

Supporting Information for: Carbon Dioxide Separation with a Two-dimensional Polymer Membrane

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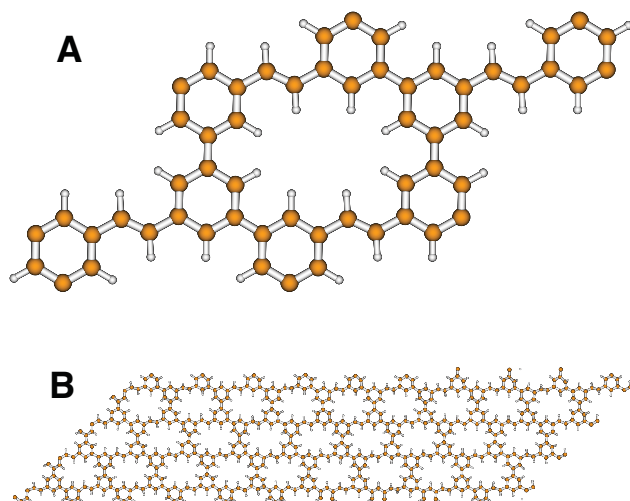


Fig. S1. (A) 2x2 supercell of PG-ES1 used for planewave pseudopotential density functional theory calculations of the charges; (B) 880-atom PG-ES1 supercell used for molecular dynamics simulations.

		ϵ (eV)	σ (Å)	q (e ⁻)
PG-ES1 ¹	C	0.0032948	3.5500	—
	H	0.0013007	2.4200	—
CO ₂ (2CLJQ ²)	C	—	—	+0.5406
	O	0.011473	2.9847	-0.2703
CO ₂ (EPM2 ³)	C	0.00242397	2.757	+0.6512
	O	0.00693756	3.033	-0.3256
N ₂ (2CLJQ ²)	N	0.003006	3.3321	-0.5475
	Q	—	—	+1.0950
O ₂ (2CLJQ ²)	O	0.003721	3.1062	-0.3577
	Q	—	—	+0.7154
CH ₄ (2CLJQ ²)	C	0.012797	3.7281	0.0
	H	—	—	—
CH ₄ (Stassen ⁴)	C	0.002862	3.50	-0.240
	H	0.001301	2.50	+0.060

Table S1. Lennard-Jones (ϵ , σ) and point-charge (q) parameters. Q denotes point charges used for reproducing the quadrupole moments in the 2CLJQ model. Charges for the PG-ES1 hydrocarbon atoms were taken from the Hirshfeld-I analysis and are shown in Table S3.

References

- (1) Fileti, E. E.; Dalpian, G. M.; Rivelino, R. Liquid Separation by a Graphene Membrane. *J. Appl. Phys.* **2010**, *108*, 113527.
- (2) Vrabec, J.; Stoll, J.; Hasse, H. A Set of Molecular Models for Symmetric Quadrupolar Fluids. *J. Phys. Chem. B* **2001**, *105*, 12126.
- (3) Harris, J. G.; Yung, K. H. Carbon Dioxide's Liquid-Vapor Coexistence Curve And Critical Properties as Predicted by a Simple Molecular Model. *J. Phys. Chem.* **1995**, *99*, 12021–12024.
- (4) Stassen, H. On the Pair Potential in Dense Fluid Methane. *J. Mol. Struct.: THEOCHEM* **1999**, *464*, 107–119.

	$k_0[S_0]a\Delta t$	α
CO ₂ (2CLJQ)	5489.21	0.000611847
CO ₂ (EPM2)	4969.54	0.000649892
N ₂ (2CLJQ)	65.9993	0.000252995
N ₂ (NQLJ)	66.1853	0.000911776
O ₂ (2CLJQ)	1394.97	0.000425758

Table S2. Langmuir-adsorption model parameters, for the curves plotted in Fig. 1B. The simulation time, $\Delta t = 20$ ns, and the area of the simulation cell, $a = 2569.05 \text{ \AA}^2$.

Table S3. Sample PG-ES1 coordinates (Å) and charges. Translation vectors are (99.36, 0.0, 0.0) Å and (25.464, 25.856, 0.0) Å.

	x	y	z	q
C	1.44822	0.888613	0.942729	-0.215400420454545
C	2.42147	0.0252085	0.415809	0.0992255795454546
C	3.5287	0.650117	-0.228837	-0.225199420454545
C	100.63	2.22219	0.427342	0.0999575795454545
C	101.8	2.84491	-0.0444291	-0.233383420454545
C	3.68432	2.04662	-0.228624	0.147543579545455
C	4.94239	2.7223	-0.396271	-0.153730420454545
H	0.806411	0.614934	1.74142	0.120045579545455
H	4.09451	0.0817093	-0.985666	0.121982579545455
H	101.785	3.89726	-0.293906	0.122866579545455
H	4.97445	3.48011	-1.23813	0.116079579545455
C	7.47568	3.11158	0.107331	0.147472579545455
C	8.65934	2.38888	-0.0392013	-0.233308420454545
C	9.9237	3.10383	-0.299506	0.0999045795454545
C	7.59857	4.51536	0.223824	-0.225149420454545
C	8.80807	5.17825	-0.211644	0.0992355795454545
C	9.80853	4.37391	-0.770647	-0.215432420454545
C	6.18942	2.50486	0.242477	-0.153658420454545
H	6.88564	5.17227	0.649145	0.121968579545455
H	10.4539	4.7715	-1.47838	0.120079579545455
H	8.69562	1.32788	0.0330193	0.122832579545455
H	6.19372	1.66609	1.00401	0.116065579545455
C	7.80262	7.42471	-0.610434	-0.215403420454545
C	8.87325	6.60228	-0.192259	0.0992265795454546
C	9.96014	7.14607	0.450248	-0.225200420454545
C	107.08	8.70914	-0.0515712	0.0999585795454545
C	108.381	9.2945	0.293571	-0.233385420454545
C	10.1875	8.5222	0.432036	0.147545579545455
C	11.4463	9.15119	0.555666	-0.153732420454545
H	6.97113	7.11257	-1.33849	0.120045579545455
H	10.8066	6.53123	0.824541	0.121983579545455
H	108.542	10.3496	0.329627	0.122867579545455
H	11.3186	10.0475	1.15602	0.116080579545455
C	13.9224	9.47113	0.165531	0.147472579545455
C	15.1202	8.73981	0.287471	-0.233307420454545
C	16.3415	9.35359	0.378631	0.0999045795454545
C	13.9586	10.8879	0.253978	-0.225148420454545
C	15.1278	11.5379	0.528791	0.0992365795454545
C	16.2472	10.6844	0.717817	-0.215432420454545
C	12.6619	8.77813	0.0395991	-0.153655420454545
H	13.1177	11.4918	-0.0559767	0.121968579545455

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H	17.1166	11.1375	1.19023	0.120079579545455
H	14.9791	7.65051	0.0928349	0.122832579545455
H	12.6906	7.88601	-0.619406	0.116065579545455
C	11.1987	1.07408	-0.85695	-0.215407420454545
C	12.2898	0.216079	-0.441794	0.0992295795454546
C	13.4866	0.855789	-0.152766	-0.225204420454545
C	11.1267	2.35311	-0.327538	0.0999605795454546
C	12.3978	2.90321	0.0293391	-0.233388420454545
C	13.603	2.23444	-0.1715	0.147549579545455
C	14.9128	2.75261	-0.166893	-0.153738420454545
H	10.4642	0.585881	-1.42392	0.120044579545455
H	14.3704	0.294698	0.186639	0.121984579545455
H	12.4276	3.93705	0.399944	0.122867579545455
H	14.9897	3.74091	0.325904	0.116080579545455
C	17.4891	2.99907	-0.563882	0.147468579545455
C	18.752	2.33637	-0.702863	-0.233303420454545
C	19.9676	2.96507	-0.276693	0.0999025795454545
C	17.5811	4.36976	-0.48855	-0.225144420454545
C	18.7249	5.01931	-0.00810403	0.0992315795454545
C	19.8863	4.25668	0.195925	-0.215427420454545
C	16.1975	2.33561	-0.705191	-0.153649420454545
H	16.6636	4.89836	-0.718825	0.121967579545455
H	20.7988	4.59326	0.724742	0.120079579545455
H	18.8256	1.44477	-1.34308	0.122832579545455
H	16.2196	1.45183	-1.30621	0.116065579545455
C	17.7367	7.19669	0.549132	-0.215406420454545
C	18.8446	6.47981	0.13232	0.0992295795454546
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C	17.5845	8.62597	0.265362	0.0999615795454546
C	18.7937	9.27603	-0.156025	-0.233389420454545
C	19.9657	8.58883	-0.450094	0.147548579545455
C	21.1545	9.26891	-0.697924	-0.153739420454545
H	17.0724	6.79271	1.28133	0.120045579545455
H	20.6585	6.65397	-1.01054	0.121983579545455
H	18.8376	10.3717	-0.276627	0.122867579545455
H	20.9803	10.2565	-1.07983	0.116080579545455
C	23.6929	9.60315	-0.393142	0.147468579545455
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C	26.1469	9.43773	-0.801475	0.0999025795454545
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C	24.9646	11.6304	-0.90131	0.0992325795454545
C	26.0369	10.8281	-1.10979	-0.215428420454545
C	22.4433	8.93146	-0.377209	-0.153650420454545
H	22.8715	11.5742	-0.392762	0.121967579545455

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H	22.489	7.88914	0.0357788	0.116064579545455
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C	113.242	15.1433	0.551661	0.0999575795454545
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C	16.2749	15.1157	0.0204044	0.147543579545455
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H	13.1363	13.2791	1.43216	0.120045579545455
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H	114.459	16.8305	-0.164985	0.122866579545455
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C	20.158	15.9823	-0.0551114	0.147472579545455
C	21.3791	15.238	-0.137204	-0.233308420454545
C	22.6035	15.9178	-0.449716	0.0999045795454545
C	20.2579	17.3839	-0.164854	-0.225149420454545
C	21.4329	18.0387	-0.453556	0.0992355795454545
C	22.572	17.269	-0.746125	-0.215432420454545
C	18.9095	15.3488	0.0399776	-0.153658420454545
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H	19.0331	14.3048	0.298212	0.116065579545455
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C	27.918	21.695	-0.0102067	-0.233307420454545
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C	26.69	23.7029	0.338112	-0.225148420454545
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H	29.934	24.0426	1.10716	0.120079579545455
H	27.8354	20.7044	-0.501235	0.122832579545455
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C	26.3238	15.0333	-0.231499	0.147549579545455
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H	27.3795	16.7083	0.513474	0.116080579545455
C	30.0341	15.9986	-0.0132458	0.147468579545455
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C	30.2172	17.3954	-0.015738	-0.225144420454545
C	31.3871	18.0356	0.379998	0.0992315795454545
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H	34.1397	22.986	-1.02678	0.116080579545455
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C	37.7676	21.9283	0.21744	-0.233303420454545
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C	37.7716	24.6614	-0.312158	0.0992325795454545
C	38.8869	23.8939	-0.66805	-0.215428420454545
C	35.2712	21.922	0.485096	-0.153650420454545
H	35.7168	24.637	0.193729	0.121967579545455

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H	39.7659	24.3829	-1.04366	0.120079579545455
H	37.7386	20.9019	0.658855	0.122832579545455
H	35.3493	21.0332	1.09604	0.116064579545455
C	21.1169	0.802817	-0.0655332	-0.215400420454545
C	47.7093	25.8177	-0.144404	0.0992255795454546
C	23.4827	0.608402	-0.446452	-0.225199420454545
C	21.2259	2.20591	-0.30653	0.0999575795454545
C	22.457	2.75134	-0.694165	-0.233383420454545
C	23.629	2.01205	-0.472732	0.147543579545455
C	24.8741	2.66065	-0.544855	-0.153730420454545
H	20.1759	0.451132	0.33374	0.120045579545455
H	24.3923	-0.00285411	-0.587626	0.121982579545455
H	22.4461	3.69501	-1.17228	0.122866579545455
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H	26.1246	1.46124	0.732783	0.116065579545455
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C	28.5443	6.46475	-0.740929	0.0992265795454546
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C	29.817	8.55399	-0.331049	0.147545579545455
C	31.067	9.21768	-0.298424	-0.153732420454545
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H	30.4347	6.56365	0.229029	0.121983579545455
H	28.7116	10.4009	-0.441117	0.122867579545455
H	31.0537	10.2433	-0.0156474	0.116080579545455
C	33.6254	9.36975	-0.481228	0.147472579545455
C	34.9165	8.76602	-0.596629	-0.233307420454545
C	36.1161	9.40482	-0.187981	0.0999045795454545
C	33.7103	10.7856	-0.385883	-0.225148420454545
C	34.8361	11.4775	0.0534426	0.0992365795454545
C	35.9305	10.6732	0.321706	-0.215432420454545
C	32.3824	8.71918	-0.463967	-0.153655420454545
H	32.9288	11.4491	-0.862733	0.121968579545455

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H	36.7452	11.1921	0.9453	0.120079579545455
H	34.9737	7.71906	-0.831931	0.122832579545455
H	32.4102	7.55202	-0.52648	0.116065579545455
C	31.1901	0.877426	-1.13494	-0.215407420454545
C	32.3611	0.1249	-0.686913	0.0992295795454546
C	33.4284	0.822206	-0.135918	-0.225204420454545
C	31.0006	2.24531	-0.790954	0.0999605795454546
C	32.1984	2.90909	-0.516087	-0.233388420454545
C	33.442	2.21117	-0.298408	0.147549579545455
C	34.6884	2.8555	-0.225734	-0.153738420454545
H	30.5834	0.507403	-1.9826	0.120044579545455
H	34.3324	0.224256	0.199851	0.121984579545455
H	32.2126	4.02764	-0.469831	0.122867579545455
H	34.6473	3.87634	0.25611	0.116080579545455
C	37.2499	3.09633	-0.567027	0.147468579545455
C	38.4466	2.31163	-0.520403	-0.233303420454545
C	39.73	2.90417	-0.143751	0.0999025795454545
C	37.3855	4.4957	-0.669951	-0.225144420454545
C	38.5639	5.11256	-0.332915	0.0992315795454545
C	39.6353	4.28156	0.154473	-0.215427420454545
C	35.9777	2.40193	-0.691298	-0.153649420454545
H	36.614	5.03035	-1.26197	0.121967579545455
H	40.4137	4.67857	0.774189	0.120079579545455
H	38.4187	1.27834	-0.869234	0.122832579545455
H	36.0272	1.43946	-1.18547	0.116065579545455
C	37.5657	7.37307	0.128212	-0.215406420454545
C	38.6435	6.5273	-0.209946	0.0992295795454546
C	39.817	7.19473	-0.647311	-0.225204420454545
C	37.41	8.69423	-0.257679	0.0999615795454546
C	38.5904	9.33308	-0.602172	-0.233389420454545
C	39.854	8.57844	-0.657053	0.147548579545455
C	41.0568	9.30714	-0.945635	-0.153739420454545
H	36.6617	6.91482	0.526003	0.120045579545455
H	40.5436	6.71827	-1.27933	0.121983579545455
H	38.6103	10.3424	-0.928565	0.122867579545455
H	40.9207	10.2375	-1.52962	0.116080579545455
C	43.6675	9.62533	-0.771455	0.147468579545455
C	44.8556	8.88457	-0.867771	-0.233303420454545
C	46.1206	9.48318	-1.14123	0.0999025795454545
C	43.6875	11.0269	-0.799428	-0.225145420454545
C	44.8869	11.6513	-0.929611	0.0992325795454545
C	46.099	10.9301	-1.20273	-0.215428420454545
C	42.3575	8.94659	-0.607332	-0.153650420454545
H	42.717	11.5208	-0.696987	0.121967579545455

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H	46.9253	11.4451	-1.62931	0.120079579545455
H	44.8215	7.84104	-0.554587	0.122832579545455
H	42.4786	7.9488	-0.332797	0.116064579545455
C	33.769	13.7773	0.411428	-0.215400420454545
C	34.8365	12.9556	0.0496497	0.0992255795454546
C	35.9704	13.6202	-0.417175	-0.225199420454545
C	33.7423	15.146	0.258086	0.0999575795454545
C	35.0169	15.7118	0.00156347	-0.233383420454545
C	36.1939	14.9674	-0.175788	0.147543579545455
C	37.5134	15.5453	0.175631	-0.153730420454545
H	32.9272	13.2271	0.896108	0.120045579545455
H	36.6174	13.0367	-1.14396	0.121982579545455
H	35.0796	16.8275	-0.0684041	0.122866579545455
H	37.4911	16.4949	0.819705	0.116079579545455
C	40.0522	15.9573	-0.198931	0.147472579545455
C	41.3239	15.4064	-0.132694	-0.233308420454545
C	42.5829	16.0748	-0.36469	0.0999045795454545
C	40.0488	17.3476	-0.103585	-0.225149420454545
C	41.2211	18.1079	-0.391417	0.0992355795454545
C	42.3709	17.4318	-0.76349	-0.215432420454545
C	38.8514	15.2573	-0.239077	-0.153658420454545
H	39.2391	17.9065	0.292484	0.121968579545455
H	43.2194	17.93	-1.30123	0.120079579545455
H	41.4548	14.3692	0.00261882	0.122832579545455
H	38.9491	14.3055	-0.809359	0.116065579545455
C	40.2015	20.3218	-0.733994	-0.215403420454545
C	41.2199	19.5301	-0.270431	0.0992265795454546
C	42.3623	20.1656	0.205964	-0.225200420454545
C	40.1926	21.7122	-0.479741	0.0999585795454545
C	41.5259	22.259	-0.479587	-0.233385420454545
C	42.6017	21.4938	-0.0599453	0.147545579545455
C	43.9094	22.0696	-0.0620339	-0.153732420454545
H	39.451	19.962	-1.46041	0.120045579545455
H	43.0071	19.4661	0.820805	0.121983579545455
H	41.7075	23.2647	-0.716925	0.122867579545455
H	43.8921	23.1156	-0.175435	0.116080579545455
C	46.4674	22.2424	-0.315069	0.147472579545455
C	47.7901	21.6185	-0.280427	-0.233307420454545
C	48.9057	22.3121	0.170679	0.0999045795454545
C	46.5126	23.6666	-0.497359	-0.225148420454545
C	47.6358	24.414	0.00177302	0.0992365795454545
C	48.7102	23.6307	0.453226	-0.215432420454545
C	45.2451	21.5668	-0.154461	-0.153655420454545
H	45.8571	24.2114	-1.14843	0.121968579545455

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H	49.4474	24.1722	1.00837	0.120079579545455
H	47.7224	20.4947	-0.462193	0.122832579545455
H	45.3327	20.4589	-0.315696	0.116065579545455
C	43.8858	14.035	-1.01944	-0.215407420454545
C	44.917	13.0935	-0.76333	0.0992295795454546
C	46.0524	13.631	-0.169279	-0.225204420454545
C	43.7883	15.2794	-0.397879	0.0999605795454546
C	44.9622	15.7167	0.19011	-0.233388420454545
C	46.1782	15.0675	-0.127271	0.147549579545455
C	47.3819	15.7081	-0.370771	-0.153738420454545
H	43.2334	13.8374	-1.92942	0.120044579545455
H	46.7842	12.9409	0.213065	0.121984579545455
H	45.0966	16.5456	0.856223	0.122867579545455
H	47.2687	16.8019	-0.515514	0.116080579545455
C	49.9987	15.9931	-0.227655	0.147468579545455
C	51.1852	15.1874	-0.176621	-0.233303420454545
C	52.4181	15.8146	0.183706	0.0999025795454545
C	50.1975	17.4563	-0.185801	-0.225144420454545
C	51.3466	18.018	0.287417	0.0992315795454545
C	52.3161	17.1204	0.724964	-0.215427420454545
C	48.7456	15.306	-0.283281	-0.153649420454545
H	49.3975	18.1378	-0.459567	0.121967579545455
H	53.0708	17.4345	1.53105	0.120079579545455
H	51.2131	14.1076	-0.385429	0.122832579545455
H	48.8269	14.2516	-0.26057	0.116065579545455
C	50.3052	20.2364	0.625615	-0.215406420454545
C	51.4725	19.456	0.416796	0.0992295795454546
C	52.6543	20.1122	0.0637046	-0.225204420454545
C	50.2043	21.6258	0.253781	0.0999615795454546
C	51.4187	22.1802	-0.208091	-0.233389420454545
C	52.7259	21.5229	-0.211243	0.147548579545455
C	53.976	22.189	-0.198288	-0.153739420454545
H	49.4209	19.8067	1.12293	0.120045579545455
H	53.5989	19.5838	0.0771943	0.121983579545455
H	51.3746	23.1767	-0.676047	0.122867579545455
H	53.8997	23.0993	0.373904	0.116080579545455
C	56.5181	22.4709	-0.5364	0.147468579545455
C	57.6887	21.7258	-0.639019	-0.233303420454545
C	58.9168	22.327	-0.750942	0.0999025795454545
C	56.644	23.8389	-0.306748	-0.225145420454545
C	57.8298	24.5457	-0.613538	0.0992325795454545
C	58.8813	23.7681	-0.989844	-0.215428420454545
C	55.1888	21.8576	-0.680379	-0.153650420454545
H	55.8216	24.3798	0.112616	0.121967579545455

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H	59.8087	24.2482	-1.46318	0.120079579545455
H	57.657	20.6691	-0.476148	0.122832579545455
H	55.2366	21.0394	-1.37704	0.116064579545455
C	41.034	0.866625	0.13279	-0.215400420454545
C	67.5775	25.9438	-0.124066	0.0992255795454546
C	43.2512	0.747633	-0.529465	-0.225199420454545
C	40.9796	2.20755	-0.0845968	0.0999575795454545
C	42.2231	2.82752	-0.274486	-0.233383420454545
C	43.4081	2.14281	-0.431822	0.147543579545455
C	44.7521	2.6539	-0.810097	-0.153730420454545
H	40.1297	0.365524	0.399741	0.120045579545455
H	44.1056	0.320529	-0.968264	0.121982579545455
H	42.229	3.94314	-0.043678	0.122866579545455
H	44.7325	3.50174	-1.47231	0.116079579545455
C	47.2753	3.09995	-0.383513	0.147472579545455
C	48.5132	2.39299	-0.112982	-0.233308420454545
C	49.7117	2.98082	-0.587042	0.0999045795454545
C	47.3191	4.50488	-0.479301	-0.225149420454545
C	48.505	5.07405	-0.942867	0.0992355795454545
C	49.5909	4.23793	-1.15923	-0.215432420454545
C	46.0521	2.33979	-0.367212	-0.153658420454545
H	46.6838	5.13399	0.15876	0.121968579545455
H	50.3657	4.44494	-2.00833	0.120079579545455
H	48.4337	1.45768	0.434784	0.122832579545455
H	46.2078	1.33742	0.0346357	0.116065579545455
C	47.5478	7.32911	-1.52768	-0.215403420454545
C	48.5742	6.50042	-1.0199	0.0992265795454546
C	49.7892	7.14322	-0.588045	-0.225200420454545
C	47.4336	8.74112	-1.22534	0.0999585795454545
C	48.7246	9.30019	-1.05843	-0.233385420454545
C	49.927	8.54993	-0.928113	0.147545579545455
C	51.2408	9.09596	-1.13534	-0.153732420454545
H	46.7498	6.92477	-2.32697	0.120045579545455
H	50.5144	6.48678	-0.0296398	0.121983579545455
H	48.7601	10.3727	-0.733275	0.122867579545455
H	51.31	9.84585	-1.93655	0.116080579545455
C	53.7343	9.53175	-0.644799	0.147472579545455
C	54.9568	8.8037	-0.594632	-0.233307420454545
C	56.1556	9.36961	0.0103246	0.0999045795454545
C	53.7791	10.8998	-0.450368	-0.225148420454545
C	54.8896	11.5015	0.119989	0.0992365795454545
C	55.9645	10.7266	0.517652	-0.215432420454545
C	52.5117	8.80289	-0.61868	-0.153655420454545
H	52.9352	11.4413	-0.602907	0.121968579545455

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H	56.7895	11.1262	1.19215	0.120079579545455
H	54.9568	7.76695	-0.91809	0.122832579545455
H	52.5742	7.79467	-0.19838	0.116065579545455
C	51.1168	0.973797	-0.940555	-0.215407420454545
C	52.1649	0.209225	-0.478143	0.0992295795454546
C	53.3245	0.860649	-0.162812	-0.225204420454545
C	51.009	2.29451	-0.595124	0.0999605795454546
C	52.2192	2.92602	-0.305323	-0.233388420454545
C	53.4105	2.20815	-0.18009	0.147549579545455
C	54.6608	2.83249	0.0719681	-0.153738420454545
H	50.2033	0.555335	-1.35945	0.120044579545455
H	54.0999	0.259123	0.451739	0.121984579545455
H	52.1703	3.97961	0.00517302	0.122867579545455
H	54.5679	3.72516	0.727602	0.116080579545455
C	57.1428	3.16592	-0.0931702	0.147468579545455
C	58.3171	2.36977	0.0890083	-0.233303420454545
C	59.5693	2.91412	0.404047	0.0999025795454545
C	57.2897	4.56375	-0.134631	-0.225144420454545
C	58.5206	5.20175	0.19338	0.0992315795454545
C	59.5643	4.34501	0.608866	-0.215427420454545
C	55.9325	2.47779	-0.374722	-0.153649420454545
H	56.5152	5.14927	-0.686784	0.121967579545455
H	60.3936	4.73028	1.21774	0.120079579545455
H	58.3098	1.31655	-0.114855	0.122832579545455
H	55.9876	1.62154	-1.05088	0.116065579545455
C	57.4291	7.37542	0.650222	-0.215406420454545
C	58.5941	6.56293	0.432254	0.0992295795454546
C	59.7241	7.32842	0.347578	-0.225204420454545
C	57.4238	8.75117	0.207645	0.0999615795454546
C	58.6012	9.37849	0.144009	-0.233389420454545
C	59.8202	8.70877	0.343558	0.147548579545455
C	61.0649	9.4532	0.395916	-0.153739420454545
H	56.5065	6.93332	0.898511	0.120045579545455
H	60.7248	6.81647	0.106727	0.121983579545455
H	58.6244	10.5347	-0.03062	0.122867579545455
H	60.9502	10.352	0.920107	0.116080579545455
C	63.6622	9.67364	0.00896763	0.147468579545455
C	64.8414	8.90884	0.244881	-0.233303420454545
C	66.0739	9.35772	-0.0805114	0.0999025795454545
C	63.7609	11.0636	-0.12845	-0.225145420454545
C	65.0099	11.6552	-0.484063	0.0992325795454545
C	66.0841	10.7179	-0.569144	-0.215428420454545
C	62.3751	9.08546	-0.135578	-0.153650420454545
H	63.0355	11.7044	0.315998	0.121967579545455

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H	66.919	11.0547	-1.17489	0.120079579545455
H	64.6994	7.93636	0.609863	0.122832579545455
H	62.2942	8.1314	-0.690977	0.116064579545455
C	53.8093	13.7382	0.423923	-0.215400420454545
C	54.9045	12.9788	0.105067	0.0992255795454546
C	56.0312	13.692	-0.252652	-0.225199420454545
C	53.6721	15.1235	0.118681	0.0999575795454545
C	54.8396	15.7344	-0.383112	-0.233383420454545
C	56.0662	15.0274	-0.382091	0.147543579545455
C	57.4095	15.6845	-0.620082	-0.153730420454545
H	53.0542	13.3035	1.04698	0.120045579545455
H	56.9741	13.2052	-0.195985	0.121982579545455
H	54.7535	16.7036	-0.825815	0.122866579545455
H	57.2949	16.5629	-1.30814	0.116079579545455
C	59.9749	15.9787	-0.435523	0.147472579545455
C	61.2553	15.3538	-0.293576	-0.233308420454545
C	62.5175	15.8857	-0.622362	0.0999045795454545
C	60.0367	17.3827	-0.655806	-0.225149420454545
C	61.276	18.0302	-0.915036	0.0992355795454545
C	62.4658	17.2049	-1.0277	-0.215432420454545
C	58.6984	15.4338	-0.0932962	-0.153658420454545
H	59.1303	17.9348	-0.652475	0.121968579545455
H	63.2639	17.5643	-1.62677	0.120079579545455
H	61.292	14.3454	0.198417	0.122832579545455
H	58.741	14.5316	0.545038	0.116065579545455
C	60.2756	20.3178	-1.26684	-0.215403420454545
C	61.3042	19.4382	-0.95074	0.0992265795454546
C	62.3654	20.0171	-0.236216	-0.225200420454545
C	60.1739	21.6855	-0.765686	0.0999585795454545
C	61.3881	22.1726	-0.284965	-0.233385420454545
C	62.5571	21.375	-0.177241	0.147545579545455
C	63.8744	21.9315	0.0722057	-0.153732420454545
H	59.5386	19.9977	-2.02953	0.120045579545455
H	62.9479	19.4324	0.494812	0.121983579545455
H	61.4198	23.1722	0.182905	0.122867579545455
H	63.832	22.8536	0.675747	0.116080579545455
C	66.4518	22.3326	-0.323448	0.147472579545455
C	67.7052	21.683	-0.20224	-0.233307420454545
C	68.8636	22.4123	0.077746	0.0999045795454545
C	66.4862	23.7738	-0.420747	-0.225148420454545
C	67.6419	24.517	-0.128718	0.0992365795454545
C	68.796	23.7988	0.230088	-0.215432420454545
C	65.1559	21.5525	-0.331648	-0.153655420454545
H	65.5543	24.1722	-0.951003	0.121968579545455

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H	69.5458	24.3947	0.766565	0.120079579545455
H	67.6963	20.618	-0.201409	0.122832579545455
H	65.2808	20.585	-0.939704	0.116065579545455
C	63.9104	13.8741	-1.00919	-0.215407420454545
C	65.0915	13.0724	-0.65568	0.0992295795454546
C	66.2132	13.8165	-0.335476	-0.225204420454545
C	63.7342	15.2066	-0.595069	0.0999605795454546
C	64.9646	15.842	-0.224247	-0.233388420454545
C	66.189	15.2151	-0.306788	0.147549579545455
C	67.4131	15.8526	-0.037858	-0.153738420454545
H	63.0219	13.3555	-1.55884	0.120044579545455
H	67.1285	13.2971	-0.141226	0.121984579545455
H	64.8647	16.8644	0.0926852	0.122867579545455
H	67.2821	16.8119	0.38379	0.116080579545455
C	69.9974	16.1215	-0.155801	0.147468579545455
C	71.1693	15.2733	-0.0555116	-0.233303420454545
C	72.427	15.8625	0.315858	0.0999025795454545
C	70.186	17.5048	-0.160492	-0.225144420454545
C	71.4153	18.121	0.17261	0.0992315795454545
C	72.3903	17.2274	0.705603	-0.215427420454545
C	68.7046	15.456	-0.301273	-0.153649420454545
H	69.3338	18.1986	-0.457576	0.121967579545455
H	73.1132	17.6089	1.41012	0.120079579545455
H	70.9846	14.2014	-0.226118	0.122832579545455
H	68.7879	14.4793	-0.811656	0.116065579545455
C	70.2649	20.4186	0.639365	-0.215406420454545
C	71.407	19.6379	0.316894	0.0992295795454546
C	72.5885	20.2249	-0.0265755	-0.225204420454545
C	70.1934	21.8146	0.23191	0.0999615795454546
C	71.4563	22.3627	-0.0990194	-0.233389420454545
C	72.6597	21.628	-0.121366	0.147548579545455
C	73.8783	22.3004	0.118401	-0.153739420454545
H	69.4524	20.0073	1.20038	0.120045579545455
H	73.5585	19.7288	-0.303734	0.121983579545455
H	71.4453	23.3631	-0.523014	0.122867579545455
H	73.8785	23.0292	0.978874	0.116080579545455
C	76.415	22.5133	-0.109299	0.147468579545455
C	77.6176	21.8901	0.0498743	-0.233303420454545
C	78.9045	22.4582	-0.237764	0.0999025795454545
C	76.5063	23.9292	-0.0330057	-0.225145420454545
C	77.6241	24.604	-0.455039	0.0992325795454545
C	78.7675	23.8398	-0.783307	-0.215428420454545
C	75.1256	22.0147	-0.384727	-0.153650420454545
H	75.6702	24.4675	0.341196	0.121967579545455

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H	79.5708	24.2464	-1.43145	0.120079579545455
H	77.6027	20.87	0.356899	0.122832579545455
H	75.123	21.3517	-1.26358	0.116064579545455
C	60.9714	0.965747	1.10014	-0.215400420454545
C	62.043	0.138571	0.768782	0.0992255795454546
C	63.1756	0.673552	0.118212	-0.225199420454545
C	60.8304	2.26124	0.534943	0.0999575795454545
C	62.0314	2.69824	-0.0973395	-0.233383420454545
C	63.2683	2.09803	-0.0744217	0.147543579545455
C	64.5426	2.68515	-0.323564	-0.153730420454545
H	60.1305	0.489555	1.67005	0.120045579545455
H	63.9336	-0.0134135	-0.202529	0.121982579545455
H	61.9869	3.63301	-0.586725	0.122866579545455
H	64.4693	3.54416	-0.989171	0.116079579545455
C	67.068	2.90084	0.0905277	0.147472579545455
C	68.2679	2.12088	-0.000582037	-0.233308420454545
C	69.5392	2.81865	-0.249077	0.0999045795454545
C	67.2596	4.26938	0.245004	-0.225149420454545
C	68.3458	4.95375	-0.241111	0.0992355795454545
C	69.3956	4.14301	-0.64978	-0.215432420454545
C	65.8269	2.28575	0.00133475	-0.153658420454545
H	66.536	4.8562	0.81057	0.121968579545455
H	70.0366	4.53982	-1.46512	0.120079579545455
H	68.2787	1.03365	0.354022	0.122832579545455
H	65.9499	1.27204	0.267855	0.116065579545455
C	67.36	7.23382	-0.233887	-0.215403420454545
C	68.5264	6.43155	-0.166737	0.0992265795454546
C	69.6953	7.16005	0.179394	-0.225200420454545
C	67.3029	8.6228	-0.0516478	0.0999585795454545
C	68.5647	9.27192	0.0148023	-0.233385420454545
C	69.7575	8.54735	0.00839113	0.147545579545455
C	71.0415	9.1203	-0.244935	-0.153732420454545
H	66.3778	6.85492	-0.543256	0.120045579545455
H	70.4643	6.76384	0.858331	0.121983579545455
H	68.5802	10.3456	0.27488	0.122867579545455
H	70.9955	9.89621	-0.987296	0.116080579545455
C	73.5769	9.4399	0.375266	0.147472579545455
C	74.7679	8.71464	0.624372	-0.233307420454545
C	76.0572	9.29337	0.701366	0.0999045795454545
C	73.798	10.8413	0.224699	-0.225148420454545
C	75.0098	11.5189	0.559812	0.0992365795454545
C	76.1152	10.734	0.75463	-0.215432420454545
C	72.2617	8.84843	0.416514	-0.153655420454545
H	73.0435	11.4759	-0.351003	0.121968579545455

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H	77.0279	11.1829	1.21331	0.120079579545455
H	74.6811	7.67746	0.891274	0.122832579545455
H	72.0989	8.35958	1.36237	0.116065579545455
C	70.8214	0.746181	-0.616993	-0.215407420454545
C	97.326	25.8116	-0.165333	0.0992295795454546
C	73.0065	0.583819	0.381308	-0.225204420454545
C	70.7723	2.08482	-0.179494	0.0999605795454546
C	71.9869	2.6642	0.143926	-0.233388420454545
C	73.1899	1.93191	0.23125	0.147549579545455
C	74.5002	2.65109	0.31024	-0.153738420454545
H	69.9723	0.342512	-1.23853	0.120044579545455
H	73.7407	-0.137852	0.793146	0.121984579545455
H	71.9401	3.69415	0.478746	0.122867579545455
H	74.4062	3.58658	0.880469	0.116080579545455
C	77.0086	2.99121	0.137559	0.147468579545455
C	78.2354	2.27452	0.262273	-0.233303420454545
C	79.4633	2.78513	0.606537	0.0999025795454545
C	77.1138	4.39368	0.320622	-0.225144420454545
C	78.3596	4.94254	0.582174	0.0992315795454545
C	79.3858	4.14089	1.08797	-0.215427420454545
C	75.7638	2.36102	-0.184726	-0.153649420454545
H	76.2909	4.96361	0.0332212	0.121967579545455
H	80.1316	4.39217	1.8167	0.120079579545455
H	78.1018	1.21677	0.29863	0.122832579545455
H	75.9738	1.33655	-0.672441	0.116065579545455
C	77.3161	7.13794	0.891038	-0.215406420454545
C	78.441	6.33716	0.60558	0.0992295795454546
C	79.639	7.00783	0.336172	-0.225204420454545
C	77.2832	8.53609	0.604756	0.0999615795454546
C	78.5544	9.07555	0.230924	-0.233389420454545
C	79.7431	8.38947	0.370138	0.147548579545455
C	80.9922	9.02914	0.303222	-0.153739420454545
H	76.7078	6.69693	1.66973	0.120045579545455
H	80.4883	6.33742	0.0169821	0.121983579545455
H	78.5306	10.1037	-0.17296	0.122867579545455
H	80.8882	10.0844	-0.0248309	0.116080579545455
C	83.4623	9.39476	0.751469	0.147468579545455
C	84.6339	8.697	0.685239	-0.233303420454545
C	85.8337	9.31713	0.391139	0.0999025795454545
C	83.5169	10.7214	1.08516	-0.225145420454545
C	84.5852	11.5658	0.657777	0.0992325795454545
C	85.7178	10.7436	0.156298	-0.215428420454545
C	82.2449	8.63802	0.743092	-0.153650420454545
H	82.6463	11.3079	1.35793	0.121967579545455

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H	86.4997	11.2056	-0.495961	0.120079579545455
H	84.543	7.55484	0.757789	0.122832579545455
H	82.3291	7.59569	1.17582	0.116064579545455
C	73.792	13.7433	0.997053	-0.215400420454545
C	74.9215	12.9431	0.594635	0.0992255795454546
C	76.134	13.6354	0.212005	-0.225199420454545
C	73.6416	15.064	0.476556	0.0999575795454545
C	74.8701	15.6647	0.027096	-0.233383420454545
C	76.1189	15.0177	0.21143	0.147543579545455
C	77.2812	15.7832	0.381057	-0.153730420454545
H	72.9555	13.4597	1.60791	0.120045579545455
H	77.0419	13.084	0.0208761	0.121982579545455
H	74.78	16.7414	-0.0944527	0.122866579545455
H	77.1053	16.6607	0.939677	0.116079579545455
C	79.7808	16.0358	0.182079	0.147472579545455
C	80.9764	15.3016	0.442683	-0.233308420454545
C	82.2992	15.9099	0.244953	0.0999045795454545
C	79.8953	17.4311	0.252903	-0.225149420454545
C	81.1139	18.1288	0.18463	0.0992355795454545
C	82.1874	17.2476	-0.110515	-0.215432420454545
C	78.5498	15.4985	-0.160968	-0.153658420454545
H	78.97	17.9202	0.613566	0.121968579545455
H	82.9965	17.6588	-0.707002	0.120079579545455
H	80.8971	14.3146	0.785695	0.122832579545455
H	78.6296	14.744	-0.997231	0.116065579545455
C	80.2216	20.3642	-0.430632	-0.215403420454545
C	81.2086	19.5679	0.194751	0.0992265795454546
C	82.258	20.2489	0.854521	-0.225200420454545
C	80.126	21.7404	-0.0882628	0.0999585795454545
C	81.297	22.3289	0.390007	-0.233385420454545
C	82.4749	21.6113	0.586503	0.147545579545455
C	83.7918	22.171	0.360341	-0.153732420454545
H	79.4759	19.9795	-1.15311	0.120045579545455
H	82.8999	19.5656	1.43089	0.121983579545455
H	81.316	23.4304	0.417639	0.122867579545455
H	83.8183	23.207	0.12731	0.116080579545455
C	86.2953	22.3775	0.68585	0.147472579545455
C	87.5689	21.7354	0.833616	-0.233307420454545
C	88.7257	22.3636	1.03273	0.0999045795454545
C	86.35	23.7504	0.460478	-0.225148420454545
C	87.5013	24.484	0.899062	0.0992365795454545
C	88.5645	23.7443	1.32381	-0.215432420454545
C	85.0263	21.6589	0.627851	-0.153655420454545
H	85.8203	24.1121	-0.460271	0.121968579545455

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H	89.3212	24.2377	2.01936	0.120079579545455
H	87.4791	20.5998	0.767515	0.122832579545455
H	85.1463	20.5861	0.745644	0.116065579545455
C	83.5104	13.7637	0.293649	-0.215407420454545
C	84.6344	13.0029	0.716306	0.0992295795454546
C	85.8208	13.6093	1.00504	-0.225204420454545
C	83.4907	15.1916	0.315541	0.0999605795454546
C	84.749	15.7844	0.550888	-0.233388420454545
C	85.9553	15.016	0.735627	0.147549579545455
C	87.2435	15.6218	0.958834	-0.153738420454545
H	82.6871	13.2407	-0.18153	0.120044579545455
H	86.7172	13.1406	1.38937	0.121984579545455
H	84.8502	16.8631	0.885863	0.122867579545455
H	87.2301	16.4363	1.6616	0.116080579545455
C	89.7238	15.913	0.422883	0.147468579545455
C	90.9113	15.1838	0.290667	-0.233303420454545
C	92.1739	15.7994	0.625694	0.0999025795454545
C	89.8353	17.3034	0.452356	-0.225144420454545
C	91.0206	17.9582	0.821239	0.0992315795454545
C	92.0785	17.1517	0.991054	-0.215427420454545
C	88.4439	15.269	0.391405	-0.153649420454545
H	88.9184	17.8774	0.0699473	0.121967579545455
H	92.9353	17.5066	1.50602	0.120079579545455
H	90.8996	14.2263	-0.29184	0.122832579545455
H	88.447	14.2113	-0.0201386	0.116065579545455
C	90.0584	20.2295	1.2916	-0.215406420454545
C	91.0486	19.3928	0.798963	0.0992295795454546
C	92.1661	20.0371	0.230314	-0.225204420454545
C	90.0048	21.6358	0.994154	0.0999615795454546
C	91.2748	22.182	0.746503	-0.233389420454545
C	92.3853	21.4047	0.454485	0.147548579545455
C	93.6552	22.0138	0.293671	-0.153739420454545
H	89.3429	19.8129	1.9541	0.120045579545455
H	92.9175	19.5076	-0.323168	0.121983579545455
H	91.4778	23.3113	0.917667	0.122867579545455
H	93.6749	22.8638	-0.422499	0.116080579545455
C	96.1516	22.3269	0.601054	0.147468579545455
C	97.3623	21.6647	0.543496	-0.233303420454545
C	98.5127	22.2396	-0.0545686	0.0999025795454545
C	96.1635	23.7468	0.38996	-0.225145420454545
C	97.2798	24.3945	-0.100713	0.0992325795454545
C	98.3521	23.5388	-0.553159	-0.215428420454545
C	94.9159	21.6419	0.712882	-0.153650420454545
H	95.3764	24.38	0.716479	0.121967579545455

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H	98.9966	23.893	-1.38357	0.120079579545455
H	97.4723	20.6365	0.852447	0.122832579545455
H	94.9853	20.5471	1.0424	0.116064579545455
C	80.9155	0.787666	1.079	-0.215400420454545
C	82.0031	0.00822346	0.717172	0.0992255795454546
C	83.1387	0.667695	0.189479	-0.225199420454545
C	80.765	2.12412	0.670876	0.0999575795454545
C	81.984	2.78987	0.44178	-0.233383420454545
C	83.1793	2.05115	0.325315	0.147543579545455
C	84.4074	2.76998	0.0885666	-0.153730420454545
H	80.3173	0.472328	1.95013	0.120045579545455
H	109.365	26.0454	-0.408455	0.121982579545455
H	81.9346	3.83441	0.206612	0.122866579545455
H	84.3499	3.77786	-0.370013	0.116079579545455
C	86.9206	3.01012	0.483889	0.147472579545455
C	88.1281	2.30834	0.690073	-0.233308420454545
C	89.2815	2.87689	0.155887	0.0999045795454545
C	86.9448	4.41206	0.445539	-0.225149420454545
C	88.1626	5.09594	0.0995361	0.0992355795454545
C	89.2154	4.21353	-0.202516	-0.215432420454545
C	85.6955	2.28196	0.214606	-0.153658420454545
H	85.9897	4.91227	0.759934	0.121968579545455
H	90.1449	4.66378	-0.61053	0.120079579545455
H	88.1957	1.35201	1.2132	0.122832579545455
H	85.7732	1.1962	0.130271	0.116065579545455
C	87.0862	7.29596	-0.0893136	-0.215403420454545
C	88.1977	6.51412	0.159464	0.0992265795454546
C	89.3872	7.18975	0.487987	-0.225200420454545
C	87.04	8.64969	0.202629	0.0999585795454545
C	88.3148	9.38851	0.362903	-0.233385420454545
C	89.5308	8.59206	0.304568	0.147545579545455
C	90.8191	9.14153	0.152429	-0.153732420454545
H	86.2271	6.87609	-0.736985	0.120045579545455
H	90.2179	6.57624	0.932551	0.121983579545455
H	88.3275	10.4671	0.444781	0.122867579545455
H	90.7561	10.1655	-0.197443	0.116080579545455
C	93.4154	9.41079	0.346589	0.147472579545455
C	94.5921	8.62856	0.311516	-0.233307420454545
C	95.8303	9.28591	0.649012	0.0999045795454545
C	93.5394	10.8076	0.199007	-0.225148420454545
C	94.6599	11.4758	0.681593	0.0992365795454545
C	95.7136	10.6203	1.07659	-0.215432420454545
C	92.1533	8.76776	0.396122	-0.153655420454545
H	92.7518	11.4255	-0.200517	0.121968579545455

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H	96.5075	11.0292	1.68547	0.120079579545455
H	94.6794	7.57299	0.0406513	0.122832579545455
H	92.1603	7.81992	0.907871	0.116065579545455
C	90.5372	0.87701	-0.591921	-0.215407420454545
C	117.165	25.8721	-0.402101	0.0992295795454546
C	92.8611	0.669828	0.00857545	-0.225204420454545
C	90.5237	2.15201	-0.0080331	0.0999605795454546
C	91.6827	2.65495	0.569805	-0.233388420454545
C	92.9643	2.01871	0.348264	0.147549579545455
C	94.2297	2.65586	0.628594	-0.153738420454545
H	89.8057	0.474143	-1.22346	0.120044579545455
H	119.175	25.9208	0.266602	0.121984579545455
H	91.6108	3.5818	1.16106	0.122867579545455
H	94.1492	3.50408	1.28356	0.116080579545455
C	96.8519	3.02921	0.367357	0.147468579545455
C	98.1594	2.43641	0.128164	-0.233303420454545
C	99.4156	2.98358	0.510073	0.0999025795454545
C	96.9182	4.43314	0.765516	-0.225144420454545
C	98.1617	5.02567	0.85046	0.0992315795454545
C	99.3395	4.20858	1.08102	-0.215427420454545
C	95.6019	2.306	0.258061	-0.153649420454545
H	96.0258	4.98175	0.73804	0.121967579545455
H	100.178	4.67652	1.64619	0.120079579545455
H	98.1859	1.51516	-0.413555	0.122832579545455
H	95.6013	1.38397	-0.318134	0.116065579545455
C	97.1896	7.29927	1.20577	-0.215406420454545
C	98.2805	6.46548	0.930629	0.0992295795454546
C	99.4916	7.1717	0.806627	-0.225204420454545
C	97.1003	8.58535	0.680738	0.0999615795454546
C	98.3522	9.1845	0.313574	-0.233389420454545
C	99.5714	8.52417	0.524633	0.147548579545455
C	100.841	9.24671	0.645244	-0.153739420454545
H	96.4578	7.00628	1.96798	0.120045579545455
H	100.424	6.65303	1.0211	0.121983579545455
H	98.3625	10.1268	-0.263015	0.122867579545455
H	100.727	10.2578	1.06029	0.116080579545455
C	103.41	9.47664	0.49117	0.147468579545455
C	104.671	8.90093	0.773158	-0.233303420454545
C	105.813	9.41537	0.166174	0.0999025795454545
C	103.39	10.804	0.0286664	-0.225145420454545
C	104.604	11.5539	-0.116599	0.0992325795454545
C	105.714	10.7133	-0.305409	-0.215428420454545
C	102.174	8.74697	0.528539	-0.153650420454545
H	102.449	11.1581	-0.351087	0.121967579545455

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H	106.604	11.2467	-0.525039	0.120079579545455
H	104.776	8.00582	1.46102	0.122832579545455
H	102.296	7.70285	0.377772	0.116064579545455
C	93.5329	13.7694	1.10156	-0.215400420454545
C	94.5802	12.9247	0.755436	0.0992255795454546
C	95.7195	13.6044	0.172976	-0.225199420454545
C	93.4767	15.1571	0.62752	0.0999575795454545
C	94.6949	15.7226	0.198851	-0.233383420454545
C	95.9187	14.9929	0.205711	0.147543579545455
C	97.0981	15.7032	-0.0927711	-0.153730420454545
H	92.6431	13.3139	1.56164	0.120045579545455
H	96.412	12.9308	-0.439069	0.121982579545455
H	94.6888	16.7643	-0.0927547	0.122866579545455
H	97.0093	16.6907	-0.499626	0.116079579545455
C	99.6386	15.9161	0.280147	0.147472579545455
C	100.854	15.2115	0.360887	-0.233308420454545
C	102.074	15.8336	-0.0748829	0.0999045795454545
C	99.7097	17.2906	0.227347	-0.225149420454545
C	100.894	17.9484	-0.0621224	0.0992355795454545
C	101.976	17.1658	-0.467301	-0.215432420454545
C	98.4269	15.257	0.303958	-0.153658420454545
H	98.7944	17.8966	0.343086	0.121968579545455
H	102.598	17.5106	-1.23145	0.120079579545455
H	100.814	14.1924	0.79799	0.122832579545455
H	98.4634	14.2232	0.538655	0.116065579545455
C	99.8725	20.1512	-0.455395	-0.215403420454545
C	100.998	19.3815	-0.0860298	0.0992265795454546
C	102.181	20.1368	0.130904	-0.225200420454545
C	99.7818	21.5237	-0.0449184	0.0999585795454545
C	101.019	22.1442	0.355358	-0.233385420454545
C	102.265	21.475	0.422504	0.147545579545455
C	103.54	22.0622	0.591631	-0.153732420454545
H	99.0673	19.7886	-1.14738	0.120045579545455
H	103.143	19.5526	0.0778711	0.121983579545455
H	100.992	23.2238	0.528024	0.122867579545455
H	103.515	22.9579	1.23519	0.116080579545455
C	106.078	22.4209	0.342234	0.147472579545455
C	107.292	21.6903	0.424976	-0.233307420454545
C	108.446	22.3209	0.799823	0.0999045795454545
C	106.18	23.837	0.392398	-0.225148420454545
C	107.358	24.4724	0.877373	0.0992365795454545
C	108.407	23.6783	1.29379	-0.215432420454545
C	104.819	21.7398	0.0725264	-0.153655420454545
H	105.36	24.3743	0.0361811	0.121968579545455

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H	109.174	23.8776	1.97808	0.120079579545455
H	107.254	20.6345	0.23855	0.122832579545455
H	104.957	20.7777	-0.444201	0.116065579545455
C	103.484	13.7877	-0.389531	-0.215407420454545
C	104.52	12.9739	0.0130899	0.0992295795454546
C	105.612	13.7348	0.445336	-0.225204420454545
C	103.302	15.1694	-0.1669	0.0999605795454546
C	104.518	15.8578	0.0144003	-0.233388420454545
C	105.653	15.1118	0.289289	0.147549579545455
C	106.969	15.7682	0.2637	-0.153738420454545
H	102.759	13.3297	-1.06364	0.120044579545455
H	106.343	13.2657	1.0939	0.121984579545455
H	104.58	16.9519	-0.191244	0.122867579545455
H	106.949	16.8014	0.461426	0.116080579545455
C	109.485	15.8833	0.107432	0.147468579545455
C	110.705	15.217	0.221022	-0.233303420454545
C	111.958	15.8469	0.473301	0.0999025795454545
C	109.52	17.3192	0.0461282	-0.225144420454545
C	110.674	17.9503	0.544925	0.0992315795454545
C	111.834	17.2262	0.874084	-0.215427420454545
C	108.222	15.2718	-0.193948	-0.153649420454545
H	108.7	17.6667	-0.547637	0.121967579545455
H	112.576	17.7095	1.41142	0.120079579545455
H	110.709	14.1622	0.0380091	0.122832579545455
H	108.135	14.4206	-0.833555	0.116065579545455
C	109.774	20.2173	0.936471	-0.215406420454545
C	110.833	19.3787	0.393738	0.0992295795454546
C	111.983	20.0624	0.0137959	-0.225204420454545
C	109.754	21.6425	0.716759	0.0999615795454546
C	110.981	22.2079	0.426394	-0.233389420454545
C	112.158	21.4477	0.106424	0.147548579545455
C	113.385	22.0752	-0.192359	-0.153739420454545
H	108.95	19.6996	1.53061	0.120045579545455
H	112.851	19.4642	-0.260288	0.121983579545455
H	111.025	23.286	0.584497	0.122867579545455
H	113.241	23.1994	-0.617079	0.116080579545455
C	115.988	22.2659	0.0441878	0.147468579545455
C	117.277	21.6171	-0.0518533	-0.233303420454545
C	118.387	22.3115	-0.47837	0.0999025795454545
C	115.947	23.6657	-0.0450413	-0.225145420454545
C	117.075	24.4128	-0.455025	0.0992325795454545
C	118.101	23.6464	-0.945448	-0.215428420454545
C	114.721	21.6615	0.0449233	-0.153650420454545
H	115.021	24.3362	0.274486	0.121967579545455

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H	118.851	24.1598	-1.59737	0.120079579545455
H	117.138	20.5514	0.0110582	0.122832579545455
H	114.709	20.6094	0.281116	0.116064579545455

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