₂₉	16.7844535	-3.4980397	14.7425143	3901	H	H ₂₇	-24.0729035	-5.3792082	-16.6844759
3849	H	H ₂₉	4.7040269	2.8168294	-21.9370353	3902	H	H ₂₇	25.4856139	-5.7950480	-14.2728110
3850	H	H ₂₉	16.7870001	3.4971369	-14.7398295	3903	H	H ₂₇	-1.4130310	-12.8688539	26.8180607
3851	H	H ₂₉	4.7003513	-2.8170823	21.9377874	3904	H	H ₂₈	-15.7516273	8.3173412	23.5211397
3852	H	H ₂₉	-21.4873234	2.1163578	-6.7165357	3905	H	H ₂₈	26.7285515	11.5424374	4.7846478
3853	H	H ₂₇	-29.5858154	-0.0802729	2.9757921	3906	H	H ₂₈	-15.7483141	-8.3164934	-23.5236630
3854	H	H ₂₇	17.3444581	-3.6781794	23.8709703	3907	H	H ₂₈	26.7286988	-11.5438769	-4.7803610
3855	H	H ₂₇	-29.5853378	0.0818644	-2.9805266	3908	H	H ₂₈	-10.9808575	-16.1712241	22.1008648
3856	H	H ₂₇	17.3484754	3.6772465	-23.8681957	3909	H	H ₂₉	-5.6763299	0.2764721	21.6724358
3857	H	H ₂₇	12.2368372	-5.0167783	26.6321986	3910	H	H ₂₉	21.2943923	4.8656977	-4.9865387
3858	H	H ₂₈	-27.1654689	10.6635266	3.4391298	3911	H	H ₂₉	-5.6728739	-0.2761664	-21.6733468
3859	H	H ₂₈	14.9513237	7.0735982	24.2883332	3912	H	H ₂₉	21.2933297	-4.8668439	4.9899504
3860	H	H ₂₈	-27.1654896	-10.6620648	-3.4434797	3913	H	H ₂₉	-15.6206090	-6.5334163	14.6731959
3861	H	H ₂₈	14.9548324	-7.0744026	-24.2859404	3914	H	H ₃₀	-15.5706630	2.0977035	22.8061571
3862	H	H ₂₈	12.2102268	-15.0573090	22.0836800	3915	H	H ₃₀	26.9415876	5.4386331	3.3968345
3863	H	H ₂₉	-15.9310274	12.5883359	9.6225717	3916	H	H ₃₀	-15.5671232	-2.0968670	-22.8086427

3917	H	H ₃₀	26.9418404	-5.4400838	-3.3925149	3970	H	H ₃₀	18.5437773	-6.2440926	-19.6030011
3918	H	H ₃₀	-11.3749526	-10.0142033	23.1795793	3971	H	H ₃₀	6.5410398	-13.6155587	23.2157205
3919	H	H ₃₁	-20.1111562	0.7161965	12.1066316	3972	H	H ₃₀	-25.0851850	-8.1657532	-8.4375419
3920	H	H ₃₁	20.2830441	0.7661720	11.8132658	3973	H	H ₃₁	-22.7811174	-2.7346240	4.9273718
3921	H	H ₃₁	-20.1092590	-0.7151147	-12.1098497	3974	H	H ₃₁	15.9976941	-4.7285133	16.5060963
3922	H	H ₃₁	20.2848900	-0.7672630	-11.8100204	3975	H	H ₃₁	6.7833474	1.9661663	-22.3798343
3923	H	H ₃₁	-0.1757468	-6.6763966	22.5152595	3976	H	H ₃₁	16.0005965	4.7276531	-16.5035392
3924	H	H ₃₀	-3.1352838	15.8772605	22.5941854	3977	H	H ₃₁	6.7796640	-1.9665304	22.3809156
3925	H	H ₃₀	18.5185958	20.3974502	-3.6633834	3978	H	H ₃₁	-22.7801747	2.7358512	-4.9310272
3926	H	H ₃₀	-3.1325214	-15.8770913	-22.5946902	3979	H	H ₃₀	-25.0301546	11.5466740	3.2179782
3927	H	H ₃₀	18.5169094	-20.3984473	3.6663523	3980	H	H ₃₀	13.5651730	8.1769367	22.7884510
3928	H	H ₃₀	-15.3851438	-21.3184781	9.0130160	3981	H	H ₃₀	-25.0302605	-11.5453274	-3.2219842
3929	H	H ₃₁	-5.7546546	19.6820368	11.7861020	3982	H	H ₃₀	13.5683849	-8.1776666	-22.7862792
3930	H	H ₃₁	10.0448991	20.9424238	4.4638293	3983	H	H ₃₀	11.4614129	-15.5331088	19.9386120
3931	H	H ₃₁	-5.7538288	-19.6817268	-11.7870255	3984	H	H ₃₁	-16.6826325	11.7466262	11.6279972
3932	H	H ₃₁	10.0444865	-20.9429649	-4.4622173	3985	H	H ₃₁	16.5397616	11.7041156	11.8723914
3933	H	H ₃₁	-4.2914878	-22.6335479	5.3587746	3986	H	H ₃₁	-16.6814021	-11.7457290	-11.6306659
3934	H	H ₃₀	2.8735070	15.6977049	22.6990091	3987	H	H ₃₁	16.5410305	-11.7050070	-11.8697353
3935	H	H ₃₀	15.6300363	21.1349377	-8.8846065	3988	H	H ₃₁	0.1398408	-16.6068234	16.6041451
3936	H	H ₃₀	2.8762992	-15.6978602	-22.6985451	3989	H	H ₃₀	-26.9179719	5.5341831	3.1574294
3937	H	H ₃₀	15.6274730	-21.1357797	8.8871150	3990	H	H ₃₀	15.3407169	2.1314522	22.9192689
3938	H	H ₃₀	-18.5045268	-20.2900277	3.9770917	3991	H	H ₃₀	-26.9177606	-5.5327352	-3.1617363
3939	H	H ₃₁	-4.1244728	6.3839224	22.4696906	3992	H	H ₃₀	15.3442748	-2.1322771	-22.9168164
3940	H	H ₃₁	20.3016278	11.1374342	-5.1433611	3993	H	H ₃₀	11.5732534	-10.0423918	23.0300657
3941	H	H ₃₁	-4.1212086	-6.3837004	-22.4703517	3994	H	H ₃₁	16.0747695	12.1511591	-12.3870957
3942	H	H ₃₁	20.3002078	-11.1385263	5.1466101	3995	H	H ₃₁	-20.3946036	10.8821004	-5.0128774
3943	H	H ₃₁	-16.1793826	-12.3491031	12.1811318	3996	H	H ₃₁	4.3202171	6.1580137	22.4255103
3944	H	H ₃₀	0.0925496	19.9154060	19.4044332	3997	H	H ₃₁	-20.3959913	-10.8810033	5.0096138
3945	H	H ₃₀	13.5890548	23.9356012	-3.9482520	3998	H	H ₃₁	4.3234795	-6.1582460	-22.4248200
3946	H	H ₃₀	0.0945834	-19.9154103	-19.4044221	3999	H	H ₃₁	16.0721286	-12.1520240	12.3896690
3947	H	H ₃₀	13.5871368	-23.9363317	3.9504236	4000	H	H ₃₀	-18.5148086	6.4856398	19.4881520
3948	H	H ₃₀	-13.6826044	-23.9081024	3.7885302	4001	H	H ₃₀	24.9371953	8.3723255	8.5258607
3949	H	H ₃₁	-16.8350671	16.4376445	4.5282939	4002	H	H ₃₀	-18.5120364	-6.4846430	-19.4911199
3950	H	H ₃₁	9.8674060	14.3896243	16.4223635	4003	H	H ₃₀	24.9381073	-8.3736679	-8.5218651
3951	H	H ₃₁	6.9683194	19.3369585	-12.3144396	4004	H	H ₃₀	-6.4264472	-13.8132677	23.0769180
3952	H	H ₃₁	9.8692548	-14.3901555	-16.4207824	4005	H	H ₃₁	-10.1693095	14.0391489	16.2727931
3953	H	H ₃₁	6.9653102	-19.3373344	12.3155609	4006	H	H ₃₁	16.9105083	16.0196783	4.7666500
3954	H	H ₃₁	-16.8352233	-16.4367375	-4.5309962	4007	H	H ₃₁	-10.1674634	-14.0386023	-16.2744176
3955	H	H ₃₀	3.1492962	27.3939764	3.0336421	4008	H	H ₃₁	16.9104102	-16.0205902	-4.7639311
3956	H	H ₃₀	-3.0100610	27.4347638	2.7971944	4009	H	H ₃₁	-6.7435956	-19.0080837	12.5909897
3957	H	H ₃₀	-0.1381679	26.5093640	8.1722413	4010	H	H ₃₀	-13.5320207	8.0633408	22.8818679
3958	H	H ₃₀	-3.0110874	-27.4346010	-2.7976814	4011	H	H ₃₀	25.1104571	11.4652538	3.1186128
3959	H	H ₃₀	-0.1382910	-26.5093567	-8.1722627	4012	H	H ₃₀	-13.5287927	-8.0626133	-22.8840311
3960	H	H ₃₀	3.1483110	-27.3941466	-3.0331336	4013	H	H ₃₀	25.1103439	-11.4666053	-3.1145905
3961	H	H ₃₁	5.7178253	19.7070981	11.5989881	4014	H	H ₃₀	-11.5820102	-15.4417292	19.9780621
3962	H	H ₃₁	4.1452756	22.6053763	-5.2357950	4015	H	H ₃₁	-6.8077908	-1.6718931	22.2222477
3963	H	H ₃₁	-9.8622798	20.9253662	4.5237584	4016	H	H ₃₁	22.6156100	2.9730782	-4.7607174
3964	H	H ₃₁	4.1432230	-22.6055992	5.2364580	4017	H	H ₃₁	-6.8041441	1.6722588	-22.2233348
3965	H	H ₃₁	-9.8626746	-20.9248360	-4.5253347	4018	H	H ₃₁	22.6146909	-2.9742954	4.7643400
3966	H	H ₃₁	5.7186304	-19.7074054	-11.5980746	4019	H	H ₃₁	-15.8106292	-4.9732962	16.3786406
3967	H	H ₃₀	-25.0861009	8.1671038	8.4335208	4020	H	H ₃₂	-10.5801446	10.6967422	26.2821334
3968	H	H ₃₀	18.5409788	6.2430951	19.6059687	4021	H	H ₃₂	26.1496811	15.2714967	-0.2935288
3969	H	H ₃₀	6.5454898	13.6152056	-23.2146670	4022	H	H ₃₂	-10.5765197	-10.6961725	-26.2838300

4023	H	H ₃₂	26.1488054	-15.2729047	0.2977207	4076	H	H ₃₅	15.2649171	16.5077532	-6.0267937
4024	H	H ₃₂	-15.5728764	-18.3803812	18.3509508	4077	H	H ₃₅	-0.0604090	-12.0407376	-19.9214166
4025	H	H ₃₃	-9.8125190	6.7173977	24.7189318	4078	H	H ₃₅	15.2630660	-16.5085750	6.0292402
4026	H	H ₃₃	25.0163248	11.1847379	-1.2326599	4079	H	H ₃₅	-15.2032536	-16.5258817	6.1320898
4027	H	H ₃₃	-9.8089162	-6.7168702	-24.7205003	4080	H	H ₃₂	-8.1414590	15.8134659	24.5542150
4028	H	H ₃₃	25.0155248	-11.1860832	1.2366606	4081	H	H ₃₂	22.7038824	20.0923078	-0.3021644
4029	H	H ₃₃	-15.2070282	-14.0680273	17.9797512	4082	H	H ₃₂	-8.1383767	-15.8130283	-24.5555162
4030	H	H ₃₄	-13.0878719	-0.2679852	19.8803519	4083	H	H ₃₂	22.7027542	-20.0935293	0.3057987
4031	H	H ₃₄	23.5506472	2.8061693	2.0210633	4084	H	H ₃₂	-14.5651438	-22.4845629	14.1971671
4032	H	H ₃₄	-13.0846641	0.2686891	-19.8824454	4085	H	H ₃₃	-6.8854536	17.1124451	20.4571333
4033	H	H ₃₄	23.5508255	-2.8074360	-2.0172955	4086	H	H ₃₃	18.3883023	20.4922499	0.8233142
4034	H	H ₃₄	-10.4662734	-6.6521159	20.3174573	4087	H	H ₃₃	-6.8830990	-17.1120733	-20.4582431
4035	H	H ₃₅	-15.1873050	2.5613553	17.3340447	4088	H	H ₃₃	18.3873302	-20.4932388	-0.8203734
4036	H	H ₃₅	22.0115014	4.5662309	5.6857140	4089	H	H ₃₃	-11.5050152	-22.5154814	10.9282787
4037	H	H ₃₅	-15.1846645	-2.5605371	-17.3364823	4090	H	H ₃₄	0.3045134	18.5581296	15.0853173
4038	H	H ₃₅	22.0121602	-4.5674156	-5.6821876	4091	H	H ₃₄	9.9962198	21.5848711	-2.4965148
4039	H	H ₃₅	-6.8277078	-9.0292663	20.2370610	4092	H	H ₃₄	0.3059296	-18.5581463	-15.0852666
4040	H	H ₃₂	6.3839132	13.8498238	26.3179217	4093	H	H ₃₄	9.9946602	-21.5854090	2.4981157
4041	H	H ₃₂	17.2349672	20.7903045	-13.9972959	4094	H	H ₃₄	-10.3013987	-21.4951692	1.9754966
4042	H	H ₃₂	6.3873779	-13.8501666	-26.3169040	4095	H	H ₃₅	2.5139034	15.6166147	17.2332857
4043	H	H ₃₂	17.2316006	-20.7912308	14.0000491	4096	H	H ₃₅	11.1569111	19.6337370	-6.1011802
4044	H	H ₃₂	-23.6196850	-18.9136154	3.0968696	4097	H	H ₃₅	2.5158256	-15.6167490	-17.2328891
4045	H	H ₃₃	2.7690301	11.6434580	24.7881535	4098	H	H ₃₅	11.1548703	-19.6343376	6.1029678
4046	H	H ₃₃	18.0609261	17.7643373	-10.7666763	4099	H	H ₃₅	-13.6714065	-18.8946385	1.8082535
4047	H	H ₃₃	2.7723758	-11.6436076	-24.7877063	4100	H	H ₃₂	-1.8179416	27.0632225	13.1260216
4048	H	H ₃₃	18.0582423	-17.7653101	10.7695736	4101	H	H ₃₂	8.1357317	28.9194518	2.3431923
4049	H	H ₃₃	-20.8312314	-16.9500508	6.0370330	4102	H	H ₃₂	-1.8172983	-27.0631247	-13.1263126
4050	H	H ₃₄	-4.6701104	12.6696769	19.7240852	4103	H	H ₃₂	8.1345432	-28.9198891	-2.3418922
4051	H	H ₃₄	17.3076905	16.3830149	-1.8468392	4104	H	H ₃₂	-6.3183747	-29.4536354	0.7595211
4052	H	H ₃₄	-4.6676432	-12.6694263	-19.7248293	4105	H	H ₃₃	-3.8925209	25.2699832	9.8942498
4053	H	H ₃₄	17.3065123	-16.3839466	1.8496128	4106	H	H ₃₃	6.6782402	26.0882712	5.1403463
4054	H	H ₃₄	-12.6394921	-17.7551597	9.8167065	4107	H	H ₃₃	-3.8922975	-25.2697739	-9.8948722
4055	H	H ₃₅	-2.6279943	15.5037444	17.1540720	4108	H	H ₃₃	6.6776608	-26.0886307	-5.1392761
4056	H	H ₃₅	13.6768274	18.7502632	-1.7048596	4109	H	H ₃₃	-2.7863947	-27.2322183	1.5040740
4057	H	H ₃₅	-2.6260798	-15.5036036	-17.1544893	4110	H	H ₃₄	4.7114260	23.2368864	1.7057795
4058	H	H ₃₅	13.6755473	-18.7509987	1.7070470	4111	H	H ₃₄	-4.3136888	23.3537086	1.0278954
4059	H	H ₃₅	-11.0501732	-19.5223281	6.1892657	4112	H	H ₃₄	-0.3968462	21.9692231	9.0695022
4060	H	H ₃₂	1.5260607	24.6710813	17.6414272	4113	H	H ₃₄	-4.3147750	-23.3534761	-1.0285885
4061	H	H ₃₂	10.6689411	28.2544392	-3.1735179	4114	H	H ₃₄	-0.3965722	-21.9692020	-9.0695648
4062	H	H ₃₂	1.5275522	-24.6711647	-17.6411753	4115	H	H ₃₄	4.7104562	-23.2371402	-1.7050237
4063	H	H ₃₂	10.6669079	-28.2550142	3.1752317	4116	H	H ₃₅	2.5977715	22.4747004	5.3662917
4064	H	H ₃₂	-12.1955332	-27.8057240	0.5672327	4117	H	H ₃₅	-0.0207315	23.2318603	0.9684614
4065	H	H ₃₃	3.8582944	20.9535841	17.5002728	4118	H	H ₃₅	-2.5761541	22.4685864	5.4021996
4066	H	H ₃₃	9.9285072	25.0047828	-6.0319328	4119	H	H ₃₅	-0.0218216	-23.2318599	-0.9684608
4067	H	H ₃₃	3.8599662	-20.9537918	-17.4996543	4120	H	H ₃₅	-2.5764884	-22.4684475	-5.4026136
4068	H	H ₃₃	9.9261887	-25.0053167	6.0335205	4121	H	H ₃₅	2.5974240	-22.4748398	-5.3658781
4069	H	H ₃₃	-13.7870799	-23.8706162	-0.5556791	4122	H	H ₃₂	12.0539340	12.8126250	24.6023339
4070	H	H ₃₄	4.2785393	12.2768497	20.0850733	4123	H	H ₃₂	13.0881215	20.2008503	-18.3128991
4071	H	H ₃₄	13.1991714	17.4127028	-9.7476595	4124	H	H ₃₂	12.0571837	-12.8132736	-24.6004043
4072	H	H ₃₄	4.2810957	-12.2770796	-20.0843906	4125	H	H ₃₂	13.0840919	-20.2015539	18.3149913
4073	H	H ₃₄	13.1966752	-17.4134118	9.7497657	4126	H	H ₃₂	-25.1419362	-16.6578207	-2.2661800
4074	H	H ₃₄	-17.4783676	-16.1548995	2.4419246	4127	H	H ₃₃	-22.8012718	14.6482168	5.3621357
4075	H	H ₃₅	-0.0629535	12.0407392	19.9214168	4128	H	H ₃₃	13.8250637	12.0098378	20.6845992

4129	H	H ₃₃	8.9768120	18.7104524	-18.2361379	4182	H	H ₃₄	10.9327305	-6.8083605	19.8717660
4130	H	H ₃₃	13.8277249	-12.0105828	-20.6823798	4183	H	H ₃₅	-22.0838650	7.1624797	1.2321869
4131	H	H ₃₃	8.9728825	-18.7109348	18.2375723	4184	H	H ₃₅	11.0412990	3.9169833	20.0814126
4132	H	H ₃₃	-22.8012114	-14.6469894	-5.3657893	4185	H	H ₃₅	-22.0840455	-7.1612921	-1.2357185
4133	H	H ₃₄	-20.8314836	6.6667957	9.3373239	4186	H	H ₃₅	11.0443089	-3.9175783	-20.0796393
4134	H	H ₃₄	17.4054559	5.6594584	15.1856161	4187	H	H ₃₅	11.0394583	-10.4072763	17.6163405
4135	H	H ₃₄	3.4263354	11.7813073	-20.3726140	4188	H	H ₃₂	-17.1656035	-2.5501986	24.6572283
4136	H	H ₃₄	17.4075866	-5.6603954	-15.1828268	4189	H	H ₃₂	30.0017444	1.2212778	2.7466817
4137	H	H ₃₄	3.4224467	-11.7814918	20.3731638	4190	H	H ₃₂	-17.1615181	2.5511225	-24.6599781
4138	H	H ₃₄	-20.8303410	-6.6656741	-9.3406628	4191	H	H ₃₂	30.0021178	-1.2228927	-2.7418752
4139	H	H ₃₅	-22.0094252	4.6287142	5.7042909	4192	H	H ₃₂	-12.8406645	-6.2655069	26.5518572
4140	H	H ₃₅	15.1931562	2.6251351	17.3394200	4193	H	H ₃₃	-17.9294538	-0.9052787	20.7336716
4141	H	H ₃₅	6.8164885	9.0930606	-20.2294538	4194	H	H ₃₃	26.7933507	1.6989215	5.6035376
4142	H	H ₃₅	15.1957939	-2.6259519	-17.3369921	4195	H	H ₃₃	-17.9260787	0.9062428	-20.7365386
4143	H	H ₃₅	6.8127581	-9.0934261	20.2305377	4196	H	H ₃₃	26.7941573	-1.7003623	-5.5992530
4144	H	H ₃₅	-22.0087615	-4.6275291	-5.7078197	4197	H	H ₃₃	-8.8681804	-6.9677447	24.9995178
4145	H	H ₃₂	15.6031085	7.1786779	-24.6394049	4198	H	H ₃₄	-17.2103832	6.2570420	15.1710446
4146	H	H ₃₂	-29.8852661	2.9822098	-0.2603851	4199	H	H ₃₄	20.6340222	7.2625823	9.3273911
4147	H	H ₃₂	14.2822699	-1.6035459	26.3730125	4200	H	H ₃₄	-17.2082869	-6.2561168	-15.1737952
4148	H	H ₃₂	-29.8854657	-2.9806023	0.2556034	4201	H	H ₃₄	20.6351282	-7.2636918	-9.3240917
4149	H	H ₃₂	14.2865826	1.6027779	-26.3707289	4202	H	H ₃₄	-3.4271804	-12.3202646	20.0492886
4150	H	H ₃₂	15.5987707	-7.1795174	24.6419031	4203	H	H ₃₅	-13.6941947	7.4309444	17.2865401
4151	H	H ₃₃	15.2391018	9.1482396	-20.8213801	4204	H	H ₃₅	20.5089916	9.4330597	5.6544706
4152	H	H ₃₃	-26.7340342	5.7707748	-1.1998801	4205	H	H ₃₅	-13.6918261	-7.4302074	-17.2887336
4153	H	H ₃₃	11.4951450	1.2920721	24.8121429	4206	H	H ₃₅	20.5093890	-9.4341635	-5.6511854
4154	H	H ₃₃	-26.7345382	-5.7693368	1.1956027	4207	H	H ₃₅	-6.8179608	-13.4573227	17.7197700
4155	H	H ₃₃	11.4990537	-1.2926907	-24.8103022	4208	H	H ₃₂	-22.5660185	9.3893087	17.7000803
4156	H	H ₃₃	15.2352717	-9.1490591	20.8238169	4209	H	H ₃₂	25.0101329	10.1068496	13.5285549
4157	H	H ₃₄	10.4693931	14.7290460	-15.5365789	4210	H	H ₃₂	-22.5636892	-9.3880955	-17.7036873
4158	H	H ₃₄	-20.6586449	11.7350897	1.8564518	4211	H	H ₃₂	25.0117616	-10.1081951	-13.5245522
4159	H	H ₃₄	10.1897127	8.6581556	19.7267418	4212	H	H ₃₂	-2.4485479	-16.7384749	24.9901025
4160	H	H ₃₄	-20.6589763	-11.7339778	-1.8597611	4213	H	H ₃₃	-18.2780152	10.3201820	17.6414752
4161	H	H ₃₄	10.1924040	-8.6587037	-19.7251114	4214	H	H ₃₃	22.6793572	11.6129614	10.1291309
4162	H	H ₃₄	10.4661113	-14.7296098	15.5382579	4215	H	H ₃₃	-18.2757406	-10.3191988	-17.6444000
4163	H	H ₃₅	-20.4516091	9.5891734	5.6266469	4216	H	H ₃₃	22.6803627	-11.6141820	-10.1254984
4164	H	H ₃₅	13.6192157	7.5808606	17.2895109	4217	H	H ₃₃	-4.4051242	-16.9843856	21.0698640
4165	H	H ₃₅	-20.4512234	-9.5880735	-5.6299181	4218	H	H ₃₄	-9.8994575	8.1977698	20.0920010
4166	H	H ₃₅	13.6215750	-7.5815946	-17.2873233	4219	H	H ₃₄	20.8933521	11.4280089	1.3265272
4167	H	H ₃₅	6.8292397	-13.5913638	17.6214651	4220	H	H ₃₄	-9.8966823	-8.1972371	-20.0935862
4168	H	H ₃₂	-26.0889703	6.9680226	13.4451044	4221	H	H ₃₄	20.8929501	-11.4291335	-1.3231797
4169	H	H ₃₂	23.4958248	6.2052874	17.8717390	4222	H	H ₃₄	-10.9967135	-14.3369701	15.5696749
4170	H	H ₃₂	-26.0871895	-6.9666186	-13.4492825	4223	H	H ₃₅	-11.0598474	3.9857093	19.9945116
4171	H	H ₃₂	23.4983518	-6.2065517	-17.8679775	4224	H	H ₃₅	22.0091511	7.2028478	1.3049599
4172	H	H ₃₂	2.5884828	-13.8723593	26.6611318	4225	H	H ₃₅	-11.0568577	-3.9851137	-19.9962855
4173	H	H ₃₃	-25.0658832	4.3041478	10.2971641	4226	H	H ₃₅	22.0089736	-7.2040308	-1.3014436
4174	H	H ₃₃	20.6889595	3.0172935	17.7684822	4227	H	H ₃₅	-10.9523950	-10.4528064	17.5718661
4175	H	H ₃₃	-25.0644721	-4.3027993	-10.3011758	4228	H	H ₄₂	-14.2993104	-2.8346107	17.0777398
4176	H	H ₃₃	20.6916483	-3.0184078	-17.7651640	4229	H	H ₄₂	22.1414873	-0.5305352	3.6915380
4177	H	H ₃₃	4.3725915	-10.3837431	25.0182753	4230	H	H ₄₂	-14.2964232	2.8353795	-17.0800260
4178	H	H ₃₄	-23.4268168	3.1376546	1.4508034	4231	H	H ₄₂	22.1421053	0.5293423	-3.6879846
4179	H	H ₃₄	12.4906678	-0.0765778	20.1182162	4232	H	H ₄₂	-7.8456911	-3.6714904	20.7152065
4180	H	H ₃₄	-23.4267489	-3.1363933	-1.4545587	4233	H	H ₄₂	-7.6032417	13.0104300	16.8658601
4181	H	H ₃₄	12.4938939	0.0759072	-20.1162257	4234	H	H ₄₂	16.2847771	15.5612038	2.0476458

4235	H	H ₄₂	-7.6012418	-13.0100205	-16.8670796	4288	N	N ₅₂	-4.2482931	-19.4060878	-13.0157694
4236	H	H ₄₂	16.2842712	-15.5620791	-2.0450442	4289	N	N ₅₂	10.3809150	-21.2085993	-2.5468381
4237	H	H ₄₂	-8.6836329	-17.7954399	10.9295310	4290	N	N ₅₂	-6.1334496	-22.4567309	4.7043022
4238	H	H ₄₂	3.9811448	8.3609082	20.4608337	4291	N	N ₅₂	-4.0714096	8.2631599	21.9433335
4239	H	H ₄₂	14.2438755	13.7163803	-10.6476776	4292	N	N ₅₂	19.5497808	12.8113180	-4.4768419
4240	H	H ₄₂	3.9839697	-8.3611220	-20.4601989	4293	N	N ₅₂	-4.0683426	-8.2629417	-21.9439808
4241	H	H ₄₂	14.2414301	-13.7171474	10.6499619	4294	N	N ₅₂	19.5483792	-12.8123701	4.4799729
4242	H	H ₄₂	-18.2258542	-12.5459393	3.8493717	4295	N	N ₅₂	-15.4804970	-14.0074215	11.4242035
4243	H	H ₄₂	3.4162663	18.3739619	12.5431443	4296	N	N ₅₂	8.2721172	14.1362239	17.5121554
4244	H	H ₄₂	6.2977266	21.2283724	-4.0371692	4297	N	N ₅₂	8.7332951	19.1333835	-11.5143195
4245	H	H ₄₂	3.4172879	-18.3741452	-12.5426003	4298	N	N ₅₂	8.2741637	-14.1366692	-17.5108298
4246	H	H ₄₂	6.2959338	-21.2287114	4.0381779	4299	N	N ₅₂	8.7304204	-19.1338530	11.5157154
4247	H	H ₄₂	-9.7140068	-20.2242095	-1.7953389	4300	N	N ₅₂	-17.0052398	-16.7019757	-2.6080954
4248	H	H ₄₂	7.4074861	20.8782744	3.2068872	4301	N	N ₅₂	4.1834320	20.6316609	10.8252845
4249	H	H ₄₂	-4.0340444	21.8695943	-2.5504094	4302	N	N ₅₂	4.1163173	23.0704957	-3.3408958
4250	H	H ₄₂	-3.3726137	19.6928664	10.0932550	4303	N	N ₅₂	-8.2988843	21.8413753	3.7995042
4251	H	H ₄₂	-4.0356374	-21.8693770	2.5497621	4304	N	N ₅₂	4.1145393	-23.0707168	3.3415530
4252	H	H ₄₂	-3.3720627	-19.6926853	-10.0937929	4305	N	N ₅₂	-8.2994471	-21.8409275	-3.8008399
4253	H	H ₄₂	7.4068720	-20.8786729	-3.2057019	4306	N	N ₅₂	4.1840527	-20.6318846	-10.8246231
4254	H	H ₄₂	-19.4720358	3.2039191	10.3278446	4307	N	N ₅₂	-23.2289313	-0.9569112	4.2588463
4255	H	H ₄₂	18.0798585	2.7942920	12.7043375	4308	N	N ₅₂	15.3898587	-3.2610284	17.6395693
4256	H	H ₄₂	1.3923677	8.5166686	-20.5333164	4309	N	N ₅₂	7.8390553	3.5652325	-22.0107900
4257	H	H ₄₂	18.0817376	-2.7952647	-12.7014438	4310	N	N ₅₂	15.3928633	3.2601999	-17.6371030
4258	H	H ₄₂	1.3886215	-8.5167443	20.5335445	4311	N	N ₅₂	7.8353458	-3.5656544	22.0120459
4259	H	H ₄₂	-19.4705496	-3.2028707	-10.3309661	4312	N	N ₅₂	-23.2281919	0.9581616	-4.2625684
4260	H	H ₄₂	-17.6523151	13.6337206	3.4195880	4313	N	N ₅₂	-18.1995527	10.7264280	10.9706775
4261	H	H ₄₂	9.7417016	11.3086162	16.9230726	4314	N	N ₅₂	16.8871034	10.3402029	13.2114251
4262	H	H ₄₂	-17.6524953	-13.6327715	-3.4224097	4315	N	N ₅₂	-18.1983730	-10.7254480	-10.9735954
4263	H	H ₄₂	9.7438051	-11.3091392	-16.9215198	4316	N	N ₅₂	16.8886598	-10.3411121	-13.2087185
4264	H	H ₄₂	7.9081464	-16.4965132	13.2099365	4317	N	N ₅₂	1.3092308	-15.6887280	17.8545644
4265	H	H ₄₂	13.4091753	5.5381664	-17.0417183	4318	N	N ₅₂	14.6673098	12.8056942	-13.5523326
4266	H	H ₄₂	-22.0628676	2.9955826	-2.2701935	4319	N	N ₅₂	-20.7815350	11.0093119	-3.1151865
4267	H	H ₄₂	8.6537918	-0.9452839	20.6183336	4320	N	N ₅₂	6.1146256	6.6988012	21.9207423
4268	H	H ₄₂	-22.0633905	-2.9943954	2.2666610	4321	N	N ₅₂	-20.7826262	-11.0081933	3.1118573
4269	H	H ₄₂	8.6571448	0.9448184	-20.6169492	4322	N	N ₅₂	6.1177751	-6.6991305	-21.9197623
4270	H	H ₄₂	13.4061460	-5.5388881	17.0438665	4323	N	N ₅₂	14.6644506	-12.8064835	13.5546818
4271	H	H ₄₂	-16.1846694	9.2442593	12.7159277	4324	N	N ₅₂	-10.4604206	12.5075210	17.4588873
4272	H	H ₄₂	17.5869359	9.6558191	10.3227728	4325	N	N ₅₂	18.2933796	14.8088702	4.0891074
4273	H	H ₄₂	-16.1831330	-9.2433881	-12.7185211	4326	N	N ₅₂	-10.4582969	-12.5069584	-17.4605610
4274	H	H ₄₂	17.5880695	-9.6567661	-10.3199529	4327	N	N ₅₂	18.2932382	-14.8098545	-4.0861788
4275	H	H ₄₂	-1.4053736	-14.4121343	17.3034674	4328	N	N ₅₂	-7.8355346	-17.8827897	13.7652264
4276	H	H ₄₂	-6.2992003	6.7595031	20.5257335	4329	N	N ₅₂	-8.6327947	-0.9915943	21.9849405
4277	H	H ₄₂	19.6747126	10.6896857	-2.3050560	4330	N	N ₅₂	23.2256287	3.2963010	-2.9241037
4278	H	H ₄₂	-6.2962785	-6.7591624	-20.5267528	4331	N	N ₅₂	-8.6292185	0.9920582	-21.9863189
4279	H	H ₄₂	19.6737644	-10.6907442	2.3082054	4332	N	N ₅₂	23.2249801	-3.2975518	2.9278285
4280	H	H ₄₂	-13.3778745	-12.5405385	13.0554169	4333	N	N ₅₂	-14.5958735	-5.8328831	17.6574053
4281	N	N ₅₂	-19.4297132	2.1270751	13.2638510	4334	N	N ₅₃	-11.7885172	5.1785802	24.3277064
4282	N	N ₅₂	20.7227014	2.5064941	11.0569022	4335	N	N ₅₃	25.8965024	9.3238701	0.2465544
4283	N	N ₅₂	-19.4277042	-2.1260298	-13.2669612	4336	N	N ₅₃	-11.7849023	-5.1779459	-24.3295938
4284	N	N ₅₂	20.7243388	-2.5076094	-11.0535830	4337	N	N ₅₃	25.8960414	-9.3252641	-0.2424046
4285	N	N ₅₂	-1.2968033	-8.2164317	22.1082903	4338	N	N ₅₃	-14.1114973	-12.7878870	19.8735935
4286	N	N ₅₂	-4.2493315	19.4063169	13.0150864	4339	N	N ₅₃	0.8768023	13.2332055	24.3031615
4287	N	N ₅₂	10.3816497	21.2080402	2.5485035	4340	N	N ₅₃	18.3595604	18.8857432	-8.5314316

4341	N	N ₅₃	0.8799811	-13.2332531	-24.3030189	4394	O	O ₅₄	15.0611707	-19.1750053	13.6247427
4342	N	N ₅₃	18.3571798	-18.8867312	8.5343721	4395	O	O ₅₄	-21.9766514	-17.1424443	1.8212571
4343	N	N ₅₃	-19.2378268	-18.6275913	7.0320006	4396	O	O ₅₄	0.6272623	23.1694228	15.5216323
4344	N	N ₅₃	3.5743509	19.4856307	19.3932902	4397	O	O ₅₄	9.5297623	26.1539107	-1.8147058
4345	N	N ₅₃	11.9017785	24.0332445	-7.0225580	4398	O	O ₅₄	0.6285063	-23.1694574	-15.5215268
4346	N	N ₅₃	3.5764092	-19.4858231	-19.3927174	4399	O	O ₅₄	9.5280608	-26.1544238	1.8162338
4347	N	N ₅₃	11.8993598	-24.0338848	7.0244631	4400	O	O ₅₄	-10.1575602	-25.9693811	0.7428973
4348	N	N ₅₃	-15.4766417	-22.9824697	0.9193133	4401	O	O ₅₄	-7.7313187	13.7045865	23.1028074
4349	N	N ₅₃	-4.6305824	18.1904892	20.3131775	4402	O	O ₅₄	21.5698975	17.7707530	-0.5181105
4350	N	N ₅₃	16.9796259	21.8189994	-0.7649890	4403	O	O ₅₄	-7.7283565	-13.7041710	-23.1040426
4351	N	N ₅₃	-4.6283103	-18.1902388	-20.3139261	4404	O	O ₅₄	21.5688605	-17.7719136	0.5215640
4352	N	N ₅₃	16.9783287	-21.8199126	0.7677054	4405	O	O ₅₄	-13.8411801	-20.0424888	13.7130982
4353	N	N ₅₃	-12.3508426	-23.1795549	8.6675423	4406	O	O ₅₄	-0.7583821	24.6932442	12.8106021
4354	N	N ₅₃	-3.6436115	26.1983098	7.7119164	4407	O	O ₅₄	7.6849351	26.7284058	0.9885442
4355	N	N ₅₃	4.5548371	26.4657769	6.1576855	4408	O	O ₅₄	-0.7576537	-24.6932019	-12.8107324
4356	N	N ₅₃	-3.6437854	-26.1981141	-7.7124981	4409	O	O ₅₄	7.6836579	-26.7288187	-0.9873174
4357	N	N ₅₃	4.5544000	-26.4660218	-6.1569576	4410	O	O ₅₄	-6.9270190	-26.9511802	0.3054029
4358	N	N ₅₃	-0.9116671	-27.5366300	0.0621810	4411	O	O ₅₄	10.1324958	11.8639118	23.1476484
4359	N	N ₅₃	-23.8045570	12.6052642	6.2791722	4412	O	O ₅₄	12.9466871	18.6459163	-16.2464337
4360	N	N ₅₃	15.4095053	10.1376508	20.6095321	4413	O	O ₅₄	10.1355599	-11.8644567	-23.1460277
4361	N	N ₅₃	8.3955799	17.1331149	-20.0237000	4414	O	O ₅₄	12.9430816	-18.6466138	16.2485120
4362	N	N ₅₃	15.4122620	-10.1384789	-20.6070711	4415	O	O ₅₄	-23.0792475	-15.6676087	-1.0525543
4363	N	N ₅₃	8.3914487	-17.1335656	20.0250379	4416	O	O ₅₄	13.9001191	5.7350049	-23.2777356
4364	N	N ₅₃	-23.8042290	-12.6039825	-6.2829881	4417	O	O ₅₄	-27.6595260	1.6921133	0.2089227
4365	N	N ₅₃	14.1733427	11.2706650	-20.7465902	4418	O	O ₅₄	13.7594728	-2.3931634	23.9354530
4366	N	N ₅₃	-26.4491337	7.6636991	0.2078833	4419	O	O ₅₄	-27.6595824	-1.6906258	-0.2133460
4367	N	N ₅₃	12.2760991	3.4981882	24.4006666	4420	O	O ₅₄	13.7634402	2.3924234	-23.9332528
4368	N	N ₅₃	-26.4495182	-7.6622745	-0.2121261	4421	O	O ₅₄	13.8960761	-5.7357524	23.2799589
4369	N	N ₅₃	12.2798117	-3.4988481	-24.3987054	4422	O	O ₅₄	-23.4181070	7.1439675	13.0751436
4370	N	N ₅₃	14.1694084	-11.2714268	20.7488549	4423	O	O ₅₄	21.8187947	6.6733391	15.8053821
4371	N	N ₅₃	-25.8902807	4.7288492	8.0734996	4424	O	O ₅₄	-23.4163957	-7.1427070	-13.0788956
4372	N	N ₅₃	19.1409237	2.7448313	19.5944089	4425	O	O ₅₄	21.8209645	-6.6745133	-15.8018878
4373	N	N ₅₃	-25.8892394	-4.7274558	-8.0776461	4426	O	O ₅₄	1.5950720	-13.5554763	24.1683304
4374	N	N ₅₃	19.1439126	-2.7458612	-19.5913451	4427	O	O ₅₄	-14.9150636	-2.8240510	23.1955833
4375	N	N ₅₃	6.7450928	-10.3536186	24.5999258	4428	O	O ₅₄	27.6692317	0.9233990	1.4249456
4376	N	N ₅₃	-18.2395997	1.4844640	20.5178169	4429	O	O ₅₄	-14.9111973	2.8248537	-23.1979722
4377	N	N ₅₃	26.4131200	3.8857666	6.5662367	4430	O	O ₅₄	27.6694097	-0.9248883	-1.4205132
4378	N	N ₅₃	-18.2363979	-1.4834827	-20.5207365	4431	O	O ₅₄	-12.7582572	-5.3062452	24.0320641
4379	N	N ₅₃	26.4139656	-3.8871886	-6.5620031	4432	O	O ₅₄	-21.6062118	8.0377766	15.7392830
4380	N	N ₅₃	-8.1777595	-9.2457644	24.5663903	4433	O	O ₅₄	23.0552974	8.4629650	13.2661350
4381	N	N ₅₃	-16.9802711	9.6704355	19.4628501	4434	O	O ₅₄	-21.6041176	-8.0366150	-15.7427372
4382	N	N ₅₃	23.6804389	11.6387648	8.0265377	4435	O	O ₅₄	23.0569773	-8.4642053	-13.2624453
4383	N	N ₅₃	-16.9776699	-9.6695216	-19.4655700	4436	O	O ₅₄	-1.4532620	-14.8125455	23.6143133
4384	N	N ₅₃	23.6810950	-11.6400386	-8.0227484	4437	C	C ₅₅	-13.2783989	1.5460268	21.5180090
4385	N	N ₅₃	-6.7039230	-16.6287443	20.9569020	4438	C	C ₅₅	24.7771157	4.9245709	1.8905386
4386	O	O ₅₄	-9.5077619	10.8984657	23.8774670	4439	C	C ₅₅	-13.2750329	-1.5453111	-21.5201421
4387	O	O ₅₄	23.5315282	15.0190252	-0.0596825	4440	C	C ₅₅	24.7771508	-4.9259031	-1.8865779
4388	O	O ₅₄	-9.5045203	-10.8979539	-23.8789906	4441	C	C ₅₅	-11.5023137	-8.8264878	20.7730759
4389	O	O ₅₄	23.5307070	-15.0202912	0.0634486	4442	C	C ₅₅	-3.0431915	13.4596592	21.4429031
4390	O	O ₅₄	-14.0267606	-17.8128017	16.2868536	4443	C	C ₅₅	17.8451376	17.8090348	-3.8224183
4391	O	O ₅₄	6.9116934	12.7164279	23.8887952	4444	C	C ₅₅	-3.0404823	-13.4594942	-21.4433980
4392	O	O ₅₄	15.0643890	19.1741947	-13.6223304	4445	C	C ₅₅	17.8435702	-17.8099959	3.8252808
4393	O	O ₅₄	6.9148286	-12.7168002	-23.8876868	4446	C	C ₅₅	-14.8037387	-18.7030064	9.0148990

4447	C	C ₅₅	3.8409077	14.7432297	20.3951171	4500	H	H ₃₇	-10.0512214	5.5747945	27.2773628
4448	C	C ₅₅	13.3202569	19.7860357	-8.8971863	4501	H	H ₃₇	27.4870982	10.6980315	-2.4842696
4449	C	C ₅₅	3.8433844	-14.7434357	-20.3945061	4502	H	H ₃₇	-10.0471469	-5.5742529	-27.2789770
4450	C	C ₅₅	13.3177612	-19.7867523	8.8993185	4503	H	H ₃₇	27.4861258	-10.6995112	2.4886742
4451	C	C ₅₅	-17.1618436	-18.6568602	2.3385645	4504	H	H ₃₇	-17.4393630	-13.6514036	19.6384243
4452	C	C ₅₅	-0.9638552	18.7500985	17.2250337	4505	H	H ₃₈	-14.1112689	-2.0359695	21.0649683
4453	C	C ₅₅	12.4283922	22.1187901	-2.3433272	4506	H	H ₃₈	25.3331314	1.2612263	1.9099113
4454	C	C ₅₅	-0.9621045	-18.7500467	-17.2251877	4507	H	H ₃₈	-14.1077885	2.0367286	-21.0672266
4455	C	C ₅₅	12.4268260	-22.1194587	2.3453167	4508	H	H ₃₈	25.3333718	-1.2625900	-1.9058520
4456	C	C ₅₅	-11.4655517	-22.4018019	3.9871531	4509	H	H ₃₈	-11.2256441	-5.4079007	22.1753354
4457	C	C ₅₅	2.9968358	25.1400652	1.5780877	4510	H	H ₃₉	-13.7528729	2.5844417	15.1919139
4458	C	C ₅₅	-3.8449713	24.8907251	3.0269227	4511	H	H ₃₉	19.4626385	4.2618782	5.4458455
4459	C	C ₅₅	0.8491070	24.0100943	8.1417861	4512	H	H ₃₉	-13.7505827	-2.5837021	-15.1941138
4460	C	C ₅₅	-3.8458303	-24.8905181	-3.0275394	4513	H	H ₃₉	19.4632852	-4.2629260	-5.4427261
4461	C	C ₅₅	0.8491202	-24.0101408	-8.1416460	4514	H	H ₃₉	-5.7129014	-8.3033979	18.0286283
4462	C	C ₅₅	2.9957385	-25.1402259	-1.5776110	4515	H	H ₃₆	4.7349274	15.8037792	26.7833390
4463	C	C ₅₅	-22.4319470	8.4391872	8.3980792	4516	H	H ₃₆	18.1696116	22.5342931	-12.3124652
4464	C	C ₅₅	17.1436804	6.8845732	17.4251745	4517	H	H ₃₆	4.7383602	-15.8040348	-26.7825760
4465	C	C ₅₅	5.2886445	13.4767218	-20.8649946	4518	H	H ₃₆	18.1664337	-22.5352714	12.3153780
4466	C	C ₅₅	17.1460989	-6.8854959	-17.4224289	4519	H	H ₃₆	-22.9055744	-21.1422329	4.2269223
4467	C	C ₅₅	5.2845780	-13.4770066	20.8658427	4520	H	H ₃₇	1.6430623	11.8651037	27.3702856
4468	C	C ₅₅	-22.4310549	-8.4379799	-8.4016729	4521	H	H ₃₇	20.7951301	18.4585315	-10.9296774
4469	C	C ₅₅	11.4957081	14.0168962	-17.7410560	4522	H	H ₃₇	1.6468043	-11.8651929	-27.3700183
4470	C	C ₅₅	-22.9486328	10.6516388	1.8089622	4523	H	H ₃₇	20.7923907	-18.4596507	10.9330083
4471	C	C ₅₅	11.4533525	7.2730571	21.4311280	4524	H	H ₃₇	-22.4398289	-17.9750995	8.1217455
4472	C	C ₅₅	-22.9489245	-10.6504040	-1.8126361	4525	H	H ₃₈	-6.7214274	13.1641201	20.8282255
4473	C	C ₅₅	11.4563901	-7.2736738	-21.4292918	4526	H	H ₃₈	19.2030644	16.8315782	-0.4765023
4474	C	C ₅₅	11.4921065	-14.0175143	17.7428939	4527	H	H ₃₈	-6.7187995	-13.1637578	-20.8293057
4475	C	C ₅₅	-24.7317561	4.0582094	3.4296573	4528	H	H ₃₈	19.2020782	-16.8326119	0.4795793
4476	C	C ₅₅	14.6967926	1.1087494	20.5588486	4529	H	H ₃₈	-12.4839191	-18.8065639	11.9478676
4477	C	C ₅₅	-24.7314233	-4.0568784	-3.4336179	4530	H	H ₃₉	-2.1152138	14.0399522	15.0679585
4478	C	C ₅₅	14.7000248	-1.1095402	-20.5564960	4531	H	H ₃₉	11.8550501	16.9018459	-1.5566669
4479	C	C ₅₅	10.0312208	-8.3771600	21.6584665	4532	H	H ₃₉	-2.1135518	-14.0398378	-15.0683002
4480	C	C ₅₅	-17.7447537	5.1494371	17.3407812	4533	H	H ₃₉	11.8538860	-16.9024835	1.5585634
4481	C	C ₅₅	22.9157411	6.6684327	8.5144626	4534	H	H ₃₉	-9.7409703	-17.5232453	5.1659588
4482	C	C ₅₅	-17.7422432	-5.1484825	-17.3436211	4535	H	H ₃₆	1.3279768	24.0924253	20.1755057
4483	C	C ₅₅	22.9167506	-6.6696652	-8.5107970	4536	H	H ₃₆	13.0157722	28.3071907	-4.3072192
4484	C	C ₅₅	-5.1748099	-11.8831010	21.7740426	4537	H	H ₃₆	1.3299017	-24.0924967	-20.1752936
4485	C	C ₅₅	-12.3769691	8.4973961	20.5020475	4538	H	H ₃₆	13.0135543	-28.3078918	4.3093074
4486	C	C ₅₅	22.4380532	11.4534619	3.3288263	4539	H	H ₃₆	-14.3445187	-27.9166263	2.0386931
4487	C	C ₅₅	-12.3741383	-8.4967293	-20.5040337	4540	H	H ₃₇	5.7668909	21.9109535	19.2780076
4488	C	C ₅₅	22.4379637	-11.4546692	-3.3252343	4541	H	H ₃₇	10.3508044	26.6471301	-8.2328388
4489	C	C ₅₅	-10.0642853	-15.0905349	17.7964877	4542	H	H ₃₇	5.7687960	-21.9112646	-19.2770798
4490	Cu	Cu ₄₈	-3.2803976	20.8951861	12.2960350	4543	H	H ₃₇	10.3480567	-26.6476872	8.2344971
4491	Cu	Cu ₄₈	9.0647620	22.5946757	2.4234598	4544	H	H ₃₇	-16.1178174	-24.9520087	-1.6129825
4492	Cu	Cu ₄₈	-3.2795556	-20.8950083	-12.2965678	4545	H	H ₃₈	5.5706711	11.7504453	22.0284323
4493	Cu	Cu ₄₈	9.0639338	-22.5951631	-2.4220104	4546	H	H ₃₈	14.2890384	17.5862908	-11.8702526
4494	Cu	Cu ₄₈	-5.7852530	-23.5586332	3.1755217	4547	H	H ₃₈	5.5735732	-11.7507456	-22.0275373
4495	H	H ₃₆	-12.8752094	9.7593261	27.0194494	4548	H	H ₃₈	14.2861896	-17.5870586	11.8725341
4496	H	H ₃₆	28.0642009	14.2222087	1.0932846	4549	H	H ₃₈	-19.8603571	-15.9486902	2.3585306
4497	H	H ₃₆	-12.8714045	-9.7586339	-27.0215076	4550	H	H ₃₉	-0.4470324	10.6368424	17.7713205
4498	H	H ₃₆	28.0636119	-14.2237183	-1.0887939	4551	H	H ₃₉	13.8281712	14.5688022	-5.0689007
4499	H	H ₃₆	-15.1927585	-18.0055679	20.8817078	4552	H	H ₃₉	-0.4447664	-10.6368185	-17.7713912

4553	H	H ₃₉	13.8265710	-14.5695466	5.0711166	4606	H	H ₃₇	15.2512435	-13.6652937	-20.1095221
4554	H	H ₃₉	-13.3823370	-14.6998484	5.8300602	4607	H	H ₃₇	7.5290464	-20.3596523	18.7758352
4555	H	H ₃₆	-6.4808373	17.5977373	25.4512005	4608	H	H ₃₇	-22.7809498	-15.8773955	-7.2574360
4556	H	H ₃₆	22.3769957	22.2685271	-1.6816909	4609	H	H ₃₈	-21.9866111	6.2187373	11.4130123
4557	H	H ₃₆	-6.4777071	-17.5973882	-25.4522407	4610	H	H ₃₈	19.8203837	5.5815665	15.1108879
4558	H	H ₃₆	22.3755248	-22.2697314	1.6852750	4611	H	H ₃₈	2.1665402	12.0429154	-22.4190780
4559	H	H ₃₆	-15.8986581	-24.1727316	12.7419361	4612	H	H ₃₈	19.8225088	-5.5826325	-15.1077175
4560	H	H ₃₇	-7.6051074	19.7757649	20.8586465	4613	H	H ₃₈	2.1622951	-12.0430315	22.4194220
4561	H	H ₃₇	18.6995247	23.0355143	1.9221011	4614	H	H ₃₈	-21.9851167	-6.2175552	-11.4165266
4562	H	H ₃₇	-7.6028305	-19.7753559	-20.8598631	4615	H	H ₃₉	-19.6893355	3.9808231	4.7042382
4563	H	H ₃₇	18.6985934	-23.0365205	-1.9191072	4616	H	H ₃₉	13.2747688	2.0953521	15.6536487
4564	H	H ₃₇	-11.0966564	-25.2702583	11.0580256	4617	H	H ₃₉	6.4147498	7.8814621	-17.9549555
4565	H	H ₃₈	0.9602142	20.7593250	14.7024917	4618	H	H ₃₉	13.2771671	-2.0960662	-15.6515247
4566	H	H ₃₈	9.0182539	23.6913685	-2.3291539	4619	H	H ₃₉	6.4114458	-7.8818069	17.9559801
4567	H	H ₃₈	0.9614489	-20.7593771	-14.7023359	4620	H	H ₃₉	-19.6887961	-3.9797643	-4.7073867
4568	H	H ₃₈	9.0166087	-23.6918541	2.3305997	4621	H	H ₃₆	-30.9842729	4.9280990	0.9740400
4569	H	H ₃₈	-9.9789481	-23.4089882	0.6889963	4622	H	H ₃₆	15.5994494	0.4064079	27.2351283
4570	H	H ₃₉	2.5229284	13.6038464	15.5603061	4623	H	H ₃₆	-30.9843836	-4.9264319	-0.9790004
4571	H	H ₃₉	10.0202496	17.2896301	-5.8494626	4624	H	H ₃₆	15.6037918	-0.4072477	-27.2326288
4572	H	H ₃₉	2.5246940	-13.6039825	-15.5599005	4625	H	H ₃₆	15.3803970	-9.5124471	25.6557366
4573	H	H ₃₉	10.0183892	-17.2901692	5.8510667	4626	H	H ₃₇	17.2892892	10.8530454	-20.9364684
4574	H	H ₃₉	-12.5436971	-16.5479028	1.5412675	4627	H	H ₃₇	-28.1078182	7.6743850	-2.4694806
4575	H	H ₃₆	-1.6501347	29.2351135	11.7935835	4628	H	H ₃₇	10.8188061	2.5932012	27.0420535
4576	H	H ₃₆	6.5955474	30.6880585	3.3533964	4629	H	H ₃₇	-28.1086258	-7.6728719	2.4649765
4577	H	H ₃₆	-1.6498124	-29.2350240	-11.7938518	4630	H	H ₃₇	10.8229950	-2.5937837	-27.0403197
4578	H	H ₃₆	6.5944395	-30.6884122	-3.3523476	4631	H	H ₃₇	17.2853536	-10.8539760	20.9392388
4579	H	H ₃₆	-4.9458089	-31.1729718	-0.5368608	4632	H	H ₃₈	11.2903441	16.9438482	-15.4063967
4580	H	H ₃₇	-5.9739132	27.1408410	10.0868818	4633	H	H ₃₈	-21.2833988	14.0075511	1.6518252
4581	H	H ₃₇	7.6084893	27.6207951	7.2979913	4634	H	H ₃₈	9.9935924	10.6893686	20.9233949
4582	H	H ₃₇	-5.9737630	-27.1405199	-10.0878363	4635	H	H ₃₈	-21.2838847	-14.0064053	-1.6552360
4583	H	H ₃₇	7.6081671	-27.6212042	-7.2967747	4636	H	H ₃₈	9.9963734	-10.6899071	-20.9217907
4584	H	H ₃₇	-1.6355169	-29.3764571	2.8994702	4637	H	H ₃₈	11.2869735	-16.9444555	15.4082034
4585	H	H ₃₈	6.7084764	24.5480085	1.6247398	4638	H	H ₃₉	-18.1058584	8.4527805	5.3707117
4586	H	H ₃₈	-5.5739959	24.8813620	-0.3106368	4639	H	H ₃₉	12.3948546	6.7740601	15.1193813
4587	H	H ₃₈	-1.1335276	22.9100129	11.1397789	4640	H	H ₃₉	-18.1054502	-8.4518072	-5.3736049
4588	H	H ₃₈	-5.5753923	-24.8810631	0.3097507	4641	H	H ₃₉	12.3969156	-6.7747263	-15.1174015
4589	H	H ₃₈	-1.1329803	-22.9099531	-11.1399535	4642	H	H ₃₉	5.7081761	-12.0951634	15.7873335
4590	H	H ₃₈	6.7074097	-24.5483701	-1.6236619	4643	H	H ₃₆	-28.0138017	7.6917276	11.8675771
4591	H	H ₃₉	2.1310589	19.9246155	5.1870551	4644	H	H ₃₆	23.0055415	6.2192528	20.4166871
4592	H	H ₃₉	0.4342866	20.6783484	0.8090606	4645	H	H ₃₆	-28.0123154	-7.6902203	-11.8720620
4593	H	H ₃₉	-2.5645497	20.0522196	4.4462135	4646	H	H ₃₆	23.0084781	-6.2204910	-20.4130024
4594	H	H ₃₉	0.4333015	-20.6783706	-0.8089978	4647	H	H ₃₆	5.0034650	-14.4520602	27.4021612
4595	H	H ₃₉	-2.5649217	-20.0520824	-4.4466193	4648	H	H ₃₇	-27.5047574	2.9460970	10.6931464
4596	H	H ₃₉	2.1308242	-19.9247305	-5.1867119	4649	H	H ₃₇	22.4458705	1.4587959	19.3284577
4597	H	H ₃₆	-27.2229139	15.6236762	3.3902252	4650	H	H ₃₇	-27.5032017	-2.9446168	-10.6975509
4598	H	H ₃₆	14.2095868	11.7988699	25.6037898	4651	H	H ₃₇	22.4488870	-1.4600037	-19.3248639
4599	H	H ₃₆	13.0139417	19.7988029	-20.8644312	4652	H	H ₃₇	5.0541317	-9.5419890	27.6213821
4600	H	H ₃₆	14.2130545	-11.7996348	-25.6015129	4653	H	H ₃₈	12.7916753	5.9142509	-21.0495119
4601	H	H ₃₆	13.0095290	-19.7995042	20.8665213	4654	H	H ₃₈	-25.2299087	2.2595565	0.1819990
4602	H	H ₃₆	-27.2232083	-15.6222129	-3.3945751	4655	H	H ₃₈	12.4383296	-1.4999385	22.0164839
4603	H	H ₃₇	-22.7812614	15.8786207	7.2537924	4656	H	H ₃₈	-25.2300089	-2.2581989	-0.1860384
4604	H	H ₃₇	15.2487608	13.6644725	20.1119671	4657	H	H ₃₈	12.4419327	1.4992687	-22.0144901
4605	H	H ₃₇	7.5331504	20.3592454	-18.7746194	4658	H	H ₃₈	12.7879799	-5.9149388	21.0515577

4659	H	H ₃₉	-19.4984034	6.9057741	1.2087905	4712	H	H ₃₇	26.0610896	-10.6584489	3.1660254
4660	H	H ₃₉	9.7663235	4.0454313	17.8211114	4713	H	H ₃₇	-17.2989147	-13.2328668	18.1230628
4661	H	H ₃₉	-19.4985805	-6.9047243	-1.2119156	4714	H	H ₃₈	-15.5452478	-1.5094072	20.6813268
4662	H	H ₃₉	9.7689575	-4.0459571	-17.8195464	4715	H	H ₃₈	25.6453342	1.4581130	3.4410862
4663	H	H ₃₉	9.7293510	-9.7758774	15.4632007	4716	H	H ₃₈	-15.5418535	1.5102438	-20.6838170
4664	H	H ₃₆	-18.3352737	-0.3571714	25.4719146	4717	H	H ₃₈	25.6458054	-1.4594932	-3.4369789
4665	H	H ₃₆	30.9597119	3.3520475	3.9228340	4718	H	H ₃₈	-10.1040304	-6.0262345	23.0920633
4666	H	H ₃₆	-18.3311762	0.3581590	-25.4748564	4719	H	H ₃₉	-13.2579105	3.2879035	16.5147746
4667	H	H ₃₆	30.9601550	-3.3537144	-3.9178714	4720	H	H ₃₉	20.2408364	5.3394663	4.5955394
4668	H	H ₃₆	-12.6291329	-8.7400309	27.3723424	4721	H	H ₃₉	-13.2554466	-3.2871904	-16.5168961
4669	H	H ₃₇	-20.7006817	-1.0625345	21.1487400	4722	H	H ₃₉	20.2412797	-5.3405552	-4.5922997
4670	H	H ₃₇	28.5563290	1.2453169	7.7396282	4723	H	H ₃₉	-6.9860762	-9.2354951	18.0338751
4671	H	H ₃₇	-20.6972328	1.0636499	-21.1520634	4724	H	H ₃₆	6.2818598	16.0522728	26.9948110
4672	H	H ₃₇	28.5575053	-1.2468533	-7.7350577	4725	H	H ₃₆	17.5401305	23.0524180	-13.6670038
4673	H	H ₃₇	-7.8603574	-7.3285693	27.5938990	4726	H	H ₃₆	6.2853139	-16.0526104	-26.9938081
4674	H	H ₃₈	-19.1831000	7.5547182	14.9146114	4727	H	H ₃₆	17.5366917	-23.0533621	13.6698141
4675	H	H ₃₈	21.2108841	8.1500211	11.4536634	4728	H	H ₃₆	-23.8228058	-21.2057233	2.9407944
4676	H	H ₃₈	-19.1811207	-7.5536858	-14.9176839	4729	H	H ₃₇	1.9676042	10.5252041	26.6017605
4677	H	H ₃₈	21.2122807	-8.1511632	-11.4502634	4730	H	H ₃₇	20.1737935	17.0314378	-11.1916560
4678	H	H ₃₈	-2.0315471	-13.7874854	21.2905798	4731	H	H ₃₇	1.9712980	-10.5253103	-26.6014438
4679	H	H ₃₉	-11.8580308	6.8939698	15.4632537	4732	H	H ₃₇	20.1710941	-17.0325242	11.1948912
4680	H	H ₃₉	18.1136723	8.7318289	4.7856037	4733	H	H ₃₇	-22.1429610	-16.4526325	7.8297645
4681	H	H ₃₉	-11.8559276	-6.8933318	-15.4651517	4734	H	H ₃₈	-6.6111687	14.6707651	20.4037173
4682	H	H ₃₉	18.1139706	-8.7328040	-4.7827009	4735	H	H ₃₈	18.5642758	18.1829075	0.0012117
4683	H	H ₃₉	-6.2584084	-12.2164975	15.4544958	4736	H	H ₃₈	-6.6086873	-14.6704098	-20.4047737
4684	H	H ₃₆	-22.2084322	9.1573233	20.2471156	4737	H	H ₃₈	18.5632926	-18.1839074	0.0017663
4685	H	H ₃₆	27.0392511	10.5762093	12.0016381	4738	H	H ₃₈	-11.9553056	-20.1255111	11.2820678
4686	H	H ₃₆	-22.2056823	-9.1561287	-20.2506691	4739	H	H ₃₉	-1.3016703	13.8535692	16.4083233
4687	H	H ₃₆	27.0406065	-10.5776643	-11.9973087	4740	H	H ₃₉	12.6196258	17.1792159	-2.9100481
4688	H	H ₃₆	-4.8354076	-17.1026808	25.9062514	4741	H	H ₃₉	-1.2997893	-13.8534993	-16.4085314
4689	H	H ₃₇	-18.4465802	12.6464555	19.0345586	4742	H	H ₃₉	12.6182359	-17.1798952	2.9120702
4690	H	H ₃₇	23.6108380	14.1633953	10.2200755	4743	H	H ₃₉	-11.3190843	-17.5614897	5.1304199
4691	H	H ₃₇	-18.4442111	-12.6454637	-19.0375078	4744	H	H ₃₆	0.5340518	25.3399322	19.6192239
4692	H	H ₃₇	23.6117161	-14.1646654	-10.2162972	4745	H	H ₃₆	12.7546861	29.2446527	-3.0626189
4693	H	H ₃₇	-5.1681139	-19.5843456	21.2665838	4746	H	H ₃₆	0.5358253	-25.3399607	-19.6191398
4694	H	H ₃₈	-9.1525470	9.1714269	22.2233396	4747	H	H ₃₆	12.7526226	-29.2453400	3.0646666
4695	H	H ₃₈	22.1958940	13.0039118	-0.0403746	4748	H	H ₃₆	-13.2895460	-29.0874385	2.1494674
4696	H	H ₃₈	-9.1494779	-9.1709339	-22.2248080	4749	H	H ₃₇	5.9889103	21.6199262	17.7438784
4697	H	H ₃₈	22.1951832	-13.0051061	0.0439280	4750	H	H ₃₇	8.9732098	26.0165446	-7.7944922
4698	H	H ₃₈	-13.0462023	-15.6933188	15.6613333	4751	H	H ₃₇	5.9905835	-21.6202499	-17.7429112
4699	H	H ₃₉	-9.8103294	3.2092550	17.8317602	4752	H	H ₃₇	8.9705570	-26.0170281	7.7959330
4700	H	H ₃₉	19.6526146	6.1011327	1.0317899	4753	H	H ₃₇	-14.9620976	-24.2562080	-2.4301208
4701	H	H ₃₉	-9.8076514	-3.2087271	-17.8333316	4754	H	H ₃₈	4.2537644	11.5939609	22.8724746
4702	H	H ₃₉	19.6524535	-6.1021911	-1.0286377	4755	H	H ₃₈	15.6908556	17.4547224	-11.1711441
4703	H	H ₃₉	-9.8450422	-8.9839141	15.7123514	4756	H	H ₃₈	4.2568082	-11.5941892	-22.8717972
4704	H	H ₃₆	-12.6330979	11.3187125	27.1318976	4757	H	H ₃₈	15.6881346	-17.4555658	11.1736514
4705	H	H ₃₆	27.8100249	15.7780433	1.2264007	4758	H	H ₃₈	-19.9455230	-16.2041285	3.9072838
4706	H	H ₃₆	-12.6293602	-11.3180329	-27.1339195	4759	H	H ₃₉	-0.0241570	12.1558705	17.6651634
4707	H	H ₃₆	27.8093720	-15.7795397	-1.2219484	4760	H	H ₃₉	13.3029558	16.0577617	-5.0003295
4708	H	H ₃₆	-15.1806232	-19.4902577	20.3353588	4761	H	H ₃₉	-0.0219758	-12.1558700	-17.6651629
4709	H	H ₃₇	-8.7664836	5.5749710	26.3604834	4762	H	H ₃₉	13.3012911	-16.0584763	5.0024526
4710	H	H ₃₇	26.0621726	10.6570461	-3.1618500	4763	H	H ₃₉	-13.2798964	-16.0645411	5.0397063
4711	H	H ₃₇	-8.7625616	-5.5744988	-26.3618900	4764	H	H ₃₆	-7.1764719	16.6175691	26.4781592

4765	H	H ₃₆	23.7452869	21.4860109	-1.8029685	4818	H	H ₃₈	19.8080486	4.3153409	16.0508585
4766	H	H ₃₆	-7.1731211	-16.6171837	-26.4793042	4819	H	H ₃₈	3.1609745	11.0652883	-23.1555333
4767	H	H ₃₆	23.7438515	-21.4872887	1.8067706	4820	H	H ₃₈	19.8103865	-4.3164065	-16.0476886
4768	H	H ₃₆	-16.5715314	-23.5946249	14.0504906	4821	H	H ₃₈	3.1566732	-11.0654571	23.1560323
4769	H	H ₃₇	-8.2685263	18.7670027	19.8453192	4822	H	H ₃₈	-22.9673254	-5.2435221	-10.6591959
4770	H	H ₃₇	18.3145983	21.7186818	2.6982062	4823	H	H ₃₉	-20.1953418	5.4741752	4.6432044
4771	H	H ₃₇	-8.2663656	-18.7665566	-19.8466501	4824	H	H ₃₉	13.2562915	3.4345585	16.4879468
4772	H	H ₃₇	18.3138556	-21.7196668	-2.6952764	4825	H	H ₃₉	6.9392901	9.3693648	-17.9844140
4773	H	H ₃₇	-10.0483418	-24.1484155	11.4144850	4826	H	H ₃₉	13.2587499	-3.4352722	-16.4858226
4774	H	H ₃₈	2.1718529	20.6173859	15.6927235	4827	H	H ₃₉	6.9359049	-9.3697377	17.9855223
4775	H	H ₃₈	9.2784173	23.9819543	-3.8512086	4828	H	H ₃₉	-20.1948947	-5.4730887	-4.6464368
4776	H	H ₃₈	2.1732583	-20.6175039	-15.6923691	4829	H	H ₃₆	-31.6144655	3.4915262	1.1753434
4777	H	H ₃₈	9.2765145	-23.9824528	3.8526899	4830	H	H ₃₆	16.2974077	-1.0102571	27.3206944
4778	H	H ₃₈	-11.4506644	-23.3434587	0.1426163	4831	H	H ₃₆	-31.6144621	-3.4898241	-1.1804110
4779	H	H ₃₉	1.2487164	13.9550043	16.4215411	4832	H	H ₃₆	16.3018322	1.0093799	-27.3180838
4780	H	H ₃₉	11.3408108	17.6543704	-5.0673206	4833	H	H ₃₆	15.3124887	-8.2809731	26.6458213
4781	H	H ₃₉	1.2505996	-13.9550711	-16.4213432	4834	H	H ₃₇	17.3707620	9.4080810	-20.3074892
4782	H	H ₃₉	11.3390449	-17.6549803	5.0691344	4835	H	H ₃₇	-27.3994547	6.4615279	-3.1887649
4783	H	H ₃₉	-12.5902861	-17.2871060	2.9341285	4836	H	H ₃₇	10.0289187	1.3564168	26.4618676
4784	H	H ₃₆	-0.7897463	29.1174460	13.1145577	4837	H	H ₃₇	-27.4003101	-6.4600528	3.1843738
4785	H	H ₃₆	7.3100619	31.0331990	1.9861213	4838	H	H ₃₇	10.0330798	-1.3569565	-26.4602618
4786	H	H ₃₆	-0.7892092	-29.1174020	-13.1146929	4839	H	H ₃₇	17.3670042	-9.4090164	20.3102746
4787	H	H ₃₆	7.3087052	-31.0335911	-1.9849579	4840	H	H ₃₈	-21.6745312	14.0745666	3.1777987
4788	H	H ₃₆	-6.5206906	-31.2652193	-0.6384715	4841	H	H ₃₈	11.4816980	11.0787171	20.5769259
4789	H	H ₃₇	-6.0864331	25.5690755	10.1926781	4842	H	H ₃₈	-21.6747816	-14.0733988	-3.1812774
4790	H	H ₃₇	7.9859544	26.1268938	6.9514688	4843	H	H ₃₈	11.4843967	-11.0793345	-20.5750897
4791	H	H ₃₇	-6.0861798	-25.5687487	-10.1936488	4844	H	H ₃₈	10.1898308	-17.4487195	16.4221396
4792	H	H ₃₇	7.9856667	-26.1273237	-6.9501892	4845	H	H ₃₉	-19.3454797	7.9078184	4.5569652
4793	H	H ₃₇	-1.9005316	-27.9156096	3.4379792	4846	H	H ₃₉	12.4002273	5.8663831	16.4124012
4794	H	H ₃₈	6.5918305	24.8346458	3.1656175	4847	H	H ₃₉	-19.3451713	-7.9067762	-4.5600698
4795	H	H ₃₈	-4.2426912	25.5249243	-0.8430999	4848	H	H ₃₉	12.4025461	-5.8670499	-16.4104187
4796	H	H ₃₈	-2.3481689	23.5878890	10.4081949	4849	H	H ₃₉	6.9423065	-11.5518144	16.6104507
4797	H	H ₃₈	-4.2441942	-25.5246954	0.8424172	4850	H	H ₃₆	-27.7836884	8.5159885	13.1954810
4798	H	H ₃₈	-2.3477769	-23.5877621	-10.4085742	4851	H	H ₃₆	23.9027161	7.3747698	19.8204102
4799	H	H ₃₈	6.5910007	-24.8350016	-3.1645554	4852	H	H ₃₆	-27.7820270	-8.5144938	-13.1999281
4800	H	H ₃₉	1.2937631	20.9688717	4.3507152	4853	H	H ₃₆	23.9055011	-7.3760560	-19.8165833
4801	H	H ₃₉	-0.0142732	21.3447229	2.1676499	4854	H	H ₃₆	3.8761221	-15.5399232	27.6054812
4802	H	H ₃₉	-1.2786596	20.9646309	4.3755440	4855	H	H ₃₇	-26.0481233	2.3389902	10.7745203
4803	H	H ₃₉	-0.0150675	-21.3447221	-2.1676527	4856	H	H ₃₇	21.8761922	1.1123666	17.8958182
4804	H	H ₃₉	-1.2790910	-20.9645611	-4.3757548	4857	H	H ₃₇	-26.0465151	-2.3375886	-10.7786911
4805	H	H ₃₉	1.2933281	-20.9689424	-4.3505016	4858	H	H ₃₇	21.8790035	-1.1135436	-17.8923166
4806	H	H ₃₆	13.0283529	12.1776483	26.5843711	4859	H	H ₃₇	4.1673599	-8.7674593	26.5674737
4807	H	H ₃₆	14.3858184	20.2335641	-20.2092254	4860	H	H ₃₈	13.6531614	7.1945118	-20.7357193
4808	H	H ₃₆	13.0319454	-12.1783494	-26.5822851	4861	H	H ₃₈	-25.5809226	3.6898322	-0.3754900
4809	H	H ₃₆	14.3814879	-20.2343388	20.2115327	4862	H	H ₃₈	11.9279134	-0.3228155	22.9294667
4810	H	H ₃₆	-27.4140826	-16.4041105	-2.0334985	4863	H	H ₃₈	-25.5811873	-3.6884545	0.3713873
4811	H	H ₃₇	-24.3600617	15.9257580	7.3493141	4864	H	H ₃₈	11.9315974	0.3221743	-22.9275612
4812	H	H ₃₇	16.1127620	13.5015243	21.4276029	4865	H	H ₃₈	13.6494476	-7.1952455	20.7378996
4813	H	H ₃₇	8.2479570	20.6602533	-20.1539024	4866	H	H ₃₉	-20.3238091	6.6360040	2.5294066
4814	H	H ₃₇	16.1154653	-13.5023903	-21.4250293	4867	H	H ₃₉	11.3457669	3.9972158	17.8546257
4815	H	H ₃₇	8.2436117	-20.6606979	20.1552281	4868	H	H ₃₉	-20.3237649	-6.6349109	-2.5326581
4816	H	H ₃₇	-24.3597343	-15.9244474	-7.3532133	4869	H	H ₃₉	11.3484075	-3.9978259	-17.8528115
4817	H	H ₃₈	-22.9687475	5.2447595	10.6555101	4870	H	H ₃₉	8.9750783	-9.9702097	16.8384842

4871	H	H ₃₆	-17.7732459	-1.3781603	26.5382611	4924	H	H ₄₃	21.2817894	-2.5232549	-2.4828762
4872	H	H ₃₆	31.7387893	2.7251671	2.6999501	4925	H	H ₄₃	-8.8926343	-6.1636291	18.6648567
4873	H	H ₃₆	-17.7689197	1.3791173	-26.5411104	4926	H	H ₄₀	6.4809382	16.3782869	23.3119790
4874	H	H ₃₆	31.7390760	-2.7268738	-2.6948751	4927	H	H ₄₀	14.2494980	22.4699805	-12.0727489
4875	H	H ₃₆	-13.9702734	-7.9479417	27.6356397	4928	H	H ₄₀	6.4837894	-16.3786346	-23.3109478
4876	H	H ₃₇	-19.8619383	-1.8066734	20.0336446	4929	H	H ₄₀	14.2463543	-22.4707465	12.0750266
4877	H	H ₃₇	27.2945754	0.3769019	7.3465617	4930	H	H ₄₀	-20.7309184	-20.5648665	1.0072216
4878	H	H ₃₇	-19.8586404	1.8077421	-20.0368246	4931	H	H ₄₁	4.4054255	13.1396070	27.8897777
4879	H	H ₃₇	27.2957360	-0.3783720	-7.3421836	4932	H	H ₄₁	19.6700809	20.2142245	-13.2049216
4880	H	H ₃₇	-7.4371584	-6.2136775	26.5553472	4933	H	H ₄₁	4.4091903	-13.1398438	-27.8890741
4881	H	H ₃₈	-18.6113447	8.6596629	15.8783887	4934	H	H ₄₁	19.6668732	-20.2152825	13.2080684
4882	H	H ₃₈	21.5852332	9.5329851	10.8025558	4935	H	H ₄₁	-24.0767494	-18.9189528	5.6815584
4883	H	H ₃₈	-18.6092730	-8.6586615	-15.8813680	4936	H	H ₄₃	-4.3710711	12.0432020	17.5066800
4884	H	H ₃₈	21.5864538	-9.5341475	-10.7990945	4937	H	H ₄₃	15.3577121	15.2714256	-1.2462435
4885	H	H ₃₈	-2.9776165	-15.0024018	20.9656119	4938	H	H ₄₃	-4.3689135	-12.0429664	-17.5073825
4886	H	H ₃₉	-12.4991972	5.7715319	16.3658856	4939	H	H ₄₃	15.3566922	-15.2722506	1.2486943
4887	H	H ₃₉	19.3695260	7.7900109	4.6389446	4940	H	H ₄₃	-10.9883495	-16.5557302	8.7059059
4888	H	H ₃₉	-12.4968825	-5.7708594	-16.3678870	4941	H	H ₄₀	-1.8820441	22.8756663	18.3146410
4889	H	H ₃₉	19.3698562	-7.7910536	-4.6358410	4942	H	H ₄₀	13.2113369	26.2045606	-1.0226842
4890	H	H ₃₉	-6.8732935	-11.4630819	16.6954578	4943	H	H ₄₀	-1.8803388	-22.8755648	-18.3149438
4891	H	H ₃₆	-23.6225079	8.8395546	19.6222882	4944	H	H ₄₀	13.2097597	-26.2052713	1.0247981
4892	H	H ₃₆	27.2597011	9.9076593	13.4142302	4945	H	H ₄₀	-11.3304161	-26.7574272	4.2339146
4893	H	H ₃₆	-23.6198349	-8.8382831	-19.6260729	4946	H	H ₄₁	3.7117855	24.5399874	18.8036437
4894	H	H ₃₆	27.2613115	-9.9091257	-13.4098683	4947	H	H ₄₁	10.5872627	28.7416810	-5.6027861
4895	H	H ₃₆	-3.6419438	-16.8497270	26.9075779	4948	H	H ₄₁	3.7134848	-24.5401862	-18.8030546
4896	H	H ₃₇	-18.4252770	12.5362381	17.4634982	4949	H	H ₄₁	10.5848230	-28.7422493	5.6044735
4897	H	H ₃₇	22.2755254	13.6670549	10.8919471	4950	H	H ₄₁	-14.2993562	-27.6505676	-0.7347586
4898	H	H ₃₇	-18.4231584	-12.5352470	-17.4664464	4951	H	H ₄₃	3.3991648	10.9538853	18.4765646
4899	H	H ₃₇	22.2765295	-13.6682533	-10.8883823	4952	H	H ₄₃	12.4603971	15.6142325	-8.5941610
4900	H	H ₃₇	-3.8539740	-19.0817811	20.5585599	4953	H	H ₄₃	3.4015360	-10.9540684	-18.4760194
4901	H	H ₃₈	-9.3438366	7.7636645	22.8973544	4954	H	H ₄₃	12.4581885	-15.6149036	8.5961598
4902	H	H ₃₈	23.0736067	11.7978625	-0.5381094	4955	H	H ₄₃	-15.8602564	-14.6148975	2.7896955
4903	H	H ₃₈	-9.3405813	-7.7631619	-22.8988494	4956	H	H ₄₀	-4.7927344	14.0296193	25.5037523
4904	H	H ₃₈	23.0728920	-11.7991042	0.5418042	4957	H	H ₄₀	22.1020013	19.1157225	-4.0413738
4905	H	H ₃₈	-13.7327496	-14.5434609	16.4854463	4958	H	H ₄₀	-4.7894084	-14.0293612	-25.5045212
4906	H	H ₃₉	-11.1542449	4.0330919	17.7536898	4959	H	H ₄₀	22.1003254	-19.1169126	4.0449174
4907	H	H ₃₉	20.1369029	6.6723290	2.4210648	4960	H	H ₄₀	-17.3116213	-20.5237789	12.2198272
4908	H	H ₃₉	-11.1516139	-4.0324918	-17.7554753	4961	H	H ₄₁	-8.3700875	18.5659705	23.6227435
4909	H	H ₃₉	20.1369296	-6.6734120	-2.4178439	4962	H	H ₄₁	21.6188314	22.4587609	1.0088431
4910	H	H ₃₉	-8.9855868	-9.9500832	16.6172075	4963	H	H ₄₁	-8.3672957	-18.5655198	-23.6240855
4911	H	H ₄₀	-13.2398369	11.6994796	23.5686036	4964	H	H ₄₁	21.6177873	-22.4599243	-1.0053814
4912	H	H ₄₀	25.0162856	15.1595572	3.4675234	4965	H	H ₄₁	-13.2513483	-24.9182503	13.2766788
4913	H	H ₄₀	-13.2366926	-11.6987662	-23.5707292	4966	H	H ₄₃	0.7607361	16.6269279	13.9136265
4914	H	H ₄₀	25.0160204	-15.1609042	-3.4635133	4967	H	H ₄₃	9.0518193	19.5102455	-2.8350083
4915	H	H ₄₀	-11.7799303	-19.0501738	19.1304548	4968	H	H ₄₃	0.7620695	-16.6269695	-13.9135013
4916	H	H ₄₁	-10.6014953	8.4065431	28.0098318	4969	H	H ₄₃	9.0503180	-19.5107323	2.8364564
4917	H	H ₄₁	27.9713632	13.5103446	-1.6389867	4970	H	H ₄₃	-9.8131148	-19.2864758	1.5352802
4918	H	H ₄₁	-10.5974614	-8.4059710	-28.0115389	4971	H	H ₄₀	1.4787825	27.0465101	11.1295189
4919	H	H ₄₁	27.9703697	-13.5118492	1.6434625	4972	H	H ₄₀	4.7858639	28.8872106	0.4373966
4920	H	H ₄₁	-17.3734091	-16.6254432	19.7325021	4973	H	H ₄₀	1.4791118	-27.0465892	-11.1292852
4921	H	H ₄₃	-12.3921029	-0.0897302	17.6599512	4974	H	H ₄₀	4.7843752	-28.8874681	-0.4366307
4922	H	H ₄₃	21.2815249	2.5221101	2.4862815	4975	H	H ₄₀	-6.2645944	-28.4525600	-2.9619904
4923	H	H ₄₃	-12.3892593	0.0903972	-17.6619370	4976	H	H ₄₁	-3.8476930	26.5747415	13.1423796

4977	H	H ₄₁	9.2363299	28.1578916	3.9455162	5030	H	H ₄₃	-21.2314210	3.3778466	1.0785472
4978	H	H ₄₁	-3.8470108	-26.5745341	-13.1429979	5031	H	H ₄₃	11.0399707	0.3824987	18.4748281
4979	H	H ₄₁	9.2354494	-28.1583886	-3.9440373	5032	H	H ₄₃	-21.2314342	-3.3767045	-1.0819448
4980	H	H ₄₁	-5.3895325	-29.2885965	2.6219889	5033	H	H ₄₃	11.0429134	-0.3830933	-18.4730573
4981	H	H ₄₃	4.2411023	21.1071445	2.1257375	5034	H	H ₄₃	10.1883844	-6.6222407	17.7676419
4982	H	H ₄₃	-3.4072177	21.3521320	0.7032894	5035	H	H ₄₀	-14.4340675	-0.0306089	25.8445444
4983	H	H ₄₃	-0.8330686	20.1058678	7.9421278	5036	H	H ₄₀	29.2791579	4.3312520	0.5049611
4984	H	H ₄₃	-3.4082546	-21.3519493	-0.7038308	5037	H	H ₄₀	-14.4299212	0.0313864	-25.8468607
4985	H	H ₄₃	-0.8328796	-20.1058242	-7.9422544	5038	H	H ₄₀	29.2790033	-4.3328259	-0.5002824
4986	H	H ₄₃	4.2403082	-21.1073738	-2.1250523	5039	H	H ₄₀	-14.8492461	-8.5726959	24.1307375
4987	H	H ₄₀	11.4017001	9.0607932	25.4717441	5040	H	H ₄₁	-19.9138957	-1.8791050	23.6943859
4988	H	H ₄₀	14.7074465	16.7332130	-19.0944304	5041	H	H ₄₁	30.4555395	1.2180536	5.7004296
4989	H	H ₄₀	11.4052986	-9.0614068	-25.4699184	5042	H	H ₄₁	-19.9100049	1.8801767	-23.6975754
4990	H	H ₄₀	14.7034923	-16.7340043	19.0967851	5043	H	H ₄₁	30.4563888	-1.2196935	-5.6955470
4991	H	H ₄₀	-26.1092964	-13.3818183	-0.3715699	5044	H	H ₄₁	-10.5464680	-7.0700118	28.2896650
4992	H	H ₄₁	-25.5351373	17.1124201	5.1840634	5045	H	H ₄₃	-15.3421866	6.1816389	13.9856106
4993	H	H ₄₁	14.6779786	13.9212365	23.7172677	5046	H	H ₄₃	18.6992691	7.1676709	8.2555623
4994	H	H ₄₁	10.8578421	21.4252323	-19.8700582	5047	H	H ₄₃	-15.3402735	-6.1808132	-13.9880676
4995	H	H ₄₁	14.6810301	-13.9220274	-23.7149116	5048	H	H ₄₃	18.7002110	-7.1686773	-8.2525672
4996	H	H ₄₁	10.8535047	-21.4258172	19.8718008	5049	H	H ₄₃	-3.3602573	-11.6763321	17.9322222
4997	H	H ₄₁	-25.5352283	-17.1110472	-5.1881449	5050	H	H ₄₀	-22.0544234	5.6231551	18.6337893
4998	H	H ₄₃	-19.1576942	5.5913257	8.2087118	5051	H	H ₄₀	26.1045367	6.8126609	11.7207697
4999	H	H ₄₃	15.7633195	4.5933413	14.0029299	5052	H	H ₄₀	-22.0517408	-5.6219679	-18.6373236
5000	H	H ₄₃	3.3946424	10.2232988	-18.6982290	5053	H	H ₄₀	26.1060443	-6.8140660	-11.7165881
5001	H	H ₄₃	15.7653176	-4.5941894	-14.0004067	5054	H	H ₄₀	-4.0546412	-13.2938800	25.9242784
5002	H	H ₄₃	3.3910948	-10.2234811	18.6987708	5055	H	H ₄₁	-21.6810914	11.3480025	19.1543262
5003	H	H ₄₃	-19.1566802	-5.5902952	-8.2117768	5056	H	H ₄₁	25.5210748	12.4757287	12.6002316
5004	H	H ₄₀	-28.9939446	2.6559297	3.5044216	5057	H	H ₄₁	-21.6786294	-11.3468356	-19.1577988
5005	H	H ₄₀	17.0977061	-0.8405677	23.8106199	5058	H	H ₄₁	25.5224183	-12.4771016	-12.5961479
5006	H	H ₄₀	-28.9935259	-2.6543703	-3.5090598	5059	H	H ₄₁	-3.8443489	-18.8472611	24.4077206
5007	H	H ₄₀	17.1015642	0.8396464	-23.8078753	5060	H	H ₄₃	-8.8875571	6.9090858	18.5558833
5008	H	H ₄₀	11.8918321	-7.6804528	25.6822649	5061	H	H ₄₃	19.2656903	9.9584196	0.8414151
5009	H	H ₄₁	17.2953424	8.6791695	-24.0670321	5062	H	H ₄₃	-8.8849595	-6.9086079	-18.5573045
5010	H	H ₄₁	-30.4633162	4.8101363	-1.5897735	5063	H	H ₄₃	19.2652917	-9.9594566	-0.8383284
5011	H	H ₄₁	13.1681558	-0.2728950	27.9321334	5064	H	H ₄₃	-10.3807185	-12.5700179	14.3276054
5012	H	H ₄₁	-30.4638363	-4.8084975	1.5848987	5065	H	H ₄₀	-12.9911249	12.6752162	24.7859951
5013	H	H ₄₁	13.1726423	0.2721864	-27.9300250	5066	H	H ₄₀	25.7875861	16.4350258	2.9438560
5014	H	H ₄₁	17.2910119	-8.6800996	24.0697986	5067	H	H ₄₀	-12.9878356	-12.6745171	-24.7880757
5015	H	H ₄₃	-18.6789516	10.8459121	2.3546799	5068	H	H ₄₀	25.7871717	-16.4364134	-2.9397270
5016	H	H ₄₃	9.7557237	8.2232430	17.5865158	5069	H	H ₄₀	-12.7999838	-20.2525271	19.2294448
5017	H	H ₄₃	-18.6791538	-10.8449063	-2.3576745	5070	H	H ₄₁	-9.4991957	9.2895936	27.3038293
5018	H	H ₄₃	9.7580928	-8.2237677	-17.5849550	5071	H	H ₄₁	26.6879226	14.3401889	-2.0357542
5019	H	H ₄₃	8.9206308	-13.7128625	14.2989967	5072	H	H ₄₁	-9.4953270	-9.2890823	-27.3053518
5020	H	H ₄₀	-24.9810029	10.0792311	11.3286321	5073	H	H ₄₁	26.6868252	-14.3416259	2.0400330
5021	H	H ₄₀	20.6784064	8.8141787	18.6733195	5074	H	H ₄₁	-17.1920332	-17.1313557	18.2477673
5022	H	H ₄₀	-24.9797283	-10.0778876	-11.3326279	5075	H	H ₄₃	-12.1241044	1.3267677	18.2982451
5023	H	H ₄₀	20.6809255	-8.8152908	-18.6700119	5076	H	H ₄₃	21.4841975	4.0769078	2.3212536
5024	H	H ₄₀	4.2983427	-16.1557029	23.9686634	5077	H	H ₄₃	-12.1212439	-1.3261145	-18.3001914
5025	H	H ₄₁	-27.8562520	4.9470168	12.6602447	5078	H	H ₄₃	21.4843448	-4.0780643	-2.3178113
5026	H	H ₄₁	24.0065198	3.8150009	19.2317054	5079	H	H ₄₃	-9.3632721	-7.6396615	18.3723897
5027	H	H ₄₁	-27.8544962	-4.9455189	-12.6646992	5080	H	H ₄₀	7.5520696	16.6387219	24.4422019
5028	H	H ₄₁	24.0093893	-3.8162938	-19.2278550	5081	H	H ₄₀	14.6402822	23.1600268	-13.4379094
5029	H	H ₄₁	3.8448206	-12.0014665	28.3179749	5082	H	H ₄₀	7.5550866	-16.6391280	-24.4409942

5083	H	H ₄₀	14.6368826	-23.1608151	13.4402567	5136	H	H ₄₃	-2.8958082	21.7462645	2.1427015
5084	H	H ₄₀	-22.1927662	-20.9400922	0.5438005	5137	H	H ₄₃	0.0818247	20.9191312	6.9469512
5085	H	H ₄₁	5.3961866	12.1496453	27.1615491	5138	H	H ₄₃	-2.8966317	-21.7461087	-2.1431652
5086	H	H ₄₁	18.6986138	19.2299647	-13.9661209	5139	H	H ₄₃	0.0818184	-20.9191359	-6.9469363
5087	H	H ₄₁	5.3998801	-12.1499365	-27.1606807	5140	H	H ₄₃	2.8139763	-21.7703064	-2.0030462
5088	H	H ₄₁	18.6953416	-19.2309725	13.9691243	5141	H	H ₄₀	11.0505709	10.0522265	26.6459243
5089	H	H ₄₁	-24.0958701	-17.6435275	4.7515727	5142	H	H ₄₀	15.7394912	17.9247158	-19.0824771
5090	H	H ₄₃	-2.9818684	12.1581398	18.2467389	5143	H	H ₄₀	11.0543024	-10.0528207	-26.6441578
5091	H	H ₄₃	15.2778519	15.7711477	-2.7411259	5144	H	H ₄₀	15.7354643	-17.9255623	19.0849951
5092	H	H ₄₃	-2.9796039	-12.1579782	-18.2472232	5145	H	H ₄₀	-26.7903265	-14.6764954	0.2157463
5093	H	H ₄₃	15.2765646	-15.7719696	2.7435707	5146	H	H ₄₁	-24.5056970	17.5685857	4.0778377
5094	H	H ₄₃	-12.2975406	-16.6471609	7.8292982	5147	H	H ₄₁	13.1521200	14.2315500	23.4584314
5095	H	H ₄₀	-1.9468375	24.4499980	18.3753113	5148	H	H ₄₁	11.3542755	21.4330044	-18.3717106
5096	H	H ₄₀	13.0642189	27.7166084	-0.6002255	5149	H	H ₄₁	13.1551078	-14.2322587	-23.4563202
5097	H	H ₄₀	-1.9452114	-24.4498944	-18.3756166	5150	H	H ₄₁	11.3501851	-21.4336155	18.3735293
5098	H	H ₄₀	13.0626371	-27.7173111	0.6023155	5151	H	H ₄₁	-24.5059915	-17.5672660	-4.0817674
5099	H	H ₄₀	-11.1184815	-28.2885295	3.9221311	5152	H	H ₄₃	-19.6785732	6.7389124	7.2600517
5100	H	H ₄₁	3.6992203	24.3864981	17.2367382	5153	H	H ₄₃	15.0455068	5.3769165	15.1686775
5101	H	H ₄₁	9.2787867	28.2000017	-4.9147572	5154	H	H ₄₃	4.6333718	11.1599184	-18.4216023
5102	H	H ₄₁	3.7006697	-24.3866962	-17.2361512	5155	H	H ₄₃	15.0476435	-5.3777254	-15.1662731
5103	H	H ₄₁	9.2764762	-28.2005013	4.9162448	5156	H	H ₄₃	4.6298175	-11.1601686	18.4223495
5104	H	H ₄₁	-12.9781918	-27.1126179	-1.4011253	5157	H	H ₄₃	-19.6777665	-6.7378534	-7.2632031
5105	H	H ₄₃	2.8858353	12.3903501	18.0669141	5158	H	H ₄₀	-30.3493791	1.9761859	3.0792051
5106	H	H ₄₃	12.1563989	16.8104993	-7.6086164	5159	H	H ₄₀	17.5123857	-1.7967870	24.9912009
5107	H	H ₄₃	2.8880561	-12.3905066	-18.0664452	5160	H	H ₄₀	-30.3490016	-1.9745525	-3.0840661
5108	H	H ₄₃	12.1542704	-16.8111544	7.6105686	5161	H	H ₄₀	17.5164805	1.7958438	-24.9883921
5109	H	H ₄₃	-15.0429329	-15.9620503	2.6805460	5162	H	H ₄₀	12.8324166	-7.1225901	26.8154698
5110	H	H ₄₀	-5.9285803	14.1334997	26.5936802	5163	H	H ₄₁	17.3520206	7.5938790	-22.9240285
5111	H	H ₄₀	23.5848822	19.3215509	-3.5438195	5164	H	H ₄₁	-29.3566981	4.0666948	-2.4325101
5112	H	H ₄₀	-5.9250791	-14.1331808	-26.5946290	5165	H	H ₄₁	12.0048169	-1.0329680	27.1861755
5113	H	H ₄₀	23.5832821	-19.3228206	3.5475992	5166	H	H ₄₁	-29.3573056	-4.0651146	2.4278063
5114	H	H ₄₀	-17.6589098	-21.0633974	13.6610357	5167	H	H ₄₁	12.0092242	1.0323217	-27.1842518
5115	H	H ₄₁	-9.2270393	17.3049548	23.2183224	5168	H	H ₄₁	17.3479419	-7.5948130	22.9268088
5116	H	H ₄₁	21.8873987	21.0248358	1.6086959	5169	H	H ₄₃	-19.7069435	9.6616636	2.1606641
5117	H	H ₄₁	-9.2242480	-17.3044596	-23.2197928	5170	H	H ₄₃	10.2781069	6.8904052	18.2554756
5118	H	H ₄₁	21.8865239	-21.0260140	-1.6051889	5171	H	H ₄₃	-19.7071101	-9.6606036	-2.1638167
5119	H	H ₄₁	-12.6630954	-23.7361772	14.1396648	5172	H	H ₄₃	10.2806680	-6.8909579	-18.2538320
5120	H	H ₄₃	-0.1230988	16.1978946	15.1476888	5173	H	H ₄₃	9.4260671	-12.6821384	15.3848125
5121	H	H ₄₃	10.6100123	19.2793515	-2.7520413	5174	H	H ₄₀	-25.6083701	10.4904128	12.7154262
5122	H	H ₄₃	-0.1215460	-16.1978876	-15.1477110	5175	H	H ₄₀	22.1152732	9.4632123	18.6783728
5123	H	H ₄₃	10.6085322	-19.2799229	2.7537431	5176	H	H ₄₀	-25.6068981	-10.4890359	-12.7195207
5124	H	H ₄₃	-10.4877052	-19.3153008	2.9608468	5177	H	H ₄₀	22.1177611	-9.4644020	-18.6748338
5125	H	H ₄₀	1.7269869	27.7175746	12.5323668	5178	H	H ₄₀	3.4886521	-16.9890857	25.0343707
5126	H	H ₄₀	5.7604672	29.9175972	-0.2469649	5179	H	H ₄₁	-26.5594290	5.1078279	13.5485561
5127	H	H ₄₀	1.7274953	-27.7176678	-12.5320889	5180	H	H ₄₁	24.0926373	4.3822230	17.7594352
5128	H	H ₄₀	5.7588221	-29.9179081	0.2478927	5181	H	H ₄₁	-26.5575337	-5.1063984	-13.5528112
5129	H	H ₄₀	-7.4874597	-29.4099754	-2.7014693	5182	H	H ₄₁	24.0952440	-4.3835198	-17.7555755
5130	H	H ₄₁	-4.2404695	27.9534945	12.4880884	5183	H	H ₄₁	2.4620051	-12.1875418	27.5764193
5131	H	H ₄₁	8.6717392	29.2552987	4.9254605	5184	H	H ₄₃	-21.4947070	4.0515799	2.4789577
5132	H	H ₄₁	-4.2399785	-27.9532675	-12.4887606	5185	H	H ₄₃	12.2678455	1.3396655	18.2287764
5133	H	H ₄₁	8.6709481	-29.2557661	-4.9240675	5186	H	H ₄₃	-21.4945294	-4.0504235	-2.4823982
5134	H	H ₄₁	-4.4321343	-30.5014662	2.3126896	5187	H	H ₄₃	12.2706952	-1.3403259	-18.2268109
5135	H	H ₄₃	2.8148203	21.7701552	2.0034951	5188	H	H ₄₃	9.2236630	-7.6567570	18.4629649

5189	H	H ₄₀	-14.9970339	-1.0977057	26.8575736	5242	H	H ₄₅	19.8167524	-17.4456510	13.3254206
5190	H	H ₄₀	30.5820066	3.4815622	0.2550202	5243	H	H ₄₅	-23.8448463	-16.2614937	6.4504669
5191	H	H ₄₀	-14.9926729	1.0985134	-26.8599789	5244	H	H ₄₇	-2.1379143	11.7751477	16.2147022
5192	H	H ₄₀	30.5818561	-3.4832083	-0.2501206	5245	H	H ₄₇	13.1778496	15.0190911	-2.6291944
5193	H	H ₄₀	-15.5893180	-7.8884258	25.3414905	5246	H	H ₄₇	-2.1359532	-11.7750320	-16.2150487
5194	H	H ₄₁	-18.8689401	-3.0668914	23.6753041	5247	H	H ₄₇	13.1766174	-15.0198009	2.6313089
5195	H	H ₄₁	30.0912700	0.2303275	4.5193872	5248	H	H ₄₇	-11.0412211	-15.6471179	6.2769807
5196	H	H ₄₁	-18.8649770	3.0679065	-23.6783241	5249	H	H ₄₄	-1.1886676	24.1195277	20.4672200
5197	H	H ₄₁	30.0919794	-0.2319459	-4.5145737	5250	H	H ₄₄	14.5190780	28.0364590	-2.2858159
5198	H	H ₄₁	-11.2270410	-5.7751714	27.6868866	5251	H	H ₄₄	-1.1866906	-24.1194640	-20.4674091
5199	H	H ₄₃	-15.1894320	5.1906031	15.2049450	5252	H	H ₄₄	14.5172052	-28.0372406	2.2881430
5200	H	H ₄₃	19.8091614	6.5476750	7.3196063	5253	H	H ₄₄	-13.3315716	-28.3855082	4.3132082
5201	H	H ₄₃	-15.1872732	-5.1897852	-15.2073805	5254	H	H ₄₅	5.7476405	23.7058752	17.2440988
5202	H	H ₄₃	19.8099820	-6.5487395	-7.3164430	5255	H	H ₄₅	8.3608522	27.8516316	-6.8370895
5203	H	H ₄₃	-4.6230023	-11.0114065	18.6072119	5256	H	H ₄₅	5.7491277	-23.7061834	-17.2431848
5204	H	H ₄₀	-23.5614918	6.0759323	18.5331582	5257	H	H ₄₅	8.3582517	-27.8520818	6.8384307
5205	H	H ₄₀	26.7056703	6.9991836	13.1665406	5258	H	H ₄₅	-14.1083993	-26.1622282	-2.9755197
5206	H	H ₄₀	-23.5588554	-6.0746636	-18.5369356	5259	H	H ₄₇	1.6747806	11.1965182	16.5557982
5207	H	H ₄₀	26.7074008	-7.0006220	-13.1622568	5260	H	H ₄₇	11.6476190	15.1112711	-6.1841474
5208	H	H ₄₀	-3.1488998	-13.9233243	27.0511418	5261	H	H ₄₇	1.6768273	-11.1966091	-16.5555252
5209	H	H ₄₁	-21.7779829	11.2766707	17.5810829	5262	H	H ₄₇	11.6458152	-15.1118993	6.1860208
5210	H	H ₄₁	24.2372806	11.9986782	13.3837316	5263	H	H ₄₇	-13.3231847	-14.6187665	3.3235190
5211	H	H ₄₁	-21.7757748	-11.2754989	-17.5845693	5264	H	H ₄₄	-4.9549918	16.1767073	26.8714776
5212	H	H ₄₁	24.2387747	-11.9999841	-13.3798409	5265	H	H ₄₄	23.0350102	21.4892749	-3.9891706
5213	H	H ₄₁	-2.4635518	-18.3987237	23.7898339	5266	H	H ₄₄	-4.9515659	-16.1764410	-26.8722695
5214	H	H ₄₃	-10.4201600	6.9464398	18.1763509	5267	H	H ₄₄	23.0332106	-21.4905147	3.9928603
5215	H	H ₄₃	19.7025763	9.6737595	2.3321793	5268	H	H ₄₄	-18.0824488	-22.9450029	12.4445167
5216	H	H ₄₃	-10.4176140	-6.9458797	-18.1780162	5269	H	H ₄₅	-9.8019070	18.1838120	21.2567381
5217	H	H ₄₃	19.7024363	-9.6748191	-2.3290279	5270	H	H ₄₅	20.3715674	21.2893156	3.2158483
5218	H	H ₄₃	-9.2851989	-12.7357849	15.4530695	5271	H	H ₄₅	-9.7994790	-18.1832839	-21.2583112
5219	H	H ₄₄	-14.4818045	11.2063583	25.7360665	5272	H	H ₄₅	20.3709374	-21.2904105	-3.2125942
5220	H	H ₄₄	27.5595846	15.0488033	3.4136836	5273	H	H ₄₅	-10.5722886	-24.1696583	13.5141277
5221	H	H ₄₄	-14.4782934	-11.2055792	-25.7383844	5274	H	H ₄₇	0.3628193	14.1440935	14.3961939
5222	H	H ₄₄	27.5593259	-15.0502875	-3.4092636	5275	H	H ₄₇	10.0273985	17.1971660	-3.3385823
5223	H	H ₄₄	-13.0816304	-19.3043706	21.3040482	5276	H	H ₄₇	0.3643638	-14.1441134	-14.3961338
5224	H	H ₄₅	-8.8340105	7.0965207	28.4258156	5277	H	H ₄₇	10.0259398	-17.1977055	3.3401872
5225	H	H ₄₅	27.6351069	12.6209452	-3.6660685	5278	H	H ₄₇	-10.3909391	-17.0903096	2.7179252
5226	H	H ₄₅	-8.8298482	-7.0960455	-28.4272293	5279	H	H ₄₄	0.1354716	28.6990723	10.4552634
5227	H	H ₄₅	27.6338450	-12.6224336	3.6705012	5280	H	H ₄₄	4.6392824	30.1019168	2.3063751
5228	H	H ₄₅	-18.8044553	-15.2165766	18.7423477	5281	H	H ₄₄	0.1355978	-28.6990786	-10.4552476
5229	H	H ₄₇	-11.5532281	1.8492655	16.1838174	5282	H	H ₄₄	4.6380247	-30.1021651	-2.3056395
5230	H	H ₄₇	19.3173879	4.1304509	2.9309991	5283	H	H ₄₄	-4.7747923	-30.0620837	-2.5377385
5231	H	H ₄₇	-11.5507351	-1.8486435	-16.1856693	5284	H	H ₄₅	-6.2300345	27.0272988	12.2964944
5232	H	H ₄₇	19.3176330	-4.1314906	-2.9279047	5285	H	H ₄₅	9.6390787	28.0286767	6.4786937
5233	H	H ₄₇	-7.7670751	-7.5254830	16.7884620	5286	H	H ₄₅	-6.2295158	-27.0269625	-12.2974979
5234	H	H ₄₄	4.7548943	16.7486146	24.6986910	5287	H	H ₄₅	9.6386144	-28.0291947	-6.4771539
5235	H	H ₄₄	16.2416225	22.9184515	-11.1402233	5288	H	H ₄₅	-3.4101993	-29.8595558	4.1556533
5236	H	H ₄₄	4.7579534	-16.7488713	-24.6979247	5289	H	H ₄₇	2.1329222	19.7196861	2.6616264
5237	H	H ₄₄	16.2386061	-22.9193244	11.1428179	5290	H	H ₄₇	-1.6919214	19.8491785	1.9097503
5238	H	H ₄₄	-20.9973625	-21.5205781	3.0209155	5291	H	H ₄₇	-0.4402294	19.2224486	5.5500706
5239	H	H ₄₅	4.0236907	10.4381280	27.3765738	5292	H	H ₄₇	-1.6926790	-19.8490874	-1.9100215
5240	H	H ₄₅	19.8198230	17.4445849	-13.3222491	5293	H	H ₄₇	-0.4403776	-19.2224242	-5.5501450
5241	H	H ₄₅	4.0275146	-10.4383452	-27.3759259	5294	H	H ₄₇	2.1322850	-19.7198016	-2.6612806

5295	H	H ₄₄	13.5832072	9.5704911	25.5378955	5348	H	H ₄₄	-13.4863203	-9.7798921	25.4987250
5296	H	H ₄₄	13.5982677	17.5580696	-20.8586557	5349	H	H ₄₅	-20.7189594	-3.2040068	21.9987536
5297	H	H ₄₄	13.5867925	-9.5712222	-25.5357198	5350	H	H ₄₅	29.6055382	-0.5931994	6.8298141
5298	H	H ₄₄	13.5939853	-17.5588007	20.8608293	5351	H	H ₄₅	-20.7152630	3.2051220	-22.0020729
5299	H	H ₄₄	-27.1813032	-13.5655500	-2.3312090	5352	H	H ₄₅	29.6066621	0.5916061	-6.8250722
5300	H	H ₄₅	-23.8908646	18.0557797	6.4731238	5353	H	H ₄₅	-8.8914214	-5.4953888	28.5347056
5301	H	H ₄₅	14.8174409	15.3887807	21.9616709	5354	H	H ₄₇	-13.1126031	4.9759547	14.4054167
5302	H	H ₄₅	9.0741703	22.4096121	-18.8190061	5355	H	H ₄₇	18.1199073	6.4469710	5.8585085
5303	H	H ₄₅	14.8201241	-15.3895767	-21.9593060	5356	H	H ₄₇	-13.1105632	-4.9752484	-14.4075201
5304	H	H ₄₅	9.0699419	-22.4100996	18.8204547	5357	H	H ₄₇	18.1204951	-6.4479465	-5.8556050
5305	H	H ₄₅	-23.8908027	-18.0544932	-6.4769543	5358	H	H ₄₇	-5.0102170	-10.3003571	16.5232226
5306	H	H ₄₇	-18.3548753	4.3836390	6.4997201	5359	H	H ₄₄	-23.2074879	6.8433751	20.6123325
5307	H	H ₄₇	14.0807615	3.1271723	13.7955447	5360	H	H ₄₄	28.1904278	8.3069559	12.1070776
5308	H	H ₄₇	4.2743241	8.5211701	-17.5352166	5361	H	H ₄₄	-23.2045470	-6.8421267	-20.6160463
5309	H	H ₄₇	14.0827998	-3.1279303	-13.7932886	5362	H	H ₄₄	28.1919267	-8.3084726	-12.1025655
5310	H	H ₄₇	4.2710591	-8.5214004	17.5359028	5363	H	H ₄₄	-4.9877684	-15.1270136	27.5060567
5311	H	H ₄₇	-18.3540693	-4.3826508	-6.5026623	5364	H	H ₄₅	-20.5184992	13.0593058	17.3897208
5312	H	H ₄₄	-31.1167038	4.1079529	3.3615824	5365	H	H ₄₅	23.1823284	13.8414343	12.8433280
5313	H	H ₄₄	17.8238595	0.2009932	26.0517698	5366	H	H ₄₅	-20.5164130	-13.0582004	-17.3930137
5314	H	H ₄₄	-31.1163912	-4.1062788	-3.3665631	5367	H	H ₄₅	23.1836371	-13.8426805	-12.8396232
5315	H	H ₄₄	17.8280171	-0.2019522	-26.0489167	5368	H	H ₄₅	-2.6678329	-19.8713451	22.1803737
5316	H	H ₄₄	13.2881862	-9.3458905	27.0647964	5369	H	H ₄₇	-9.8222126	5.4507454	16.6317730
5317	H	H ₄₅	18.2728955	10.2038922	-22.8180274	5370	H	H ₄₇	18.3050916	7.9431441	2.1523125
5318	H	H ₄₅	-30.1101043	6.7259211	-2.6122399	5371	H	H ₄₇	-9.8198449	-5.4502171	-16.6333444
5319	H	H ₄₅	11.8374536	1.3556483	28.5782634	5372	H	H ₄₇	18.3050112	-7.9441295	-2.1493792
5320	H	H ₄₅	-30.1108855	-6.7242997	2.6074119	5373	H	H ₄₇	-8.4854843	-10.8294637	14.6123793
5321	H	H ₄₅	11.8419582	-1.3562847	-28.5763717	5374	H	H ₄₄	-13.8861651	9.9738359	24.9448261
5322	H	H ₄₅	18.2686923	-10.2048743	22.8209468	5375	H	H ₄₄	26.7675378	13.7585931	2.9576332
5323	H	H ₄₇	-17.9847686	8.4189162	2.8584470	5376	H	H ₄₄	-13.8827050	-9.9730876	-24.9470556
5324	H	H ₄₇	10.1951317	6.1293928	16.1551966	5377	H	H ₄₄	26.7672648	-13.7600339	-2.9533446
5325	H	H ₄₇	-17.9847579	-8.4179497	-2.8613197	5378	H	H ₄₄	-12.8851053	-17.8391138	20.7433704
5326	H	H ₄₇	10.1973965	-6.1299423	-16.1535588	5379	H	H ₄₅	-8.0674198	7.5796291	27.1355263
5327	H	H ₄₇	7.7870243	-11.4149673	14.5451555	5380	H	H ₄₅	26.0796054	12.8722507	-3.6097330
5328	H	H ₄₄	-26.9028171	9.2364419	10.5809459	5381	H	H ₄₅	-8.0634808	-7.5791950	-27.1368184
5329	H	H ₄₄	21.1250060	7.5378510	20.4436997	5382	H	H ₄₅	26.0783334	-12.8736541	3.6139093
5330	H	H ₄₄	-26.9016212	-9.2349943	-10.5852535	5383	H	H ₄₅	-18.0153210	-15.2426201	17.3776168
5331	H	H ₄₄	21.1278760	-7.5389881	-20.4403148	5384	H	H ₄₇	-12.4998804	0.7443085	15.5674765
5332	H	H ₄₄	5.7733223	-15.4441917	25.4789233	5385	H	H ₄₇	19.4270227	2.7795174	3.7433536
5333	H	H ₄₅	-27.2807655	2.7601460	12.9573541	5386	H	H ₄₇	-12.4974309	-0.7436347	-15.5694847
5334	H	H ₄₅	24.2936331	1.8816392	18.0563070	5387	H	H ₄₇	19.4274736	-2.7805625	-3.7402442
5335	H	H ₄₅	-27.2788347	-2.7586779	-12.9617233	5388	H	H ₄₇	-6.9301686	-6.4527688	17.5920967
5336	H	H ₄₅	24.2964212	-1.8829461	-18.0524190	5389	H	H ₄₄	5.8137757	17.6615400	25.4301786
5337	H	H ₄₅	2.9822226	-9.8989478	28.5108537	5390	H	H ₄₄	16.2023729	24.1310153	-12.1491276
5338	H	H ₄₇	9.8230748	7.4830596	-15.7118466	5391	H	H ₄₄	5.8169004	-17.6618526	-25.4292493
5339	H	H ₄₇	-19.4205302	4.6630394	0.6707169	5392	H	H ₄₄	16.1991251	-24.1318870	12.1517212
5340	H	H ₄₇	9.5976381	1.7760307	17.4379482	5393	H	H ₄₄	-22.0168683	-22.4219351	2.2222289
5341	H	H ₄₇	-19.4206782	-4.6619954	-0.6738207	5394	H	H ₄₅	3.4092677	11.2830372	28.5528946
5342	H	H ₄₇	9.6003432	-1.7765474	-17.4364100	5395	H	H ₄₅	21.0068667	18.4577358	-13.1233121
5343	H	H ₄₇	9.8201522	-7.4835869	15.7134124	5396	H	H ₄₅	3.4132337	-11.2832210	-28.5523474
5344	H	H ₄₄	-16.4603692	0.9816905	25.6086828	5397	H	H ₄₅	21.0037718	-18.4588661	13.1266755
5345	H	H ₄₄	29.9422881	4.9429207	2.5959927	5398	H	H ₄₅	-24.4176249	-17.4551974	7.3002398
5346	H	H ₄₄	-16.4563185	-0.9808040	-25.6113230	5399	H	H ₄₇	-3.4440689	12.2793423	15.4901014
5347	H	H ₄₄	29.9424377	-4.9445308	-2.5912051	5400	H	H ₄₇	13.1384245	15.1278481	-1.0569585

5401	H	H ₄₇	-3.4422528	-12.2791568	-15.4906537	5454	H	H ₄₄	-28.2477294	-14.3231407	-1.4455060
5402	H	H ₄₇	13.1374420	-15.1285558	1.0590665	5455	H	H ₄₅	-22.7399865	17.4918992	5.5454641
5403	H	H ₄₇	-9.6957608	-16.1397647	6.9345020	5456	H	H ₄₅	13.5331086	14.7857202	21.2617774
5404	H	H ₄₄	-0.5037644	22.7474205	20.0906835	5457	H	H ₄₅	9.2075831	21.4683268	-17.5543991
5405	H	H ₄₄	14.0568475	26.7298132	-3.0425034	5458	H	H ₄₅	13.5357149	-14.7864489	-21.2596077
5406	H	H ₄₄	-0.5017678	-22.7473923	-20.0907710	5459	H	H ₄₅	9.2036195	-21.4688225	17.5558750
5407	H	H ₄₄	14.0549138	-26.7305698	3.0447554	5460	H	H ₄₅	-22.7400397	-17.4906748	-5.5491097
5408	H	H ₄₄	-13.5541480	-26.8775715	3.9007317	5461	H	H ₄₇	-18.2659625	5.7959159	5.7995490
5409	H	H ₄₅	5.8058271	24.0141480	18.7845987	5462	H	H ₄₇	13.2312400	4.3159358	14.3937424
5410	H	H ₄₅	9.6012453	28.5414914	-7.5131618	5463	H	H ₄₇	5.0349772	9.6837904	-16.7852867
5411	H	H ₄₅	5.8075423	-24.0144595	-18.7836746	5464	H	H ₄₇	13.2333138	-4.3166493	-14.3916152
5412	H	H ₄₅	9.5985010	-28.5420087	7.5147030	5465	H	H ₄₇	5.0317691	-9.6840619	16.7860966
5413	H	H ₄₅	-15.4070852	-26.8349541	-2.3989674	5466	H	H ₄₇	-18.2653478	-5.7949339	-5.8024688
5414	H	H ₄₇	1.6501122	9.9117112	17.4687279	5467	H	H ₄₄	-29.7338363	4.7500693	2.9310523
5415	H	H ₄₇	12.6278695	14.1072719	-6.9023908	5468	H	H ₄₄	16.6706440	0.9106254	25.2292621
5416	H	H ₄₇	1.6523750	-9.9118008	-17.4684592	5469	H	H ₄₄	-29.7336226	-4.7484692	-2.9358138
5417	H	H ₄₇	12.6260090	-14.1079513	6.9044124	5470	H	H ₄₄	16.6746362	-0.9115227	-25.2265916
5418	H	H ₄₇	-14.2788780	-13.6219853	4.0836872	5471	H	H ₄₄	13.0587855	-9.6491237	25.5268051
5419	H	H ₄₄	-4.5877687	16.2986161	25.3386378	5472	H	H ₄₅	18.7787826	8.9763809	-21.9728315
5420	H	H ₄₄	21.5252446	21.2754587	-3.5717791	5473	H	H ₄₅	-29.4613648	5.8377215	-3.7379760
5421	H	H ₄₄	-4.5845855	-16.2983699	-25.3393690	5474	H	H ₄₅	10.6827807	0.3188054	28.3160721
5422	H	H ₄₄	21.5235291	-21.2766165	3.5752229	5475	H	H ₄₅	-29.4622757	-5.8361359	3.7332571
5423	H	H ₄₄	-16.9397336	-22.6232987	11.4004762	5476	H	H ₄₅	10.6872973	-0.3193802	-28.3143619
5424	H	H ₄₅	-9.4617309	19.5547344	21.9515195	5477	H	H ₄₅	18.7747798	-8.9773917	21.9758403
5425	H	H ₄₅	20.5930515	22.8252789	2.9519839	5478	H	H ₄₇	-17.3283151	9.6193817	3.6373457
5426	H	H ₄₅	-9.4592719	-19.5542249	-21.9530362	5479	H	H ₄₇	10.3553155	7.5698345	15.5402096
5427	H	H ₄₅	20.5922964	-22.8263880	-2.9486812	5480	H	H ₄₇	-17.3282436	-9.6184492	-3.6401202
5428	H	H ₄₅	-11.1339166	-25.6056423	13.1972792	5481	H	H ₄₇	10.3574029	-7.5703918	-15.5385517
5429	H	H ₄₇	1.7248464	14.6111558	13.7520429	5482	H	H ₄₇	6.9704576	-12.6624732	14.0395079
5430	H	H ₄₇	8.7280131	17.6826648	-4.0896196	5483	H	H ₄₄	-27.5430039	10.2025236	11.6527927
5431	H	H ₄₇	1.7262583	-14.6112472	-13.7517752	5484	H	H ₄₄	22.2179630	8.6369560	20.7427364
5432	H	H ₄₇	8.7264059	-17.6831343	4.0910168	5485	H	H ₄₄	-27.5416827	-10.2010407	-11.6572075
5433	H	H ₄₇	-10.4533084	-17.1755384	1.1440631	5486	H	H ₄₄	22.2208148	-8.6381516	-20.7391790
5434	H	H ₄₄	0.8637151	29.5383782	11.5794499	5487	H	H ₄₄	5.3204011	-16.7314236	26.2725888
5435	H	H ₄₄	5.1113108	31.2939388	1.3817988	5488	H	H ₄₅	-25.7360185	3.0816096	12.9084155
5436	H	H ₄₄	0.8639830	-29.5384245	-11.5793126	5489	H	H ₄₅	23.4322746	2.4039521	16.8409009
5437	H	H ₄₄	5.1098455	-31.2942135	-1.3809823	5490	H	H ₄₅	-25.7341174	-3.0802231	-12.9125462
5438	H	H ₄₄	-5.9750341	-31.0400605	-2.8564068	5491	H	H ₄₅	23.4348395	-2.4052127	-16.8371510
5439	H	H ₄₅	-5.6472458	25.5661675	12.3719998	5492	H	H ₄₅	2.2990801	-9.9672759	27.0893668
5440	H	H ₄₅	9.6267908	26.7352112	5.5803429	5493	H	H ₄₇	-19.3169448	4.5789470	2.2456741
5441	H	H ₄₅	-5.6466454	-25.5658625	-12.3729105	5494	H	H ₄₇	10.9023930	2.1057808	16.6089736
5442	H	H ₄₅	9.6262389	-26.7357283	-5.5788069	5495	H	H ₄₇	-19.3168395	-4.5779070	-2.2487703
5443	H	H ₄₅	-3.9806561	-28.3948015	4.0591023	5496	H	H ₄₇	10.9049329	-2.1063682	-16.6072239
5444	H	H ₄₇	3.4783870	19.4307132	3.4365513	5497	H	H ₄₇	8.4117081	-7.7828561	16.3653439
5445	H	H ₄₇	-1.6608158	19.9647477	0.3349570	5498	H	H ₄₄	-16.5801606	0.5081180	27.1135972
5446	H	H ₄₇	-1.8167970	18.9426486	6.2719211	5499	H	H ₄₄	31.3561663	4.8496149	1.8919780
5447	H	H ₄₇	-1.6618460	-19.9646581	-0.3352240	5500	H	H ₄₄	-16.5758495	-0.5072248	-27.1162580
5448	H	H ₄₇	-1.8168168	-18.9425514	-6.2722084	5501	H	H ₄₄	31.3562048	-4.8513035	-1.8869496
5449	H	H ₄₇	3.4778885	-19.4309000	-3.4359967	5502	H	H ₄₄	-14.7805533	-9.7217536	26.4070031
5450	H	H ₄₄	13.2489510	9.9165675	27.0426154	5503	H	H ₄₅	-19.2664866	-3.5103380	21.4609889
5451	H	H ₄₄	14.9987915	18.2174567	-21.1739603	5504	H	H ₄₅	28.4653448	-0.8077288	5.7590084
5452	H	H ₄₄	13.2527529	-9.9172811	-27.0404909	5505	H	H ₄₅	-19.2628644	3.5113759	-21.4640805
5453	H	H ₄₄	14.9944193	-18.2182629	21.1763570	5506	H	H ₄₅	28.4663030	0.8061980	-5.7544561

5507	H	H ₄₅	-9.2034494	-4.8540001	27.1261723	5560	O	O ₅₆	11.4956194	13.0567257	-16.9457729
5508	H	H ₄₇	-13.1340156	6.4029601	13.7367576	5561	O	O ₅₆	-22.1287730	9.9323655	1.2049105
5509	H	H ₄₇	17.3502762	7.6415186	6.5401586	5562	O	O ₅₆	10.6335499	6.5538281	20.8269437
5510	H	H ₄₇	-13.1321564	-6.4022541	-13.7388564	5563	O	O ₅₆	-22.1291219	-9.9311750	-1.2084518
5511	H	H ₄₇	17.3509093	-7.6424529	-6.5373765	5564	O	O ₅₆	10.6365303	-6.5544005	-20.8252402
5512	H	H ₄₇	-4.2190932	-11.5012248	15.8782825	5565	O	O ₅₆	11.4921952	-13.0573438	16.9476107
5513	H	H ₄₄	-21.6493625	6.9648275	20.3890558	5566	O	O ₅₆	-23.6484425	3.6356489	3.7858353
5514	H	H ₄₄	27.2029643	8.5961357	10.9097359	5567	O	O ₅₆	14.5212051	0.9529554	19.3655865
5515	H	H ₄₄	-21.6464710	-6.9636631	-20.3925192	5568	O	O ₅₆	-23.6480346	-3.6343765	-3.7896211
5516	H	H ₄₄	27.2042464	-8.5976008	-10.9053728	5569	O	O ₅₆	14.5242581	-0.9537373	-19.3632587
5517	H	H ₄₄	-5.5581810	-14.9582805	26.0436900	5570	O	O ₅₆	9.1236126	-7.9029781	21.0024274
5518	H	H ₄₅	-20.5309765	13.2034317	18.9549054	5571	O	O ₅₆	-17.1103178	4.3659371	16.6055746
5519	H	H ₄₅	24.5032368	14.3700389	12.1751322	5572	O	O ₅₆	22.0861600	5.8276086	8.1123399
5520	H	H ₄₅	-20.5286622	-13.2023269	-18.9581927	5573	O	O ₅₆	-17.1078903	-4.3650156	-16.6083194
5521	H	H ₄₅	24.5044106	-14.3713584	-12.1712034	5574	O	O ₅₆	22.0871398	-5.8287973	-8.1088025
5522	H	H ₄₅	-3.9763866	-20.4035838	22.8696777	5575	O	O ₅₆	-4.9795258	-10.8558330	21.0932383
5523	H	H ₄₇	-8.5398051	5.0141810	17.4360650	5576	O	O ₅₆	-12.1589005	8.5302464	19.2784043
5524	H	H ₄₇	18.4144620	7.9155926	0.5809067	5577	O	O ₅₆	21.2798366	11.2100565	3.7099438
5525	H	H ₄₇	-8.5372841	-5.0137225	-17.4374263	5578	O	O ₅₆	-12.1562677	-8.5295933	-19.2803447
5526	H	H ₄₇	18.4141351	-7.9165834	-0.5779590	5579	O	O ₅₆	21.2798260	-11.2112020	-3.7065341
5527	H	H ₄₇	-9.8771575	-10.4250011	13.9945617	5580	O	O ₅₆	-9.1240164	-14.7830710	17.0432971
5528	O	O ₅₆	-12.2047512	1.6805694	20.8665651	Molecular Orbitals					
5529	O	O ₅₆	23.6645400	5.0476996	1.3055598						
5530	O	O ₅₆	-12.2015028	-1.6799113	-20.8685275	Table 7: Energies of the calculated molecular orbitals.					
5531	O	O ₅₆	23.6644767	-5.0489729	-1.3017715						
5532	O	O ₅₆	-11.4631706	-8.6340975	19.5254164	Level	Label	Symmetry	Energy /eV		
5533	O	O ₅₆	-2.5974623	12.4957758	20.7795492	8356	LUMO+15	None	nan		
5534	O	O ₅₆	17.1977283	16.7859072	-4.1415638	8355	LUMO+14	None	nan		
5535	O	O ₅₆	-2.5948072	-12.4956351	-20.7799704	8354	LUMO+13	None	nan		
5536	O	O ₅₆	17.1961569	-16.7868332	4.1443211	8353	LUMO+12	None	nan		
5537	O	O ₅₆	-14.6019643	-17.5488893	8.5732147	8352	LUMO+11	None	nan		
5538	O	O ₅₆	3.9158213	14.4926528	19.1912779	8351	LUMO+10	None	-38.6610		
5539	O	O ₅₆	12.2921658	19.2553713	-8.4740286	8350	LUMO+9	None	-38.6610		
5540	O	O ₅₆	3.9181178	-14.4928635	-19.1906510	8349	LUMO+8	None	-38.6610		
5541	O	O ₅₆	12.2897702	-19.2560324	8.4759949	8348	LUMO+7	None	-38.6610		
5542	O	O ₅₆	-16.2085685	-18.1042062	1.7876836	8347	LUMO+6	None	-38.6610		
5543	O	O ₅₆	-1.5006104	17.9269337	16.4600324	8346	LUMO+5	None	-38.7033		
5544	O	O ₅₆	12.1647934	21.0604347	-1.7422244	8345	LUMO+4	None	-38.7033		
5545	O	O ₅₆	-1.4989315	-17.9268528	-16.4602736	8344	LUMO+3	None	-38.7033		
5546	O	O ₅₆	12.1633848	-21.0610892	1.7441717	8343	LUMO+2	None	-38.7033		
5547	O	O ₅₆	-10.6652385	-21.5012050	4.3023627	8342	LUMO+1	None	-38.7033		
5548	O	O ₅₆	2.5836878	24.1282772	0.9979056	8341	LUMO	None	-38.7033		
5549	O	O ₅₆	-3.9849205	23.7164050	3.3908019	8340	HOMO	None	-39.0973		
5550	O	O ₅₆	1.4021618	22.9571723	7.8004613	8339	HOMO-1	None	-39.0973		
5551	O	O ₅₆	-3.9856553	-23.7161910	-3.3914378	8338	HOMO-2	None	-39.0973		
5552	O	O ₅₆	1.4021784	-22.9572478	-7.8002365	8337	HOMO-3	None	-39.0973		
5553	O	O ₅₆	2.5825478	-24.1284158	-0.9974944	8336	HOMO-4	None	-39.0973		
5554	O	O ₅₆	-21.2802435	8.6497065	7.9884313	8335	HOMO-5	None	-39.0973		
5555	O	O ₅₆	16.1872816	7.1525107	16.6821686	8334	HOMO-6	None	-39.1624		
5556	O	O ₅₆	5.0933501	13.4062053	-19.6421190	8333	HOMO-7	None	-39.1624		
5557	O	O ₅₆	16.1895667	-7.1533808	-16.6795824	8332	HOMO-8	None	-39.1624		
5558	O	O ₅₆	5.0894828	-13.4064786	19.6429305	8331	HOMO-9	None	-39.1624		
5559	O	O ₅₆	-21.2794278	-8.6485602	-7.9918459	8330	HOMO-10	None	-39.1624		
						8329	HOMO-11	None	-39.1624		

8328	HOMO-12	None	-39.2332	8326	HOMO-14	None	nan
8327	HOMO-13	None	nan	8325	HOMO-15	None	nan

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