Periodic DFT investigation of the effect of aluminium content on the properties of the acid zeolite H-FER.

L. Grajciar,[a] C. O. Areán,[b] A. Pulido[a] and P. Nachtigall[a]

Supplementary Information:

Table S1. Relative deprotonation energy for the most stable configuration of BA sites for each Si/Al ratio (H-FER(71), H-FER(35) and H-FER(8) models) and Al distribution considered.

H-FER sample	Aluminium location[a]	Oxygen position[b]	ΔE_{deprot}[c] (kJ/mol)	ΔE_{deprot}[d] (kJ/mol)	ν_{OH} (cm^{-1})	Al-O-Si angle (deg.)	Cluster size[e]	Si(***n***Al)[f]	NNN Al[g]
H-FER(8)	**T1**	O(3)	41	34	3539	133	9T	2	2
	T2	O(7)	38	30	3613	132	12T	2	1
	T2	O(7)	75	70	3615	133	9T	3	3
	T3	O(4)	45	37	3593	141	9T	2	2
	T3	O(2)	0	0[h]	3610	136	6T	1	0
	T4	O(6)	7	3	3592	138	10T	1	1
	T4	O(6)	32	34	3618	137	14T	2	4
	T4	O(8)	42	48	3408	135	18T	2*	3
H-FER(35)	**T4**-$(Si)_2$-T4	O(6)	17	23	3605	136	12T	1	0
	T4-$(Si)_2$-**T4**	O(6)	17	25	3606	136	12T	1	0
	T3-$(Si)_1$-T4	O(8)	12	21	3259	134	11T	1*	1
	T3-$(Si)_1$-**T4**	O(6)	35	39	3615	136	12T	2	1
	T3-$(Si)_1$-T3	O(4)	20	33	3604	136	8T	2	1
	T3-$(Si)_1$-**T3**	O(8)	31	48	2969	135	11T	1*	1
	T2-$(Si)_1$-T4	O(7)	40	37	3601	137	11T	2	1
	T2-$(Si)_1$-**T4**	O(8)	6	17	3274	135	9T	1*	1
	T2-$(Si)_2$-T2	O(7)	16	7	3599	137	12T	1	0
	T2-$(Si)_2$-**T2**	O(7)	16	7	3598	138	12T	1	0
	T2-$(Si)_3$-T2'	O(7)	23	15	3606	133	12T	1	0
	T2-$(Si)_3$-**T2'**	O(3)	13	0	3585	139	12T	1	0
H-FER(71)	**T1**	O(3)	13	7	3558	137	12T	1	0
	T2	O(7)	17	14	3606	134	12T	1	0
	T3	O(8)	15	22	3607	133	11T	1	0
	T4	O(6)	12	16	3600	137	12T	1	0

[a] Framework position of the primary Al atom is depicted in bold; location of the secondary Al atom forming a BA site pair and number of SiO_4 tetrahedra separating Al atoms is also indicated for H-FER(35). [b] Numbering scheme from ref. 60 adopted. [c] Relative deprotonation energy of the BA site with respect to the most acidic BA site calculated at the periodic DFT level. [d] Relative deprotonation energy of the BA site with respect to the most acidic BA site calculated at the periodic QM-Pot level. [f] Value of the *n* parameter of the Si(*n*Al) descriptor for the BA site. Stars denote BA sites involved in intra-zeolite H-bonding. [g] Number of next nearest neighbor (NNN) Al atoms with respect to Al atom of the BA site. [h] The absolute value of deprotonation energy is 1222 kJ/mol.

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Supplementary Information:

Table S2. The characteristics the most stable configuration of BA sites for each Si/Al ratio (H-FER(71), H-FER(35) and H-FER(8) models) and Al distribution considered.

H-FER sample	E[c] (eV)	Aluminium location[b]	Oxygen position[c]	ν_{OH}[d] (cm^{-1})	$\nu_{OH\_1D\text{-}Num}$[e] (cm^{-1})
H-FER(8)	-1725.357	**T1**	O(3)	3539	-
		T2	O(7)	3613	-
		T2	O(7)	3615	-
		T3	O(4)	3593	-
		T3	O(2)	3610	-
		T4	O(6)	3592	-
		T4	O(6)	3618	-
		T4	O(8)	3408	-
H-FER(35)	-1713.758	**T4**-$(Si)_2$-T4	O(6)	3605	-
		T4-$(Si)_2$-**T4**	O(6)	3606	-
	-1713.860	**T3**-$(Si)_1$-T4	O(8)	3259	-
		T3-$(Si)_1$-**T4**	O(6)	3615	-
	-1714.025	**T3**-$(Si)_1$-T3	O(4)	3604	-
		T3-$(Si)_1$-**T3**	O(8)	2969	-
	-1713.950	**T2**-$(Si)_1$-T4	O(7)	3601	-
		T2-$(Si)_1$-**T4**	O(8)	3274	-
	-1713.846	**T2**-$(Si)_2$-T2	O(7)	3599	-
		T2-$(Si)_2$-**T2**	O(7)	3598	-
	-1713.846	**T2**-$(Si)_3$-T2'	O(7)	3606	-
		T2-$(Si)_3$-**T2'**	O(3)	3585	-
H-FER(71)	-1712.068	**T1**	O(3)	3558	3450
	-1712.080	**T2**	O(7)	3606	3532
	-1712.055	**T3**	O(8)	3607	3534
	-1712.036	**T4**	O(6)	3600	3529

[a] The value of the absolute electronic energy (PAW wavefunction). [b] Framework position of the primary Al atom is depicted in bold; location of the secondary Al atom forming a BA site pair and number of SiO_4 tetrahedra separating Al atoms is also indicated for H-FER(35). [b] Numbering scheme from ref. 60 adopted. [c] Relative deprotonation energy of the BA site with respect to the most acidic BA site calculated at the periodic DFT level. [d] The value of the OH stretching frequency calculated using ω/r correlation, ref. 19. [e] The value of the OH stretching frequency calculated from the numerical solution of the 1D nuclear Schrödinger equation.

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Supplementary Information:

The lattice parameters of the rectangular cell (α=β=γ=90°) and cartesian coordinates of atoms in the cell for the most stable configuration of BA sites for each Si/Al ratio (H-FER(71), H-FER(35) and H-FER(8) models) and Al distribution considered are provided.

The data record for each sample starts with a header providing the number of atoms on the first line and name of the sample with the values of the lattice parameters on the second line. The cartesian coordinates for each atom of the sample follow.

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 H-FER(71)_T1   19.147 14.304 15.153
H       10.14382778  6.31003859  3.75186301
O        9.39231671  3.84554723  3.96136326
O        9.42288088  4.09534647 11.47666429
O        9.32357813 10.26501078  3.56762595
O        9.34753060 10.11763027 11.16543915
O       11.32929171  8.56018965  3.77929141
O       11.39338577  8.47099701 11.36559765
O       11.02317947  5.87539100  3.74569375
O       11.36953690  5.85343868 11.29619749
O       11.39857726 10.91386034  5.05231576
O       11.42744313 10.81594603 12.62351026
O       11.59481731 10.83420573  2.39895138
O       11.60347953 10.71864380  9.96003477
O       11.81520917  3.69890787  5.05410089
O       11.72526812  3.58096373 12.63180743
O       11.53421991  3.61699656  2.39036855
O       11.51052835  3.54695197  9.96550988
O       12.26890764 11.31860171  7.49729923
O       12.26676407 11.30599097 15.06028563
O       12.45338251  3.17726289  7.53752005
O       12.44705645  3.18791530 15.12869446
O       12.90571155  1.36055403  5.63947619
O       12.93498826  1.32347070 13.30594364
O       12.76880432  1.33296300  1.87071959
O       12.78895382  1.29657225  9.38345415
O       12.79781097 13.08773467  5.59127834
O       12.74438962 13.05731735 13.11271543
O       12.88220404 13.06052904  1.79874035
O       12.81245824 13.02084589  9.46918194
O       13.32678792  6.91443405  5.13470262
O       13.29719339  7.10832102 12.60843210
O       13.25175000  6.95775206  2.27313541
O       13.21771156  7.17924938  9.94011065
O       14.19139739  0.03426490  3.71517745
O       14.16766223  0.06098201 11.30346909
O       14.00550358 10.70903767  5.57473108
O       14.03029874 10.72199520 13.15595343
O       14.16488463 10.73318496  1.66404994
O       14.17408266 10.74704765  9.24522758
O       14.37682248  3.57318198  5.74423456
O       14.30735557  3.60249977 13.29491076
O       14.15220560  3.59888474  2.00665712
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O	14.13315731	3.58460177	9.56883698
O	14.28497431	7.18762144	7.56606349
O	14.28167680	7.18959515	15.02019030
O	15.11151578	14.28240498	6.16616726
O	15.09000039	14.14745049	13.74646966
O	15.07427387	0.14728471	1.24816388
O	15.05290072	14.33892893	8.83798749
O	15.46985715	8.48799312	5.57814700
O	15.51862076	8.52785025	13.07095410
O	15.47723308	8.42429942	1.89441516
O	15.52119169	8.47441258	9.55340180
O	15.71615072	5.88116001	5.74957180
O	15.62691942	5.90980036	13.10202818
O	15.60927080	5.81144628	1.71385692
O	15.50883739	5.85985731	9.53562999
O	15.83865796	10.34079324	3.69933749
O	15.88035818	10.46021002	11.27662207
O	16.05775344	4.13745805	3.75498732
O	16.06772692	3.98080819	11.33163796
O	16.60349970	10.81354760	6.15800936
O	16.62488165	10.84101776	13.75893423
O	16.78622064	10.64421729	1.26973479
O	16.79244805	10.68498902	8.82463426
O	16.98886352	3.59092951	6.15253298
O	16.90879111	3.69985340	13.80844193
O	16.71305761	3.43644511	1.31594175
O	16.68279947	3.60067617	8.80841538
O	16.96009351	13.02289275	0.08994509
O	16.97756619	13.02754325	7.57415665
O	16.93568522	1.29935987	7.50960262
O	16.94532120	1.28600970	14.92061402
O	18.90520201	11.24354965	7.36297494
O	18.90900772	11.26797333	14.98653256
O	18.97807728	2.93193713	0.08671868
O	18.98397012	2.92898819	7.75499806
O	1.90353213	12.84780775	0.12165116
O	1.87978183	12.86077486	7.53094841
O	1.80907505	1.15191418	7.43459398
O	1.80108206	1.13617840	15.10159312
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O	2.05050105	10.66636907	13.76135781
O	1.84883317	10.42985394	1.25965477
O	1.84501717	10.57206549	8.89242552
O	1.91060066	3.53035830	6.20877555
O	1.99492183	3.43396705	13.76667445
O	2.14822148	3.42262694	1.28093180
O	2.21996115	3.35222341	8.85901522
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O	2.86614726	3.91808027	11.33899267
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O	2.71227688	10.01386198	11.30969276
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O	3.25913708	8.34723937	13.31395595
O	3.35514103	8.32276780	1.89290644
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O	3.30535835	5.71819102	5.59778075
O	3.23361051	5.72782423	13.25369505
O	3.34408714	5.70581515	1.93755687

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O	3.67337647	14.14568902	13.77848111
O	3.76060012	14.33248537	1.29173982
O	3.68425178	14.28211707	8.86478500
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O	4.41198546	10.76339000	1.77418427
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O	4.78218045	3.52086238	9.55504782
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O	4.59485521	14.17717168	11.32411801
O	5.62766664	6.93334946	5.07871421
O	5.49589573	7.02522521	12.65707697
O	5.63171429	7.00868280	2.41301008
O	5.49504365	7.13526199	9.99092224
O	6.03148335	12.90944598	5.67830171
O	5.96463787	12.88647188	13.22384703
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O	5.90747361	12.88032799	9.38876827
O	5.98922078	1.17073759	5.63048197
O	5.91788593	1.15523146	13.22907116
O	6.07275233	1.15736525	1.91770175
O	5.98631052	1.14873552	9.46772236
O	6.29838965	11.01399467	7.52978688
O	6.30376826	11.01032313	15.08372443
O	6.46538058	2.94240786	7.56525086
O	6.46423035	2.93815118	15.12403179
O	7.21736287	10.61269974	5.10191737
O	7.24306976	10.62808524	12.66504828
O	6.97487574	10.53139426	2.42881431
O	7.03606903	10.55641552	10.00181697
O	7.04389915	3.52945313	5.07581492
O	7.18275551	3.41516887	12.65215945
O	7.32050746	3.43731373	2.40103696
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O	7.50723296	8.33057876	3.78575964
O	7.42744811	8.30920710	11.36829130
O	7.59656652	5.74843899	3.71558024
O	7.31360804	5.68352041	11.26813325
Al	12.38352947	7.20840326	3.73229487
Si	12.33310657	7.15596800	11.30308867
Si	10.93602104	10.11179291	3.70422999
Si	10.95557624	10.02958138	11.28001191
Si	10.95616847	4.16427673	3.78611527
Si	11.02077577	4.27136654	11.34049864
Si	12.62857226	11.49995495	5.92342231
Si	12.62919253	11.47530142	13.48900085
Si	12.73361880	11.47463276	1.45593941
Si	12.72169124	11.44969327	9.04865161
Si	12.91092774	2.94454915	5.99957090
Si	12.86056511	2.92481449	13.57617183
Si	12.75532274	2.92631465	1.54636062

Si	12.73186054	2.90094838	9.11738996
Si	13.75360164	0.01357588	5.28087158
Si	13.73415858	14.32291669	12.86830757
Si	13.73182147	0.04582172	2.15539407
Si	13.70675574	0.00181916	9.74499674
Si	14.67023590	7.12127755	5.98405738
Si	14.68219047	7.18675056	13.45625452
Si	14.62560298	7.09858738	1.45875124
Si	14.63524202	7.17411591	9.14118335
Si	15.47264907	10.07815075	5.26035014
Si	15.50945391	10.13530215	12.82542469
Si	15.55579505	10.02632752	2.13131017
Si	15.58338344	10.08951992	9.72298496
Si	15.77738918	4.31174146	5.34313095
Si	15.71993846	4.30199296	12.88702330
Si	15.63131323	4.26215869	2.19418478
Si	15.59476645	4.26030359	9.80118895
Si	16.00969376	14.32256756	7.52270477
Si	16.00953506	14.32225327	15.07839338
Si	17.30657060	11.43902001	7.47881817
Si	17.30778679	11.44042995	15.10439808
Si	17.38495023	2.85628580	7.55062120
Si	17.37290440	2.84080690	15.10952249
Si	1.39950645	11.30798829	7.50766793
Si	1.40587943	11.30779871	15.10964321
Si	1.46214009	2.73667463	7.56127024
Si	1.46209917	2.72697042	15.13284182
Si	2.78134219	14.20332432	7.51053138
Si	2.78750664	14.19697718	15.14514713
Si	3.19037469	9.91846664	5.26841554
Si	3.16333195	9.90999142	12.86521695
Si	3.08803543	9.90451795	2.16290081
Si	3.05853459	9.89596877	9.72895787
Si	3.15040699	4.11776248	5.34860928
Si	3.17996904	4.13581266	12.91640320
Si	3.26667771	4.10478106	2.22260303
Si	3.29138223	4.12482279	9.78592673
Si	4.24256545	7.00131948	5.93927338
Si	4.16132083	7.02243399	13.58299117
Si	4.24224333	7.00735140	1.55749334
Si	4.16451359	7.04183643	9.06409403
Si	5.10082742	14.19074402	5.31405615
Si	5.03513393	14.17864762	12.89077619
Si	5.11201754	14.21684832	2.18235219
Si	5.03987669	14.20501490	9.75908534
Si	6.03144141	11.30566763	5.95608415
Si	6.02515470	11.28414356	13.50656456
Si	5.91735944	11.29808158	1.48274978
Si	5.91993278	11.28037806	9.08711444
Si	5.99367346	2.74516884	6.02680584
Si	6.03594633	2.74091594	13.56825074
Si	6.12886951	2.73751750	1.54473617
Si	6.14352581	2.73497979	9.14558272
Si	6.56093985	7.01799235	3.74828762
Si	6.42722896	7.03570763	11.32186366
Si	7.75904651	9.94398647	3.72211687
Si	7.75768533	9.90129197	11.30162873
Si	7.79989767	4.12861954	3.78377910

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Si       7.81883625  4.14214825 11.34512932

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 H-FER(71)_T2   19.147 14.304 15.153
H        10.41663065  3.08013888  5.70642672
O         9.23179849  4.09855205  3.58020272
O         9.29405240  4.05968324 11.09508608
O         9.37731249 10.11542707  3.93094072
O         9.38909595 10.11794106 11.47918892
O        11.31249072  8.33288761  3.67643242
O        11.31252810  8.32165197 11.27929341
O        11.62733058  5.72166034  3.87366020
O        11.33853147  5.70218153 11.40277542
O        11.69151060 10.56028032  5.07748803
O        11.71435249 10.56975456 12.63598334
O        11.45288029 10.66506187  2.40978325
O        11.48385312 10.63459051  9.97037740
O        11.25711950  3.25250079  5.23874069
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O        11.58890407  3.48318290  9.97193905
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O        12.43635834 10.94675180 15.13753943
O        12.29300040  2.88336229 15.02194650
O        12.31982396  2.80485433  7.57046951
O        12.78618917  1.09910096  5.57697750
O        12.70636353  1.10635337 13.07622793
O        13.02337870  1.07027794  1.65214169
O        12.79355928  1.14904505  9.58741970
O        12.88542867 12.83734802  5.66902027
O        12.87662950 12.84697742 13.33212360
O        12.84261738 12.82493608  1.83256100
O        12.76736564 12.88693035  9.40944914
O        13.31726300  7.36348990  5.08571793
O        13.21570906  7.08833818 12.65104619
O        13.33327851  7.16712746  2.42708192
O        13.18008021  6.96795585  9.97339817
O        14.17764166 14.15339886  3.72055481
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O        14.30308875 10.61489315 13.28821969
O        14.07575777 10.48324237  2.04661961
O        14.11035460 10.61104952  9.60662483
O        13.86714930  3.55411330  5.48739202
O        13.94206852  3.45671732 12.99387717
O        14.26054663  3.41157651  1.53610083
O        14.18874025  3.40097218  9.33310006
O        14.16634563  7.01005066 15.09615918
O        14.17483900  6.99189218  7.54390923
O        15.08913752 14.26390481  6.18678699
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Si 17.41580213 11.31764893 9.48938174
Si 17.43667982 11.28678288 1.91923903
Si 17.45030344 2.78172144 6.41741894
Si 17.47291543 2.77885347 13.97711102
Si 17.56053477 2.76038582 9.54673876
Si 17.53515492 2.74539663 1.94472155
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Si 17.89637598 7.05424612 11.75760641
Si 0.13741197 9.93454840 4.16425773
Si 0.11086709 9.94862924 11.72370573
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Si	18.54652701	2.86772212	2.97063121
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Si	1.00228692	10.10478580	5.09710885
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Si	1.24049346	1.49135521	12.80762250
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Si	3.08199392	5.70121328	12.77215818
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Si 14.01101238 5.68771280 10.54543995
Si 15.28360717 8.53974826 2.92928577
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Si 15.36018237 2.79222446 2.99406463
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O	6.38818272	10.07384801	6.02759962
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Al	10.10208560	8.45974068	5.60177919
Al	11.86907939	7.04017776	11.19298283

Si	6.81624938	8.51542888	13.41998847
Si	10.02533231	8.44840918	13.44854645
Si	10.07895711	14.18977379	5.87913500
Si	10.11036801	14.19239190	13.43563111
Si	11.52999344	11.39950883	5.86084734
Si	11.42289306	11.28906364	13.44606810
Si	11.96052703	1.16272073	8.08548518
Si	11.95606769	1.17552697	0.54297403
Si	11.79936147	1.13999226	3.64968461
Si	11.81525218	1.16031433	11.19628628
Si	11.81573913	6.82452245	8.01486673
Si	11.79439958	6.91130259	0.31721951
Si	11.99154682	6.87609222	3.49579286
Si	12.96407005	4.02007743	7.33484571
Si	12.91013665	4.04320445	14.95150916
Si	12.93604821	3.92953784	4.26004488
Si	12.87644883	3.95821590	11.91677603
Si	13.79437664	11.34879204	8.09305394
Si	13.75415339	11.28521930	0.47613594
Si	13.76798953	11.36885100	3.60000744
Si	13.69209326	11.23727793	11.23303450
Si	14.83754226	14.16043741	7.42402509
Si	14.82275415	14.15223185	15.01400348
Si	14.70152403	14.21720054	4.28711544
Si	14.66485368	14.16204943	11.91865149
Si	14.53915221	8.38509023	7.36006074
Si	14.63006139	8.35603133	14.91306687
Si	14.71388485	8.42958142	4.22064962
Si	14.80167140	8.37722617	11.81723560
Si	15.16309866	4.11750551	2.03411371
Si	15.12297287	4.19424405	9.63732533
Si	16.42917968	1.26466703	9.67944500
Si	16.48037451	1.28455839	2.05191017
Si	16.44423046	7.05067002	9.58087946
Si	16.40955267	7.02988468	2.07907790
Si	0.51583858	1.36150779	9.67258134
Si	0.54629717	1.35477544	2.10107377
Si	0.51426480	7.12328535	9.55871016
Si	0.48885631	7.11686398	2.00725504
Si	1.85088009	4.22273046	9.63363895
Si	1.85586228	4.21329840	2.05763589
Si	2.19636877	14.29940258	7.46250853
Si	2.22335498	14.29083671	15.01701686
Si	2.37060921	14.30752252	4.33208686
Si	2.35136400	14.31163276	11.89063849
Si	2.33277444	8.50820355	7.32828030
Si	2.28007995	8.49486809	14.92745821
Si	2.14308628	8.51312455	4.20806302
Si	2.16051090	8.51450652	11.79938024
Si	3.22410869	11.44835344	8.05495188
Si	3.22927671	11.43115435	0.47868597
Si	3.23938666	11.38055283	3.60731175
Si	3.23675296	11.38403344	11.18138709
Si	4.13476401	4.18072123	7.41194399
Si	4.13708358	4.17295021	14.98482056
Si	4.14539455	4.20751086	4.27996637
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Si	5.08295142	1.27709787	8.11183006

Si 5.10864220 1.27514256 0.52758950
Si 5.22443842 1.33850153 3.66233639
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Si 5.15785450 7.08390641 8.02514951
Si 5.11360579 7.07382290 0.46969603
Si 4.99681957 7.14073564 3.58220005
Si 5.03423248 7.14765493 11.16079476
Si 5.50442168 11.40962752 5.84235504
Si 5.51177359 11.41306896 13.40953955
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Si 6.82545374 8.51532841 5.82897061

218
H-FER(35)_T2-$(Si)_2$-T2 19.147 14.304 15.153
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O 10.79571227 9.84599650 13.05266985
O 10.87346956 0.37377270 6.98661719
O 10.87267414 0.38823518 14.55808469
O 10.69595721 0.40376521 4.32449830
O 10.69564688 0.39913628 11.89517711
O 10.63846385 7.40170377 6.97459951
O 10.64651339 7.40451691 14.54289039
O 10.44372786 7.34005743 4.10640772
O 10.44206971 7.33634533 11.67911352
O 11.68177586 0.65002904 9.46776101
O 11.67890327 0.63961889 1.89216055
O 11.42731945 6.68630804 1.79666012
O 11.43538245 6.68050890 9.37352869
O 11.97406306 5.15233486 7.28742973
O 11.96676402 5.14658471 14.86855416
O 12.07444894 5.23344580 3.93549641
O 12.08100202 5.23720545 11.51838201
O 12.14440666 2.57495824 7.69868128
O 12.16185835 2.57210482 0.13648845
O 11.96647186 2.62650205 3.62751317
O 11.95918720 2.63023993 11.21406654
O 12.48011201 11.36953397 6.90372392
O 12.48157747 11.34300255 14.47576491
O 12.40975473 11.53315346 4.23682047
O 12.40730587 11.53630455 11.81087577
O 13.41522939 3.67280130 5.61125270
O 13.41802122 3.67325461 13.19206512
O 13.47921207 0.29422604 7.54889497
O 13.47399255 0.27867070 15.12234534
O 13.33401899 0.38198732 3.97437687
O 13.33403178 0.38931200 11.55074427
O 13.23778188 7.47525199 7.63190068
O 13.24299013 7.46166570 0.06108185
O 13.01684052 7.73077357 3.71853936

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O	13.34098634	11.12861479	9.38219195
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O	14.30487747	4.12968603	0.46364295
O	14.25256364	3.92606032	3.12901988
O	14.24802834	3.91691005	10.70433160
O	14.85912110	12.37003263	7.57527813
O	14.85828570	12.35751687	15.13566428
O	14.78175215	12.51243987	3.59632411
O	14.77742526	12.51829246	11.16452832
O	14.56195354	9.77078163	7.44535639
O	14.56819767	9.75777079	15.04230482
O	14.51034359	9.91003961	3.86369950
O	14.51023011	9.91663561	11.44969146
O	15.28939907	14.15517714	5.65528269
O	15.28865974	14.15456319	13.22803932
O	14.89098630	7.90788316	5.57642292
O	14.88946279	7.90946513	13.15578697
O	16.07570115	0.31727598	8.11375582
O	16.06879910	0.30369940	0.54050570
O	15.88012852	0.52803848	3.20695294
O	15.87841317	0.53341720	10.77998085
O	15.85289075	7.51185815	7.98036014
O	15.85853945	7.49501159	0.40221046
O	15.59718888	7.62887433	3.05397707
O	15.59485538	7.63843333	10.63222421
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O	16.14651309	2.70114579	9.29531474
O	16.15623096	5.30751590	1.91717525
O	16.13551789	5.31782998	9.48995495
O	18.14969010	1.01910653	1.98332438
O	18.15396513	1.02273975	9.56756785
O	17.95988995	7.21067380	1.93199789
O	17.95377338	7.20643594	9.50667216
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O	0.81985813	2.98166017	1.94961092
O	0.95059962	5.60083437	9.68788893
O	0.95538200	5.60286955	2.10422479
O	1.23811268	0.75624482	8.14304895
O	1.24261249	0.75845671	0.57200561
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O	1.32052144	0.70585068	10.82101676
O	1.03891106	7.78035321	8.16808272
O	1.04253808	7.78817463	0.59108492
O	0.91577051	8.01802046	3.26197263
O	0.90764154	8.01915105	10.83800948
O	1.86982606	8.20085956	5.71467010
O	1.87258766	8.19646636	13.28506097
O	1.97555099	0.10901720	5.71718094
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O	2.23840366	12.68879624	0.12635356
O	2.37688856	12.68509916	3.77053501
O	2.39234328	12.68657517	11.35630760
O	2.24895364	10.06524680	7.58597223
O	2.25682046	10.06728986	15.14476046
O	2.45780319	10.06948400	3.93819030

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O	3.82728584	0.45696299	0.02241437
O	3.87382587	0.52507876	3.91254914
O	3.87947678	0.53460280	11.50349574
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O	3.64902389	7.80879072	0.06334585
O	3.46442655	7.60472726	3.65057931
O	3.45913762	7.60664216	11.21156220
O	3.65670136	4.11966829	5.69874864
O	3.65955597	4.12006217	13.27544863
O	4.46531837	11.42505993	6.97156981
O	4.47367055	11.43611181	14.55196339
O	4.69822658	11.47002736	4.30804925
O	4.70407527	11.45024829	11.88769300
O	4.90484568	2.89770522	7.71286390
O	4.90892764	2.89264913	0.13477622
O	5.12477935	2.87227101	3.84913017
O	5.13232545	2.88008989	11.42592731
O	4.98086686	5.51416866	7.54804626
O	4.98016351	5.50808936	15.13163054
O	5.04855801	5.49226483	3.87525771
O	5.05078852	5.50109846	11.45735741
O	5.56589133	1.07574595	9.51215749
O	5.57062114	1.07149968	1.93436481
O	5.46379522	7.25219750	9.50058019
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O	6.38420617	0.80126019	7.02455975
O	6.38636040	0.79422356	14.59912466
O	6.47846729	0.64820734	4.35979939
O	6.48577443	0.65381792	11.93399799
O	6.24312205	7.79686456	7.05585395
O	6.24467103	7.78523036	14.62949148
O	5.98372433	7.92320399	4.40199742
O	5.97159291	7.93999361	11.97740520
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O	6.44357086	10.12872673	5.79790450
O	6.45301478	10.12734221	13.39154843
Al	10.02311170	8.34541021	5.68630199
Al	10.02066274	8.34313131	13.25653200
Si	6.76647682	8.53202249	13.27160036
Si	10.14474098	14.05719415	5.69472107
Si	10.14793860	14.05999671	13.27025422
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Si	11.51426551	11.26239189	13.15570239
Si	12.04852208	0.96507280	7.91678159
Si	12.05071889	0.96203838	0.34344474
Si	11.92255474	1.00016770	3.45601554
Si	11.92160719	1.00492422	11.03286806
Si	11.81416908	6.69819795	7.77427594
Si	11.81332493	6.69541683	0.19861956

Si	11.83435870	6.71213990	3.34508556
Si	11.83712430	6.71291817	10.92272702
Si	12.95697967	3.87141000	7.16268185
Si	12.96084909	3.87342058	14.74399395
Si	12.93701129	3.84941262	4.07030201
Si	12.93669519	3.84928004	11.65187101
Si	13.79878212	11.15680375	7.81913991
Si	13.79959903	11.14615522	0.24349267
Si	13.75216923	11.26853110	3.37332348
Si	13.75070203	11.27084648	10.94921212
Si	14.91853352	13.95846850	7.22405201
Si	14.91518994	13.94825819	14.79522901
Si	14.81274402	14.06072814	4.10626833
Si	14.81142249	14.06511310	11.67868048
Si	14.62281087	8.17521827	7.15984349
Si	14.62651001	8.16500129	14.74188955
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Si	14.52001125	8.30763925	11.62943150
Si	15.20579649	4.00431807	1.80938950
Si	15.20098660	4.00368623	9.38516859
Si	16.55373543	1.13624635	9.43483591
Si	16.54871283	1.12802656	1.85724125
Si	16.37759673	6.91998186	9.40031464
Si	16.38598834	6.91194633	1.82480841
Si	0.61945277	1.36611943	9.51528183
Si	0.61409538	1.36762738	1.93966011
Si	0.45503417	7.14157607	9.54465340
Si	0.46126084	7.14454919	1.96659442
Si	1.83468189	4.25477649	9.52639180
Si	1.83162094	4.25109142	1.94826638
Si	2.32472419	14.26229388	7.29047075
Si	2.32498351	14.26330099	14.86722044
Si	2.38759289	14.26675425	4.15840341
Si	2.39452018	14.26893087	11.73907427
Si	2.20737629	8.46649759	7.28140783
Si	2.21120453	8.46714362	14.85059072
Si	2.18994025	8.48219676	4.14827640
Si	2.18663999	8.48264681	11.71814417
Si	3.16206165	11.36613373	7.93176325
Si	3.16449330	11.36807701	0.35231697
Si	3.30276440	11.37753616	3.47875841
Si	3.30883010	11.37487011	11.05674397
Si	4.05192184	4.20814495	7.27420809
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Si	4.16862512	4.15155733	4.15389113
Si	4.17340048	4.15758383	11.73147659
Si	5.16257469	1.31108847	7.95696585
Si	5.16570603	1.30609361	0.37954122
Si	5.25297283	1.28368833	3.51190184
Si	5.25714874	1.29031611	11.09133044
Si	5.07781841	7.09589733	7.92856393
Si	5.07715099	7.09121173	0.35294011
Si	4.98845385	7.07058818	3.47031162
Si	4.98639076	7.07715323	11.04425356
Si	5.50798396	11.44266871	5.72453541
Si	5.51517282	11.43941205	13.30360153
Si	6.95291293	14.29977482	5.75525232
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218
H-FER(35)_T2-$(Si)_3$-T2' 19.147 14.304 15.153
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O 10.80652245 0.43916339 7.04409625
O 10.80952016 0.39174132 14.61519363
O 10.52648065 0.49244906 4.38126228
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O 10.46712371 7.46463806 14.56809214
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O 11.99315202 2.66454118 0.12187809
O 11.85347397 2.69643182 3.82409715
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O 13.16163539 0.39546162 4.02838191
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O 12.93917054 7.77936886 7.38774774
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O 14.75151231 12.47044410 0.05147148
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O	14.56257330	9.92747884	11.44384376
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O	15.70020557	0.49643272	10.80726949
O	15.46504463	7.52333051	8.19168355
O	15.59597352	7.53662153	0.62330407
O	15.98854967	7.78830508	3.26528884
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O	15.99660951	5.39194233	9.65987390
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O	0.82955262	5.50724893	9.60775488
O	0.94875136	5.51321353	2.03154816
O	0.97272639	0.58542593	8.14549771
O	1.05320604	0.51736644	0.62059292
O	1.30952067	0.72293725	3.27439942
O	1.33066039	0.64937275	10.79226346
O	1.17289999	7.71854646	8.18743917
O	1.09229292	7.74220326	0.57011432
O	0.80164595	7.89178174	3.22053783
O	0.70077238	7.89774246	10.80978604
O	1.62234280	8.33497267	5.68104348
O	1.71734838	8.24666185	13.22914921
O	1.92161511	0.09208264	5.74710041
O	1.91745112	0.16808869	13.31275006
O	2.16866177	12.61582417	7.67755893
O	2.32038382	12.61584022	15.12149538
O	2.32773627	12.67748000	3.78685489
O	2.37706926	12.65045641	11.47686531
O	2.36085658	10.00414643	7.60996948
O	2.34386878	9.99979953	15.12411060
O	2.23623364	10.05562601	3.75819008
O	2.20574525	10.03281909	11.33405226
O	2.67829876	4.21809553	8.19541152
O	2.71732992	4.20150190	0.56533421
O	2.74895489	3.98348080	3.23156846
O	2.66272362	4.07378937	10.87182903
O	3.64668740	11.35508194	9.50984228
O	3.65183728	11.32925796	1.90250948
O	3.60013196	0.49540274	7.78931717
O	3.66597589	0.53727824	0.14654811
O	3.86106087	0.48586161	3.99097607
O	3.88211635	0.47780260	11.56433236

O	3.66233847	7.71137968	7.24716680
O	3.63947729	7.68614077	14.97773164
O	3.37058219	7.63854804	3.80228208
O	3.28558521	7.59564447	11.15902930
O	3.55918520	4.08586285	5.72437737
O	3.67416621	4.17532245	13.28472291
O	4.50532375	11.51242643	7.03571220
O	4.61131529	11.32519321	14.62726188
O	4.53436225	11.28390682	4.37316582
O	4.54238518	11.16019895	11.96237761
O	4.89351733	2.80849117	7.64996959
O	4.96450885	2.85451840	0.05833897
O	5.06840802	2.86258354	3.89884041
O	4.99649886	2.89824332	11.35596381
O	4.97366591	5.41973435	7.55821555
O	5.03033208	5.45644360	0.05403524
O	4.88810214	5.47719804	3.86233235
O	4.89070928	5.50376270	11.29902566
O	5.51775598	1.03556860	9.53173484
O	5.50405164	1.07942617	1.97431267
O	5.21943788	7.32501726	9.39623851
O	5.21281590	7.30506732	1.94588102
O	6.15367841	0.55291991	7.03512734
O	6.24198536	0.61700564	14.65637239
O	6.46695578	0.66028296	4.38435308
O	6.47285998	0.80481450	11.97899957
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O	6.28149783	7.76647668	14.73702298
O	5.95773501	7.84577123	4.39799565
O	5.83892040	7.92694631	11.88180298
O	6.42973052	12.65242553	5.63126200
O	6.32013032	12.78866453	13.15188448
O	6.34656895	10.02774006	5.84457696
O	6.66520915	10.24766958	13.29734611
Al	10.02620230	8.39063243	5.54855893
Al	6.82660956	8.33513670	13.21643028
Si	10.08282810	8.33523943	13.24348094
Si	10.05981693	14.11207648	5.76362502
Si	10.07394992	14.08511433	13.32594755
Si	11.46988877	11.31192574	5.72874241
Si	11.41753330	11.23881915	13.31012281
Si	11.94279406	1.09239752	7.98215128
Si	11.93189432	1.06717693	0.41729662
Si	11.77454472	1.09540742	3.54353913
Si	11.77355432	1.12703765	11.11803735
Si	11.75787627	6.84682541	7.94739629
Si	11.72205752	6.86313549	0.24866372
Si	11.92695579	6.88001028	3.37066146
Si	11.94203302	6.90846932	11.08033327
Si	12.87927253	3.99925322	7.25477213
Si	12.83814599	3.99033684	14.86059387
Si	12.87291553	3.93069967	4.10689546
Si	12.79572690	3.97575594	11.75677864
Si	13.74839361	11.29615667	7.93970472
Si	13.73597836	11.23397892	0.34680770
Si	13.72179378	11.28109944	3.47640604
Si	13.66353126	11.22796115	11.07430410
Si	14.82781381	14.09779275	7.32022256

Si 14.81136204 14.06805534 14.89562536
Si 14.66672799 14.14452317 4.18306914
Si 14.63667619 14.12783546 11.78812146
Si 14.47999621 8.32631134 7.19672449
Si 14.56038016 8.27271199 14.78217366
Si 14.70382748 8.35879328 4.08120302
Si 14.76309761 8.33432268 11.68377259
Si 15.12911108 4.00572165 1.93183616
Si 15.10022919 4.05276441 9.51931573
Si 16.45292381 1.18953942 9.54868694
Si 16.47601042 1.19055809 1.94564818
Si 16.34331515 6.96407978 9.44190137
Si 16.36066653 6.93971971 1.92426605
Si 0.51130683 1.28539376 9.54059911
Si 0.53674160 1.28488678 1.96266515
Si 0.38933028 7.06120335 9.44112117
Si 0.43491787 7.04533749 1.87806796
Si 1.74839232 4.17795736 9.53163823
Si 1.81016989 4.15101413 1.91362921
Si 2.17425013 14.20848024 7.33258070
Si 2.24129712 14.22541437 14.87964308
Si 2.35666053 14.25397185 4.19421764
Si 2.37301146 14.25317478 11.77410550
Si 2.21201277 8.44054899 7.19036658
Si 2.21143438 8.41086095 14.76886904
Si 2.02158382 8.48068615 4.11296385
Si 1.99177355 8.44213280 11.64168723
Si 3.17377571 11.36356841 7.94857053
Si 3.21386156 11.31252559 0.34136353
Si 3.19006476 11.33472936 3.46662953
Si 3.17619788 11.29929152 11.06150137
Si 4.02217240 4.13214805 7.28442838
Si 4.09574685 4.18342560 14.85477375
Si 4.06462639 4.11408642 4.17535390
Si 4.05444752 4.17753582 11.70559400
Si 5.03762443 1.22530719 7.98813001
Si 5.08258482 1.28178099 0.42264264
Si 5.21478019 1.27900162 3.56022680
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Si 5.02628361 7.02781714 7.81967825
Si 5.06353388 7.06637558 0.34477199
Si 4.86414774 7.06836341 3.50499116
Si 4.83177993 7.10400355 10.96252515
Si 5.45294513 11.36228690 5.71776773
Si 5.45075735 11.44346149 13.25930707
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218
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O 2.08390913 10.44230341 5.07650077

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O	2.77637499	11.03518185	7.54046399
O	2.68881127	3.01968077	7.43672050
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O	3.17770894	1.32944354	1.86414198
O	3.20395964	12.79446801	5.56792975
O	2.98838730	13.05944435	1.80713703
O	3.57295584	7.40211334	5.03088197
O	3.53623811	6.82916965	2.39336730
O	4.49277806	14.22785945	3.72042102
O	4.67394863	10.64587424	5.73486947
O	4.37219910	10.84438850	2.12404040
O	4.39698130	3.26826371	5.35815064
O	4.70663799	3.43385705	1.65307035
O	4.51792543	7.16488478	7.47775547
O	5.39929018	14.21522820	6.19080812
O	5.36628475	14.19627779	1.23709250
O	5.98775994	8.34882982	5.60429039
O	5.70429795	8.35456366	1.93209730
O	5.67443341	5.78721121	5.45875286
O	5.92377988	5.78132814	1.89804933
O	6.57322107	10.30224166	3.88301067
O	6.56061492	3.80484787	3.55441445
O	7.30358433	10.53819495	6.34802829
O	7.21036271	10.74152681	1.31121714
O	7.23587029	3.44207298	6.12749591
O	7.32911120	3.66370866	1.09118071
O	7.26466953	12.88562740	7.52948277
O	7.37626676	1.18436623	7.50078663
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O	11.60686556	10.61667890	1.30725687
O	11.67963355	3.39281757	6.14434004
O	11.39670150	3.49997131	1.25151298
O	12.36899697	3.91343909	3.66490290
O	12.33120480	10.13759471	3.78659012
O	12.70656060	8.31723738	5.69360698
O	12.87163966	8.35873602	1.88215868
O	12.85845976	5.70146661	5.57738935
O	12.71887592	5.74293649	1.75946896
O	13.27691872	0.00436063	6.17755361
O	13.27718642	14.27359522	1.28709973
O	14.15306676	7.00447477	7.51892713
O	13.97559163	10.65692067	5.83391324
O	14.19608747	10.66117430	1.97845789
O	14.26592996	3.45356096	5.45791643
O	14.02344275	3.42723231	1.61651411
O	14.21076280	14.17786438	3.73203309
O	15.02823604	7.18179332	5.05111053
O	15.04278600	6.87968183	2.39689745
O	15.46321635	12.84808596	5.68250086
O	15.53918603	12.94552923	1.76819542
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O	15.54197046	1.26517872	1.87100330
O	15.92853206	11.04052724	7.58099420
O	15.97383048	3.04066446	7.46657453
O	16.53127459	10.51115868	5.08066910
O	16.82067150	10.73689687	2.42493597
O	16.89045711	3.38801754	5.01778239
O	16.57758237	3.64036662	2.36644661
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O	16.94722089	5.77499641	3.87833705
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O	18.99321003	10.08951298	11.50131484
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O	1.80004019	5.79582867	11.44435843
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O	1.89992541	10.77660875	10.01853272
O	1.88515814	3.41343503	12.59576490
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O	2.76388984	3.09077666	15.06147928
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O	3.19268615	1.29343214	9.41668932
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O	4.47400889	14.20440690	11.30127399
O	4.67682771	10.66420792	13.49804595
O	4.51188292	10.68065125	9.52470665
O	4.49990571	3.47664772	13.08012669
O	4.66822948	3.48033409	9.12999761
O	4.51856868	6.94036099	15.12834377
O	5.46164090	14.26841894	13.72884639
O	5.45725837	14.27951225	8.87082291
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O	5.85940693	8.39206872	9.43477035
O	5.87925227	5.74477219	13.16791231
O	5.99464445	5.77927645	9.22364460
O	6.26911605	10.11660424	11.42826606
O	6.28124145	4.00568594	11.18739688
O	7.30979355	10.62971979	13.79064393
O	7.12092957	10.67570676	9.01485626
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O	7.34330146	12.97190375	15.06364113
O	7.26704997	1.27470618	15.16190419
O	9.42128031	11.35295199	0.01571751
O	9.36985426	2.87707711	14.83470964
O	11.58528802	12.83710643	15.02606421
O	11.31968022	1.15288852	15.14719817
O	11.49572879	10.49177938	13.80667551
O	11.71461337	10.76409105	8.85109254
O	11.71213283	3.38549221	13.76362378
O	11.52062293	3.65339494	8.80291689
O	12.37942270	3.89681083	11.28167217
O	12.30538803	10.14057174	11.32936224
O	12.78980356	8.28399155	13.16415347
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O	12.88374936	5.67874388	13.20385342

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O	14.15803794	7.05821186	15.10176255
O	14.09911331	10.59100426	13.24825847
O	14.26667964	10.64238535	9.63046113
O	14.28364785	3.43212236	13.05840614
O	14.12626880	3.50962904	9.30361762
O	14.20265878	14.20158240	11.30393978
O	15.10471870	7.05916248	12.64872121
O	15.10285293	7.16566277	9.96829194
O	15.45665425	12.86606726	13.25657321
O	15.65493537	12.89661186	9.47958938
O	15.67213333	1.17445957	13.14306764
O	15.43724551	1.20338495	9.31370611
O	15.90643860	11.03129413	15.13580492
O	15.98784154	2.99861470	15.06180661
O	16.70021508	10.61453103	12.66648329
O	16.89629204	10.62025605	9.99242600
O	16.90691119	3.45855342	12.63781120
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O	17.03114900	8.33599288	11.35020057
O	16.92100419	5.72714032	11.25671582
Al	5.88641835	4.10326983	5.30367552
Al	5.88020047	10.03922903	2.13460585
Si	6.08690003	9.93843428	5.48247664
Si	4.91247730	7.03153807	1.54354602
Si	1.30983810	9.92827553	3.73608028
Si	1.36349178	4.21183872	3.71665581
Si	2.64073683	7.08827282	3.73010578
Si	3.16273231	11.23104937	5.97581802
Si	2.97561187	11.43566571	1.60112668
Si	2.99242649	2.68480635	5.86521680
Si	3.17313002	2.89253365	1.44938008
Si	4.03646128	14.16299723	5.28841425
Si	4.01630514	14.26226993	2.15747956
Si	4.92825999	7.12085269	5.89433785
Si	6.08185510	4.19517115	1.95924608
Si	6.35481021	14.23072766	7.51551970
Si	7.76136947	11.35905744	7.69453912
Si	7.81857979	2.75598946	7.45523854
Si	10.96174488	11.37232379	7.55176794
Si	11.03808106	2.78427840	7.51502051
Si	12.37292323	14.18578049	7.52497782
Si	12.60580981	9.91038032	5.37295456
Si	12.75821071	9.94464763	2.22783555
Si	12.79899790	4.11342803	5.22212264
Si	12.64033807	4.14732425	2.07882666
Si	13.68905231	7.04630549	5.95955390
Si	13.69987090	7.01549801	1.49267927
Si	14.63888325	14.19335569	5.30100869
Si	14.64215230	14.23829926	2.16517593
Si	15.47345533	11.26194593	6.03811553
Si	15.60934098	11.33831511	1.53290414
Si	15.67739353	2.76533014	5.89301880
Si	15.53037165	2.83497340	1.44141576
Si	15.96767531	7.05051921	3.72728088
Si	17.28012667	9.92961879	3.76314871

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Si 1.43969477 9.95244540 11.34533284
Si 1.41661586 4.22873291 11.26686318
Si 2.77686597 7.07777916 11.30435475
Si 3.18637188 11.29728515 13.65803626
Si 3.09726889 11.36369410 9.10106092
Si 3.08125206 2.79486124 13.49319069
Si 3.17095942 2.86199837 8.97547605
Si 4.07818508 14.20352220 12.87821575
Si 4.07563209 14.26391600 9.72596252
Si 6.05660082 9.94226172 13.02931033
Si 5.92974105 9.96041922 9.85490387
Si 5.93229053 4.17206398 12.75783628
Si 6.05678621 4.19111631 9.58912021
Si 6.34110666 14.23426290 15.09693102
Si 7.80274682 11.40673608 15.14653675
Si 7.76618229 2.79457451 14.93721667
Si 11.02538713 11.32011202 15.12535270
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Si 12.68141065 9.88277187 12.88904784
Si 12.78584187 9.99431031 9.78446587
Si 12.82165643 4.09875136 12.83156087
Si 12.72447494 4.21501024 9.72639585
Si 13.73987014 7.01896334 13.52871012
Si 13.73760825 7.10398517 9.08982339
Si 14.66016084 14.22406319 12.86718241
Si 14.64671091 14.14668259 9.73791677
Si 15.53656283 11.27418686 13.57201891
Si 15.68005648 11.29861704 9.16511663
Si 15.70643834 2.76794418 13.47951468
Si 15.55792490 2.79650526 9.01858422
Si 16.02704404 7.06999227 11.30635802
Si 17.39618092 9.91716363 11.37452690
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218
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O 2.13239965 3.59528645 2.39038536
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O 3.14423762 12.87148777 5.44577602
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218
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