

Input example for VASP

SYSTEM = [Cr(ox)_3]@[Fe_2L_3][BF_4]

GGA = PE

NBANDS = 512

NELM = 999

NELMIN = 4

NELMDL = -7

ENCUT = 600

EDIFF = 1.E-08

LASPH = .TRUE.

LREAL = .FALSE.

ISIF = 2

NSW = 900

IBRION = 2

POTIM = 0.45

EDIFFG = -1.E-03

ALGO = Normal

LMAXMIX = 4

PREC = Accurate

ADDGRID = .TRUE.

ISMear = 0

LORBIT = 11

SIGMA = 1.E-02

ISPIN = 2

NUPDOWN = 3.0

MAGMOM = 3.0 187*0.0

ICHARG = 2

ISTART = 0

LDAU = .TRUE.

LDAUL = 2 2 -1 -1 -1 -1 -1 -1

LDAUTYPE = 2

LDAUPRINT = 2

LDAUU = 1.24 1.96 0.00 0.00 0.00 0.00 0.00 0.00

LDAUJ = 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

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[Cr(ox)_3]@[Fe_2L_3][BF_4] PBE@LS

Cr 12.520941 16.957615 12.989253

Fe 12.669253 11.622034 12.802159

Fe 12.485214 22.156937 13.103484

O 11.581433 15.820116 14.314031

O 10.858534 18.050077 13.147087

O 9.677529 15.692079 15.528019

O 8.914516 18.174192 14.291382

O 11.827475 15.924255 11.446540

O 13.241722 18.128852 11.543011

O 11.743748 15.930995 9.186416

O 13.268222 18.366579 9.296953

O 14.193854 15.898799 13.083649

O 13.432515 18.036349 14.398404

O 16.212399 15.841036 14.101377

O 15.391308 18.208509 15.510906

N 14.388938 10.634488 12.810868

N 13.579580 12.603001 14.216986

N 13.211663 13.487003 15.168004

N 11.885621 20.202642 15.377296

N 11.549297 21.150818 14.482100

N 10.807650 23.201636 13.165337

N 11.844416 10.461516 14.184497

N 10.965405 12.537512 12.987959

N 10.296552 13.492116 12.306701

N 10.779706 20.268086 11.418372

N 11.746975 21.189801 11.582120

N 13.267531 23.231463 11.637960

N 11.920163 10.536406 11.320191

N 13.319521 12.671029 11.299887

N 14.237002 13.646244 11.130646

N 14.811637 20.289880 12.452818

N	14.175019	21.197678	13.216093
N	13.349532	23.212727	14.536954
C	10.392748	16.256482	14.708725
C	9.966049	17.603477	14.025312
C	12.099519	16.425706	10.249710
C	12.938428	17.752193	10.305375
C	15.111127	16.350067	13.928137
C	14.662118	17.638060	14.707439
C	14.765427	9.640622	11.978033
C	16.007829	9.019072	12.060339
C	16.915900	9.430549	13.035552
C	16.542822	10.451773	13.905125
C	15.280038	11.031798	13.775266
C	14.758562	12.075787	14.624205
C	15.143783	12.633467	15.849450
C	14.135291	13.535059	16.184155
C	14.000331	14.345039	17.393327
C	14.772210	14.020819	18.525954
C	14.641733	14.755220	19.700866
C	13.747396	15.824104	19.770014
C	12.974900	16.169264	18.650065
C	13.104452	15.419069	17.472381
C	12.044446	17.317886	18.681853
C	11.236861	17.578927	19.800130
C	10.346579	18.653410	19.789209
C	10.251898	19.478647	18.672589
C	11.059508	19.239807	17.544291
C	11.951746	18.160808	17.565456
C	10.963689	20.136670	16.394389
C	9.992390	21.099905	16.120353
C	10.395637	21.706989	14.925609
C	9.909530	22.801194	14.123740
C	8.664592	23.419884	14.275636
C	8.315668	24.471583	13.435114
C	9.227435	24.877522	12.456308
C	10.448911	24.221082	12.352910
C	12.391543	9.376418	14.773352
C	11.714909	8.608229	15.716527
C	10.421514	8.971501	16.087819
C	9.839596	10.084039	15.486355
C	10.563755	10.802105	14.534127
C	10.056757	11.929150	13.785448
C	8.793712	12.507274	13.609012
C	8.967703	13.508267	12.654235
C	7.963635	14.386713	12.057395
C	6.598169	14.100263	12.250318
C	5.620555	14.899616	11.666016
C	5.980371	15.998725	10.885236
C	7.335019	16.308897	10.689008
C	8.315404	15.492874	11.272085
C	7.745096	17.492976	9.903576
C	7.102649	17.842568	8.705135
C	7.529291	18.953892	7.976552
C	8.590428	19.731314	8.432293
C	9.240646	19.403970	9.637261
C	8.807206	18.285663	10.359771
C	10.325441	20.255803	10.121692
C	11.052255	21.225677	9.430709
C	11.921519	21.783189	10.376176
C	12.873158	22.865335	10.374342
C	13.364719	23.503796	9.231450
C	11.174341	9.415286	11.424961
C	10.714139	8.710944	10.315174
C	11.014707	9.177361	9.036440
C	11.787251	10.330103	8.910520
C	12.233910	10.981226	10.061051
C	13.102429	12.135087	10.075245
C	13.891400	12.781760	9.116103
C	14.617151	13.745526	9.814022
C	15.651436	14.649568	9.317338
C	17.191020	16.517019	9.631687
C	16.166258	15.686342	10.105748
C	17.668796	17.624103	10.486543
C	19.034414	17.907886	10.640285
C	17.131570	19.434129	12.032482
C	16.729699	18.399770	11.179280
C	16.157627	20.270001	12.730368

C	14.165856	24.235659	11.750397
C	15.120476	21.773873	13.998005
C	12.798309	24.209768	15.265348
C	14.638457	22.843651	14.833684
C	14.283001	24.539454	9.367222
C	16.182190	14.453345	8.027482
C	17.719530	16.293278	8.351539
C	19.445069	18.934806	11.491961
C	18.507004	19.691796	12.188015
C	16.376866	21.219450	13.728612
C	14.689316	24.909745	10.652529
C	13.480225	24.873548	16.279284
C	15.375449	23.471324	15.842885
C	17.207876	15.267048	7.555731
C	14.794205	24.500113	16.576232
H	12.443992	14.154708	14.973602
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H	14.414673	14.313792	11.902767
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H	14.030440	9.302410	11.255051
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H	15.246066	14.494668	20.570431
H	13.668250	16.412429	20.685163
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H	9.713157	18.843250	20.656306
H	9.558343	20.319105	18.682958
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H	7.348439	24.963177	13.535224
H	9.001590	25.693745	11.771959
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H	12.192828	7.706146	16.091611
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H	6.300820	13.238505	12.846827
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H	6.285983	17.224632	8.329667
H	7.033148	19.212872	7.040591
H	8.902460	20.605368	7.860821
H	9.289139	18.024070	11.301580
H	10.969627	21.468439	8.379285
H	13.030250	23.166305	8.251557
H	10.977148	9.026199	12.418849
H	10.160314	7.789894	10.486590
H	10.669848	8.643823	8.150789
H	15.784889	15.850481	11.114483
H	15.670270	18.190218	11.031049
H	11.776692	24.483626	15.012867
H	12.058799	10.728540	7.933682
H	13.936099	12.579352	8.053972
H	19.774908	17.300686	10.117959
H	14.462550	24.506208	12.761160
H	14.681599	25.045265	8.488244
H	15.803097	13.649085	7.397895
H	18.506674	16.944261	7.968674
H	20.508043	19.140114	11.622422
H	18.844892	20.493642	12.843963
H	17.321378	21.457124	14.200251
H	15.407996	25.711824	10.812881
H	12.978257	25.670577	16.825472
H	16.390146	23.132204	16.046283
H	17.608576	15.103875	6.554766
H	15.350921	24.998532	17.369325
B	12.285770	6.269992	13.001248
F	13.148256	7.287159	12.455657

F	12.344269	5.120635	12.199363
F	12.700798	5.992225	14.329715
F	10.950968	6.792184	13.021292

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[Cr(ox)_3]@[Fe_2L_3][BF_4] PBE@HS

Cr	12.534994	16.945440	12.980668
Fe	12.669930	11.662697	12.803175
Fe	12.467664	22.079588	13.103845
O	11.539350	15.827481	14.280846
O	10.865127	18.037286	13.037561
O	9.627192	15.780489	15.488298
O	8.893932	18.204252	14.128614
O	11.887947	15.923007	11.408726
O	13.336849	18.105070	11.568947
O	11.797635	16.004133	9.150005
O	13.382719	18.394714	9.328972
O	14.205749	15.892651	13.140330
O	13.367477	18.012037	14.444361
O	16.206533	15.886201	14.193770
O	15.273924	18.185832	15.644017
N	14.384103	10.669268	12.811322
N	13.578412	12.633866	14.221818
N	13.202687	13.503301	15.182633
N	11.743491	20.099697	15.528982
N	11.434937	21.057220	14.638029
N	10.596525	23.263256	13.367013
N	11.838307	10.511731	14.188740
N	10.971659	12.586019	12.981771
N	10.303702	13.524063	12.277700
N	10.771220	20.170738	11.208071
N	11.716271	21.107482	11.405310
N	13.187286	23.352155	11.398215
N	11.910073	10.597314	11.314590
N	13.334374	12.713267	11.311128
N	14.275128	13.667585	11.153090
N	15.000358	20.204444	12.509500
N	14.344613	21.128475	13.230378
N	13.556869	23.286999	14.580802
C	10.357504	16.299394	14.651668
C	9.951867	17.624478	13.909884
C	12.166038	16.456914	10.228171
C	13.033813	17.764827	10.322063
C	15.093261	16.363479	14.005358
C	14.589134	17.626656	14.794451
C	14.755745	9.675813	11.975911
C	16.002442	9.061315	12.045793
C	16.919382	9.480221	13.009779
C	16.549839	10.499018	13.883809
C	15.281899	11.070603	13.767977
C	14.759904	12.109100	14.623926
C	15.139922	12.654823	15.855942
C	14.124210	13.544545	16.201241
C	13.976885	14.328646	17.425609
C	14.769454	14.004483	18.544131
C	14.624314	14.703572	19.738356
C	13.696371	15.740706	19.839759
C	12.906927	16.089684	18.733135
C	13.048287	15.371958	17.536340
C	11.955638	17.219312	18.797081
C	11.137452	17.436178	19.917188
C	10.236970	18.502271	19.934432
C	10.143301	19.363500	18.844657
C	10.962489	19.169203	17.716983
C	11.863259	18.096954	17.709375
C	10.874233	20.089569	16.586909
C	9.957130	21.116786	16.350236
C	10.340364	21.688095	15.129606
C	9.793522	22.791667	14.359048
C	8.519486	23.333995	14.586431
C	8.067267	24.367626	13.774355
C	8.890920	24.839739	12.746645
C	10.142664	24.255616	12.581029
C	12.382548	9.431032	14.787656
C	11.714582	8.692091	15.759992
C	10.434242	9.081152	16.149708
C	9.852885	10.185881	15.533197

C	10.567255	10.873560	14.551966
C	10.061848	11.991066	13.787759
C	8.798314	12.562395	13.594922
C	8.973102	13.543080	12.619180
C	7.967021	14.398108	11.992947
C	6.602390	14.116506	12.200209
C	5.620741	14.885456	11.583066
C	5.975766	15.953184	10.757762
C	7.328833	16.262179	10.551367
C	8.313973	15.473470	11.163605
C	7.731723	17.428041	9.735904
C	7.098475	17.744026	8.523036
C	7.516638	18.846910	7.776682
C	8.559891	19.650839	8.229238
C	9.198450	19.357562	9.448348
C	8.774692	18.245968	10.187309
C	10.267274	20.222634	9.940060
C	10.945515	21.260100	9.287407
C	11.831936	21.781937	10.235053
C	12.771520	22.893547	10.186501
C	13.232562	23.456535	8.988360
C	11.144540	9.489024	11.413030
C	10.647609	8.818275	10.298111
C	10.931132	9.305972	9.023158
C	11.728742	10.442344	8.904486
C	12.212821	11.058931	10.058757
C	13.104913	12.194925	10.081522
C	13.909307	12.832536	9.129329
C	14.658561	13.770835	9.837601
C	15.719526	14.649221	9.350721
C	17.320307	16.461917	9.680408
C	16.272071	15.657852	10.150529
C	17.825381	17.557798	10.533891
C	19.195685	17.824353	10.679151
C	17.321141	19.395173	12.059098
C	16.902067	18.353694	11.222750
C	16.350110	20.245342	12.741934
C	14.062355	24.372539	11.432829
C	15.286250	21.784184	13.952795
C	13.073769	24.294822	15.334915
C	14.840576	22.876736	14.794963
C	14.129446	24.518641	9.040069
C	16.237441	14.453102	8.055476
C	17.837067	16.235154	8.395989
C	19.624333	18.855595	11.517025
C	18.699850	19.635993	12.206522
C	16.557388	21.259689	13.678696
C	14.552471	24.991435	10.286086
C	13.822225	24.939821	16.312435
C	15.650636	23.477684	15.770244
C	17.289074	15.236234	7.589630
C	15.138803	24.518548	16.535184
H	12.431084	14.166088	14.991363
H	12.467510	19.390984	15.260635
H	10.838410	14.234015	11.747779
H	10.639749	19.433566	11.947830
H	14.457762	14.327586	11.930520
H	14.434953	19.485977	11.995252
H	14.013910	9.334584	11.261075
H	16.224769	8.246016	11.360213
H	17.901942	9.014989	13.086067
H	17.229162	10.862632	14.653316
H	16.034494	12.439806	16.425419
H	15.488121	13.187790	18.484116
H	15.243952	14.441896	20.596771
H	13.604930	16.305509	20.768450
H	12.410498	15.631035	16.689863
H	11.186394	16.749056	20.762643
H	9.593345	18.655781	20.801477
H	9.435820	20.191881	18.873501
H	12.523235	17.937808	16.856001
H	9.121158	21.394933	16.979176
H	7.892338	22.923467	15.376565
H	7.076974	24.795737	13.931519
H	8.572478	25.644771	12.086383
H	10.823610	24.591529	11.797838
H	13.361050	9.115548	14.437292

H	12.189820	7.793717	16.147094
H	9.886552	8.516622	16.903812
H	8.848950	10.519212	15.792557
H	7.874966	12.301584	14.095242
H	6.308371	13.281904	12.835459
H	4.568262	14.656281	11.754087
H	5.203274	16.573164	10.300820
H	9.363454	15.704336	10.973557
H	6.295230	17.106496	8.151450
H	7.029244	19.077216	6.828504
H	8.870563	20.513324	7.639816
H	9.244040	18.009927	11.142450
H	10.808377	21.576420	8.261180
H	12.902135	23.043510	8.036140
H	10.958438	9.085341	12.403848
H	10.073572	7.907957	10.460745
H	10.551085	8.802394	8.134342
H	15.900627	15.823223	11.163126
H	15.839638	18.156986	11.077159
H	12.042805	24.587798	15.134069
H	11.986276	10.857691	7.931086
H	13.950402	12.638048	8.065719
H	19.925506	17.202285	10.159373
H	14.373049	24.699585	12.426072
H	14.504324	24.966663	8.119473
H	15.826590	13.672794	7.415790
H	18.642189	16.866487	8.017631
H	20.690860	19.046420	11.641166
H	19.050813	20.439178	12.854201
H	17.505735	21.566429	14.100984
H	15.254590	25.819369	10.371130
H	13.379282	25.750349	16.889351
H	16.662312	23.106743	15.929319
H	17.680322	15.072598	6.584763
H	15.751353	24.991368	17.302842
B	12.228987	6.345839	13.030495
F	13.105907	7.330004	12.449121
F	12.245139	5.178225	12.253845
F	12.659594	6.086189	14.357903
F	10.907426	6.901309	13.061806

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	[Fe(ox)_3]@[Fe_2L_3][BF_4]	PBE@LS
Fe	12.524988	16.930661
Fe	12.670915	11.602064
Fe	12.482698	22.172353
O	11.485916	15.789853
O	10.839099	18.096919
O	9.606962	15.731608
O	8.857737	18.187407
O	11.897220	15.900666
O	13.205498	18.181254
O	11.758842	15.982134
O	13.298890	18.388796
O	14.235693	15.870437
O	13.495789	18.089200
O	16.275211	15.887250
O	15.422933	18.226777
N	14.391580	10.617753
N	13.577038	12.583097
N	13.205735	13.464555
N	11.894932	20.213934
N	11.554302	21.163981
N	10.802662	23.212936
N	11.844252	10.446668
N	10.970715	12.520056
N	10.302635	13.470463
N	10.777559	20.279151
N	11.742642	21.203294
N	13.263471	23.244182
N	11.918043	10.525433
N	13.324097	12.653427
N	14.247118	13.623720
N	14.801356	20.303816
N	14.169060	21.211607
N	13.350230	23.224230
C	10.325285	16.265608

C	9.923228	17.633384	14.043305
C	12.129542	16.443564	10.180884
C	12.948550	17.789592	10.255665
C	15.158907	16.363883	13.986459
C	14.702077	17.672973	14.739628
C	14.768295	9.623433	11.978109
C	16.015668	9.010841	12.053682
C	16.928215	9.432447	13.020596
C	16.554691	10.454242	13.889609
C	15.286805	11.024776	13.766862
C	14.763509	12.068334	14.615554
C	15.151043	12.633603	15.836586
C	14.135055	13.524969	16.176167
C	14.000371	14.336814	17.383650
C	14.775360	14.015806	18.515098
C	14.648069	14.753737	19.688065
C	13.753563	15.822529	19.755935
C	12.977464	16.163920	18.637258
C	13.103639	15.410173	17.461547
C	12.047184	17.312655	18.668606
C	11.236658	17.570109	19.785497
C	10.346006	18.644258	19.775480
C	10.254367	19.472060	18.660594
C	11.064755	19.236625	17.533428
C	11.957907	18.158338	17.554016
C	10.969140	20.136664	16.386171
C	9.991163	21.093367	16.112800
C	10.394967	21.709950	14.923484
C	9.904128	22.803841	14.124264
C	8.654555	23.413995	14.274179
C	8.301098	24.465280	13.434844
C	9.213137	24.879553	12.459498
C	10.439467	24.231573	12.358412
C	12.389807	9.362203	14.777294
C	11.718003	8.607689	15.735028
C	10.432211	8.985042	16.118725
C	9.851267	10.096340	15.513455
C	10.570243	10.800375	14.546982
C	10.064437	11.925488	13.794185
C	8.804130	12.510636	13.621590
C	8.976801	13.499360	12.653830
C	7.973822	14.377549	12.055454
C	6.608229	14.090724	12.247401
C	5.630989	14.890979	11.663720
C	5.991774	15.990834	10.884406
C	7.346581	16.301117	10.689108
C	8.326585	15.484250	11.271472
C	7.757486	17.486202	9.905759
C	7.121824	17.831087	8.702452
C	7.549332	18.942569	7.974641
C	8.605164	19.723566	8.436288
C	9.249100	19.400446	9.645880
C	8.813619	18.283081	10.368530
C	10.330068	20.255821	10.131851
C	11.059681	21.219806	9.435490
C	11.923032	21.786957	10.380155
C	12.874214	22.869404	10.374101
C	13.370574	23.499720	9.228603
C	11.167806	9.406917	11.417113
C	10.690703	8.718074	10.304474
C	10.978109	9.198071	9.027484
C	11.755941	10.347858	8.905359
C	12.219734	10.983062	10.058004
C	13.093317	12.133189	10.076226
C	13.877486	12.787125	9.118208
C	14.616422	13.736989	9.821400
C	15.650818	14.641316	9.326224
C	17.184882	16.513444	9.638094
C	16.163114	15.680012	10.113714
C	17.659608	17.623548	10.490715
C	19.024874	17.908575	10.645027
C	17.119178	19.436608	12.031446
C	16.718788	18.400096	11.180164
C	16.145912	20.273584	12.728773
C	14.162384	24.248197	11.746187
C	15.114427	21.777197	14.000754
C	12.801103	24.220857	15.269547

C	14.635459	22.845647	14.839904
C	14.288969	24.535786	9.361236
C	16.182186	14.444072	8.036745
C	17.713010	16.289700	8.357673
C	19.434163	18.938297	11.494009
C	18.494385	19.696029	12.186938
C	16.367650	21.215001	13.734134
C	14.690553	24.914645	10.645790
C	13.482146	24.875569	16.290105
C	15.371223	23.463514	15.856235
C	17.204899	15.260545	7.563273
C	14.792290	24.492081	16.591951
H	12.422702	14.113729	14.980821
H	12.639755	19.517682	15.117886
H	10.832559	14.169858	11.752159
H	10.632084	19.556229	12.181727
H	14.443025	14.273336	11.919980
H	14.227706	19.600110	11.912396
H	14.029859	9.278591	11.261560
H	16.240843	8.193281	11.371716
H	17.910068	8.966675	13.103397
H	17.230535	10.819699	14.661820
H	16.052948	12.435087	16.400732
H	15.465054	13.172917	18.481472
H	15.255004	14.496047	20.556708
H	13.677505	16.414884	20.668796
H	12.479073	15.664256	16.604108
H	11.282527	16.907152	20.650319
H	9.710461	18.832355	20.641535
H	9.559875	20.311750	18.670464
H	12.607305	17.969055	16.698889
H	9.096841	21.288148	16.690088
H	7.972197	23.043814	15.038177
H	7.330250	24.950541	13.533174
H	8.983400	25.696037	11.776464
H	11.168523	24.535764	11.610819
H	13.372272	9.055206	14.430460
H	12.193996	7.705816	16.113265
H	9.879837	8.405836	16.858324
H	8.842688	10.420187	15.768001
H	7.884852	12.258990	14.133876
H	6.310692	13.228730	12.843573
H	4.577388	14.659373	11.823839
H	5.221817	16.632146	10.453264
H	9.377343	15.718115	11.093397
H	6.310844	17.208551	8.322408
H	7.058350	19.199269	7.035201
H	8.919620	20.596826	7.864931
H	9.288900	18.025738	11.315006
H	10.984875	21.451174	8.380876
H	13.040824	23.155218	8.249410
H	10.979717	9.008254	12.409422
H	10.132211	7.798820	10.471461
H	10.617620	8.677538	8.140130
H	15.781376	15.845447	11.122237
H	15.659615	18.190222	11.030699
H	11.782259	24.502068	15.013137
H	12.016581	10.757168	7.929953
H	13.909297	12.599996	8.052936
H	19.766159	17.299835	10.125631
H	14.455633	24.524719	12.756413
H	14.691485	25.035762	8.480466
H	15.805039	13.637686	7.408548
H	18.496844	16.943750	7.973041
H	20.496911	19.145867	11.624537
H	18.830498	20.499795	12.841582
H	17.310762	21.440663	14.214305
H	15.409333	25.717573	10.802963
H	12.982891	25.673514	16.837803
H	16.382688	23.116879	16.063803
H	17.606066	15.096933	6.562368
H	15.347899	24.983280	17.390508
B	12.273324	6.268957	13.010877
F	13.142915	7.273600	12.452455
F	12.313993	5.113821	12.216748
F	12.694281	5.996406	14.338376
F	10.944404	6.805942	13.036197

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[Fe(ox)_3]@[Fe_2L_3][BF_4] PBE@HS

Fe	12.539703	16.913076	12.980491
Fe	12.669522	11.655529	12.803203
Fe	12.467665	22.084851	13.104671
O	11.452688	15.795012	14.267585
O	10.836335	18.071314	13.088306
O	9.572311	15.816280	15.526857
O	8.841714	18.210876	14.144951
O	11.944829	15.890827	11.338189
O	13.308847	18.140383	11.515579
O	11.788686	16.039852	9.085334
O	13.389571	18.401916	9.270841
O	14.246123	15.857609	13.220017
O	13.431819	18.046861	14.446613
O	16.273667	15.923474	14.222415
O	15.319982	18.189968	15.683527
N	14.383760	10.664779	12.812290
N	13.572744	12.624007	14.224558
N	13.193643	13.489666	15.187397
N	11.754768	20.106673	15.530990
N	11.443354	21.064165	14.641543
N	10.596992	23.265337	13.369596
N	11.836471	10.508200	14.189091
N	10.971718	12.577708	12.975426
N	10.304137	13.512222	12.266370
N	10.763544	20.177446	11.217603
N	11.707851	21.114924	11.412599
N	13.182683	23.355758	11.400870
N	11.909510	10.594127	11.313603
N	13.340351	12.703936	11.314655
N	14.285670	13.654006	11.159046
N	14.995591	20.212327	12.498332
N	14.342076	21.136336	13.220801
N	13.555835	23.289690	14.578273
C	10.298406	16.303113	14.667532
C	9.909543	17.645262	13.931467
C	12.180804	16.460714	10.168148
C	13.034473	17.785903	10.271656
C	15.144175	16.366866	14.048054
C	14.635491	17.646687	14.822131
C	14.755414	9.672411	11.975883
C	16.002707	9.059129	12.044364
C	16.919987	9.479021	13.007555
C	16.551147	10.498758	13.881089
C	15.282619	11.069243	13.766441
C	14.759423	12.107460	14.622193
C	15.140700	12.657648	15.851946
C	14.119425	13.539113	16.201911
C	13.973504	14.323067	17.426316
C	14.767049	13.998625	18.544087
C	14.625181	14.699965	19.737366
C	13.698374	15.737948	19.839127
C	12.908661	16.087228	18.733001
C	13.047352	15.368351	17.536715
C	11.959625	17.218578	18.796351
C	11.139925	17.435106	19.915471
C	10.238668	18.500526	19.931053
C	10.146907	19.361678	18.841206
C	10.968839	19.168616	17.715180
C	11.869895	18.096769	17.708865
C	10.881429	20.089585	16.585759
C	9.959360	21.111981	16.348274
C	10.343768	21.688399	15.130527
C	9.794512	22.791592	14.360776
C	8.520029	23.332619	14.588307
C	8.067388	24.366947	13.777411
C	8.890157	24.840126	12.749541
C	10.142350	24.257136	12.583528
C	12.380990	9.428682	14.789376
C	11.713568	8.691872	15.763592
C	10.434002	9.082786	16.153886
C	9.853250	10.188205	15.537618
C	10.567190	10.873692	14.554543
C	10.062953	11.990846	13.788506
C	8.801071	12.566558	13.597470

C	8.975182	13.539207	12.613703
C	7.968639	14.393578	11.987560
C	6.604208	14.110451	12.194020
C	5.622136	14.880348	11.578866
C	5.976593	15.949072	10.754749
C	7.329497	16.259725	10.549830
C	8.315184	15.470941	11.161127
C	7.732230	17.427071	9.737066
C	7.102560	17.741629	8.521905
C	7.522967	18.843793	7.775753
C	8.564389	19.648211	8.231210
C	9.198355	19.356986	9.453252
C	8.772615	18.246331	10.192071
C	10.265198	20.222973	9.946863
C	10.946300	21.256570	9.291111
C	11.828619	21.783615	10.239471
C	12.768099	22.895342	10.189547
C	13.229597	23.457651	8.991419
C	11.141638	9.487653	11.411806
C	10.643046	8.818805	10.296598
C	10.927065	9.307242	9.022061
C	11.724895	10.443703	8.903811
C	12.210276	11.058671	10.058396
C	13.103785	12.193745	10.082927
C	13.905956	12.835454	9.131419
C	14.663021	13.765373	9.842343
C	15.723637	14.643461	9.354816
C	17.320736	16.459590	9.681108
C	16.273606	15.654989	10.152540
C	17.823626	17.557618	10.532926
C	19.193769	17.823147	10.681233
C	17.316321	19.396368	12.054862
C	16.898665	18.354861	11.218063
C	16.344863	20.247381	12.735458
C	14.058225	24.375672	11.435565
C	15.283760	21.786831	13.948082
C	13.072233	24.296364	15.333450
C	14.839351	22.878848	14.791652
C	14.125340	24.520696	9.042960
C	16.242036	14.445930	8.059892
C	17.838374	16.231363	8.397391
C	19.620743	18.854256	11.520063
C	18.694845	19.635640	12.206425
C	16.553389	21.257825	13.676095
C	14.548509	24.993997	10.288663
C	13.821329	24.941783	16.310171
C	15.649576	23.479779	15.766439
C	17.291541	15.230917	7.592390
C	15.138417	24.521233	16.531183
H	12.408960	14.137394	15.004260
H	12.489362	19.407366	15.265765
H	10.838682	14.208837	11.720878
H	10.625648	19.448129	11.965096
H	14.483120	14.299955	11.943024
H	14.427555	19.502373	11.974251
H	14.013092	9.331140	11.261602
H	16.224796	8.243597	11.358936
H	17.902328	9.013443	13.083944
H	17.231454	10.862861	14.649902
H	16.040537	12.452394	16.417023
H	15.484355	13.180837	18.483709
H	15.247166	14.439416	20.594487
H	13.608871	16.303299	20.767585
H	12.410042	15.629025	16.690228
H	11.187980	16.747664	20.760963
H	9.593287	18.653746	20.796664
H	9.438815	20.189460	18.868380
H	12.531246	17.938679	16.856424
H	9.119118	21.382869	16.974682
H	7.893869	22.921641	15.378809
H	7.077701	24.795672	13.935672
H	8.571452	25.645584	12.089645
H	10.822941	24.593452	11.800056
H	13.359164	9.112573	14.438657
H	12.188372	7.793412	16.151035
H	9.886036	8.518797	16.908170
H	8.849819	10.522733	15.798131

H	7.879014	12.315379	14.105086
H	6.310879	13.274343	12.827713
H	4.569890	14.651201	11.750932
H	5.203737	16.568693	10.298182
H	9.364480	15.704184	10.972691
H	6.301171	17.102830	8.148330
H	7.038961	19.072984	6.825747
H	8.877300	20.509814	7.641863
H	9.238832	18.012408	11.149246
H	10.813440	21.566790	8.262401
H	12.899244	23.044136	8.039522
H	10.955323	9.083895	12.402506
H	10.067959	7.909017	10.458619
H	10.547538	8.803760	8.132997
H	15.900491	15.823184	11.164076
H	15.836318	18.159181	11.070278
H	12.040427	24.587968	15.134041
H	11.982128	10.859508	7.930290
H	13.939543	12.650905	8.065633
H	19.924305	17.200031	10.163635
H	14.369069	24.702880	12.428815
H	14.499167	24.969865	8.122807
H	15.832521	13.663629	7.421835
H	18.642700	16.862981	8.018044
H	20.687100	19.044270	11.647405
H	19.044513	20.438507	12.854959
H	17.502026	21.558499	14.102279
H	15.250459	25.822310	10.374076
H	13.378240	25.752167	16.887248
H	16.661718	23.109559	15.924100
H	17.681551	15.067348	6.587130
H	15.751880	24.995657	17.297018
B	12.225011	6.348701	13.030272
F	13.100401	7.331889	12.444448
F	12.234966	5.181627	12.253158
F	12.662312	6.088378	14.355283
F	10.904591	6.906635	13.068853

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[Cr(ox)_3]@[Fe_2L_3][BF_4] PBE+U@LS

Cr	12.543806	16.956531	12.975342
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Fe	12.459145	22.145123	13.116441
O	11.613226	15.819062	14.314808
O	10.867371	18.038390	13.120599
O	9.716332	15.701957	15.540144
O	8.914280	18.138942	14.250401
O	11.849554	15.914923	11.430767
O	13.260402	18.130870	11.522407
O	11.754306	15.930250	9.171417
O	13.274731	18.363867	9.276034
O	14.228676	15.905627	13.076271
O	13.445796	18.044259	14.391468
O	16.236086	15.857595	14.115883
O	15.390511	18.210017	15.528266
N	14.387909	10.606395	12.820385
N	13.613878	12.606243	14.230650
N	13.277487	13.501683	15.179034
N	11.862951	20.164154	15.391083
N	11.524152	21.114583	14.501889
N	10.751614	23.186615	13.200875
N	11.819230	10.479256	14.221099
N	10.959574	12.576315	13.010061
N	10.289200	13.517971	12.316888
N	10.778376	20.250042	11.377566
N	11.723893	21.187021	11.567586
N	13.235503	23.257747	11.643879
N	11.884245	10.564770	11.309412
N	13.333121	12.685468	11.299890
N	14.259565	13.648307	11.125809
N	14.815882	20.291629	12.446641
N	14.172046	21.189981	13.212279
N	13.338850	23.195871	14.576706
C	10.423817	16.254380	14.706057
C	9.978643	17.585673	13.998612
C	12.114469	16.421108	10.234957
C	12.951745	17.750840	10.287285

C	15.133904	16.360388	13.931058
C	14.671704	17.644843	14.711894
C	14.741439	9.598246	11.997776
C	15.976717	8.960354	12.075338
C	16.898502	9.375289	13.035701
C	16.546796	10.410945	13.897556
C	15.288463	11.002962	13.772792
C	14.789113	12.062228	14.621719
C	15.203260	12.621187	15.837749
C	14.214763	13.542456	16.181380
C	14.101265	14.363782	17.384684
C	14.912197	14.074787	18.498990
C	14.788206	14.815384	19.670978
C	13.862263	15.856239	19.754827
C	13.055333	16.169924	18.650344
C	13.178562	15.413803	17.476353
C	12.092326	17.291220	18.689102
C	11.272350	17.521146	19.804777
C	10.345659	18.564663	19.792212
C	10.230088	19.391361	18.678378
C	11.053728	19.186652	17.555145
C	11.979388	18.136190	17.576587
C	10.945006	20.088264	16.410083
C	9.969118	21.049028	16.141777
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C	10.827193	9.302338	9.030033
C	11.661676	10.412841	8.923636
C	12.156301	11.006227	10.085952
C	13.073298	12.125951	10.114160
C	13.870001	12.764485	9.154725
C	14.624643	13.702368	9.858275
C	15.669206	14.597687	9.366302
C	17.188072	16.483882	9.668763
C	16.159205	15.657043	10.141088
C	17.652212	17.611763	10.504373
C	19.016279	17.910826	10.645560
C	17.109042	19.449213	12.015509
C	16.710195	18.393013	11.187315
C	16.134804	20.286765	12.711981
C	14.081037	24.319151	11.779152
C	15.095334	21.778520	13.991982
C	12.782259	24.184105	15.342000
C	14.615759	22.829749	14.856877
C	14.196718	24.644809	9.400841
C	16.227920	14.372850	8.093487
C	17.741449	16.233945	8.403529
C	19.423553	18.959977	11.470801
C	18.482664	19.724269	12.154875

C	16.352610	21.225718	13.721039
C	14.591686	25.016415	10.689181
C	13.470241	24.818868	16.370931
C	15.361351	23.425986	15.880296
C	17.255214	15.184957	7.622114
C	14.784998	24.432661	16.646980
H	12.482262	14.130782	15.020489
H	12.628877	19.495514	15.128687
H	10.811631	14.188371	11.759194
H	10.625765	19.541014	12.117305
H	14.462727	14.238741	11.954515
H	14.222567	19.612762	11.890691
H	13.871455	9.118852	11.403565
H	16.030419	7.958052	11.531391
H	17.778625	8.772675	13.169129
H	17.200030	10.718476	14.650592
H	16.116299	12.396552	16.364075
H	15.685713	13.277938	18.415612
H	15.521121	14.626375	20.477865
H	13.879924	16.489040	20.634210
H	12.538897	15.642257	16.635595
H	11.427793	16.886492	20.681839
H	9.790312	18.757399	20.687782
H	9.564072	20.225356	18.714935
H	12.653850	17.970735	16.706577
H	9.088763	21.236896	16.742819
H	7.918274	22.949072	15.104501
H	7.229020	24.862883	13.632742
H	8.852608	25.668993	11.876234
H	11.059632	24.549121	11.676847
H	13.239981	9.040234	14.541284
H	12.046959	7.801573	16.292747
H	9.753101	8.584589	17.018542
H	8.761504	10.583143	15.861561
H	7.820766	12.333590	14.132553
H	6.266346	13.258596	12.742481
H	4.567594	14.654439	11.617468
H	5.257965	16.599019	10.228265
H	9.386176	15.741651	11.081395
H	6.471387	17.113913	8.121082
H	7.291484	19.059437	6.807703
H	9.090469	20.497503	7.697327
H	9.246188	18.064245	11.264031
H	11.000044	21.509365	8.354507
H	12.980849	23.252801	8.269381
H	10.839092	9.061922	12.411135
H	9.918679	7.919132	10.443260
H	10.439438	8.815563	8.135232
H	15.752575	15.842943	11.136358
H	15.651238	18.171223	11.053682
H	11.757776	24.462390	15.102979
H	11.938647	10.824329	7.953835
H	13.896562	12.580386	8.088610
H	19.758946	17.298040	10.133141
H	14.369410	24.584867	12.794199
H	14.585584	25.166441	8.526594
H	15.869255	13.547628	7.479032
H	18.530387	16.882430	8.020314
H	20.485558	19.177711	11.589219
H	18.815964	20.544999	12.789570
H	17.294991	21.451491	14.202757
H	15.290539	25.834445	10.856312
H	12.974317	25.600092	16.944720
H	16.376115	23.079216	16.070070
H	17.678198	15.001387	6.633811
H	15.347168	24.905118	17.452207
B	12.670891	6.397522	12.724121
F	13.034563	6.932403	11.446035
F	12.680894	4.998022	12.689980
F	13.601227	6.881531	13.699634
F	11.365592	6.880667	13.063046

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[Fe(ox)_3]@[Fe_2L_3][BF_4]	PBE+U@HS
Fe	12.529247 16.930714 12.970671
Fe	12.619120 11.631656 12.857316
Fe	12.472899 22.105789 13.129507

O	11.463830	15.807116	14.275058
O	10.816788	18.065732	13.065702
O	9.579156	15.817924	15.527049
O	8.827301	18.196281	14.131248
O	11.945554	15.886165	11.341551
O	13.302675	18.148114	11.505300
O	11.833663	15.997633	9.084395
O	13.433617	18.360830	9.258624
O	14.246631	15.898614	13.233971
O	13.392030	18.091757	14.436600
O	16.261530	15.999880	14.258906
O	15.281877	18.290617	15.660838
N	14.324187	10.580505	12.898735
N	13.558511	12.613065	14.270207
N	13.211998	13.505762	15.218342
N	11.714598	20.093239	15.509599
N	11.411647	21.068564	14.635478
N	10.605865	23.339282	13.426881
N	11.737921	10.514025	14.267462
N	10.919498	12.596361	13.005691
N	10.266448	13.519663	12.272872
N	10.713676	20.197396	11.194599
N	11.618758	21.162135	11.420925
N	13.132422	23.378798	11.440177
N	11.843429	10.570060	11.345341
N	13.330667	12.665078	11.351646
N	14.285757	13.601811	11.187258
N	15.012430	20.225828	12.440884
N	14.373164	21.139362	13.189151
N	13.644090	23.294586	14.630142
C	10.302007	16.305788	14.665293
C	9.898324	17.636850	13.917339
C	12.203304	16.438832	10.166621
C	13.053466	17.766128	10.262287
C	15.130229	16.429749	14.063316
C	14.604948	17.716885	14.813282
C	14.658074	9.533641	12.117422
C	15.888214	8.887233	12.211256
C	16.825454	9.338029	13.138430
C	16.490290	10.409824	13.962952
C	15.234117	11.003187	13.830295
C	14.738236	12.079942	14.661211
C	15.147215	12.645713	15.875620
C	14.148517	13.555572	16.220782
C	14.022356	14.360060	17.434052
C	14.836232	14.061924	18.544142
C	14.700456	14.776443	19.730505
C	13.759227	15.801453	19.833126
C	12.950386	16.125589	18.733282
C	13.084722	15.395090	17.543871
C	11.979930	17.238893	18.793113
C	11.153318	17.442635	19.909387
C	10.226651	18.486113	19.916446
C	10.117278	19.339088	18.821487
C	10.948087	19.160584	17.699809
C	11.873284	18.109597	17.701388
C	10.851609	20.079476	16.568558
C	9.936661	21.114889	16.344570
C	10.324408	21.702881	15.135602
C	9.794931	22.843148	14.399045
C	8.534436	23.400306	14.659381
C	8.108525	24.493544	13.912519
C	8.945159	25.003850	12.915645
C	10.176808	24.389424	12.705689
C	12.254381	9.442357	14.902027
C	11.562030	8.748257	15.891364
C	10.287355	9.175270	16.257631
C	9.733966	10.272537	15.601363
C	10.473254	10.914091	14.606592
C	9.994710	12.023142	13.808683
C	8.735625	12.594033	13.582862
C	8.930476	13.550304	12.586959
C	7.938558	14.384647	11.912273
C	6.572391	14.068719	12.043845
C	5.608402	14.815406	11.373357
C	5.983844	15.889792	10.566091
C	7.338621	16.231129	10.434007

C	8.305991	15.468533	11.104258
C	7.762486	17.394567	9.626626
C	7.199665	17.667396	8.369923
C	7.644074	18.760043	7.624023
C	8.642516	19.593627	8.120554
C	9.209351	19.344934	9.384432
C	8.758930	18.244343	10.123760
C	10.232534	20.243810	9.912848
C	10.883019	21.309779	9.288466
C	11.734267	21.853025	10.261557
C	12.642309	22.985769	10.231446
C	13.009253	23.640556	9.045432
C	11.045817	9.486419	11.431755
C	10.535030	8.837137	10.310375
C	10.843869	9.323808	9.041909
C	11.678781	10.433982	8.935354
C	12.171656	11.028437	10.097814
C	13.093837	12.143921	10.126548
C	13.909625	12.761933	9.170357
C	14.673820	13.692256	9.873502
C	15.746760	14.552826	9.380465
C	17.325850	16.390845	9.666052
C	16.269040	15.603570	10.145809
C	17.821454	17.518456	10.482964
C	19.192724	17.788882	10.614773
C	17.325896	19.398407	11.957028
C	16.900569	18.335038	11.151565
C	16.365753	20.258247	12.644168
C	13.989408	24.416750	11.479707
C	15.331955	21.783329	13.895943
C	13.183540	24.259349	15.445314
C	14.919956	22.853155	14.791425
C	13.888855	24.714610	9.103357
C	16.302393	14.295771	8.112049
C	17.874885	16.108340	8.405908
C	19.626467	18.846170	11.415663
C	18.705249	19.645827	12.086547
C	16.596304	21.265382	13.584731
C	14.391425	25.115100	10.346339
C	13.959789	24.844368	16.441152
C	15.761210	23.395632	15.774897
C	17.357436	15.067137	7.634716
C	15.276207	24.400975	16.603426
H	12.432544	14.159301	15.033897
H	12.450078	19.392040	15.232935
H	10.811521	14.201137	11.719439
H	10.584421	19.457035	11.928230
H	14.496061	14.247603	11.964656
H	14.432406	19.517585	11.926704
H	13.901493	9.160950	11.432323
H	16.071555	8.021099	11.578824
H	17.796227	8.851571	13.232816
H	17.185447	10.790878	14.710022
H	16.046685	12.427319	16.436290
H	15.564710	13.254014	18.484136
H	15.337841	14.535433	20.581936
H	13.672568	16.375632	20.756476
H	12.431058	15.636514	16.703980
H	11.215667	16.760993	20.758623
H	9.574879	18.628011	20.779130
H	9.387298	20.147881	18.841708
H	12.541975	17.963472	16.852719
H	9.104768	21.390680	16.979824
H	7.898825	22.961491	15.427176
H	7.130755	24.938698	14.097856
H	8.650082	25.856773	12.306232
H	10.858322	24.746623	11.932132
H	13.228580	9.089841	14.574279
H	12.023758	7.865662	16.329070
H	9.723220	8.651531	17.029265
H	8.736877	10.636940	15.845500
H	7.802349	12.351205	14.073933
H	6.265675	13.222811	12.658170
H	4.553877	14.560786	11.485138
H	5.223855	16.488348	10.062197
H	9.358687	15.725332	10.974191
H	6.435923	17.002541	7.964495

H	7.215273	18.957173	6.640872
H	8.977637	20.443414	7.526320
H	9.169123	18.041531	11.113402
H	10.756095	21.632930	8.263246
H	12.615000	23.287844	8.093524
H	10.851091	9.087517	12.423560
H	9.933863	7.941951	10.455273
H	10.456925	8.836294	8.147169
H	15.866525	15.814567	11.138162
H	15.836748	18.136581	11.018795
H	12.151642	24.571628	15.278113
H	11.957382	10.844291	7.965517
H	13.945721	12.565499	8.106811
H	19.919798	17.148630	10.113644
H	14.359973	24.691022	12.468383
H	14.188446	25.230648	8.191062
H	15.918830	13.476127	7.505422
H	18.684822	16.727410	8.018005
H	20.693606	19.041271	11.527234
H	19.059555	20.468164	12.707653
H	17.554642	21.565312	13.988835
H	15.085624	25.949049	10.438086
H	13.540326	25.626554	17.071916
H	16.772053	23.008177	15.892558
H	17.777041	14.858279	6.650017
H	15.913573	24.829746	17.377093
B	12.702739	6.446183	12.759362
F	13.063180	6.978668	11.479376
F	12.727116	5.046817	12.731962
F	13.626461	6.944402	13.734205
F	11.392181	6.917850	13.093939

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[Cr(ox)_3]@[Fe_2L_3][BF_4] PBE(D3)+U@LS

Cr	12.544827	16.935652	12.973621
Fe	12.667620	11.745545	12.811738
Fe	12.456776	22.029771	13.115823
O	11.605801	15.806046	14.330578
O	10.850643	18.011504	13.122425
O	9.728131	15.709105	15.587383
O	8.876906	18.089883	14.217264
O	11.841170	15.904847	11.411517
O	13.267565	18.107688	11.504974
O	11.713007	15.941356	9.153832
O	13.321647	18.322690	9.257568
O	14.250155	15.895548	13.073461
O	13.458653	18.018826	14.403142
O	16.274743	15.871967	14.080442
O	15.387224	18.166173	15.569305
N	14.377454	10.734846	12.714237
N	13.675913	12.715571	14.153113
N	13.362744	13.600996	15.113474
N	11.789739	20.063233	15.331251
N	11.465138	20.999607	14.427178
N	10.752902	23.052812	13.100045
N	11.913580	10.607921	14.263721
N	10.996101	12.682032	13.096823
N	10.305580	13.613022	12.416137
N	10.866487	20.154311	11.337465
N	11.815926	21.077238	11.551080
N	13.316762	23.128246	11.699832
N	11.800317	10.694442	11.363799
N	13.242790	12.792816	11.285674
N	14.168340	13.747499	11.090596
N	14.802822	20.193882	12.538662
N	14.136702	21.076267	13.297821
N	13.245362	23.059368	14.622302
C	10.417590	16.244015	14.729344
C	9.954742	17.554146	13.992658
C	12.100229	16.415092	10.213903
C	12.969495	17.725046	10.266739
C	15.161265	16.355093	13.922467
C	14.683217	17.617338	14.731094
C	14.678940	9.733248	11.865815
C	15.916955	9.097468	11.866895
C	16.893668	9.508875	12.773191
C	16.596162	10.542452	13.657858

C	15.333675	11.134122	13.610795
C	14.878544	12.191244	14.485111
C	15.336485	12.761198	15.681727
C	14.344826	13.662012	16.070222
C	14.241526	14.478319	17.272532
C	15.102181	14.246211	18.361161
C	14.953162	14.971387	19.540128
C	13.954392	15.940224	19.654929
C	13.105981	16.200907	18.569631
C	13.254400	15.462677	17.389837
C	12.072378	17.252929	18.610466
C	11.216000	17.426124	19.707232
C	10.215258	18.398896	19.666208
C	10.067657	19.214203	18.547397
C	10.935576	19.069150	17.450099
C	11.927730	18.084814	17.494731
C	10.828520	19.965841	16.306777
C	9.840935	20.901387	15.992988
C	10.278741	21.524678	14.816629
C	9.812121	22.615896	13.996920
C	8.543395	23.197976	14.075643
C	8.220805	24.246645	13.221063
C	9.178405	24.687498	12.303208
C	10.421691	24.065424	12.273328
C	12.493414	9.539074	14.842474
C	11.883856	8.813901	15.862057
C	10.627211	9.208135	16.315796
C	10.010473	10.306301	15.721849
C	10.668966	10.980979	14.694849
C	10.126025	12.097782	13.951910
C	8.856598	12.676858	13.811686
C	8.994250	13.646227	12.817669
C	7.991472	14.505181	12.201684
C	6.622592	14.266967	12.423181
C	5.662234	15.036421	11.772194
C	6.043776	16.056455	10.898455
C	7.403989	16.323519	10.688376
C	8.365230	15.540750	11.338206
C	7.867934	17.428570	9.827646
C	7.317805	17.683706	8.563233
C	7.837216	18.707373	7.768185
C	8.891270	19.493266	8.226547
C	9.436234	19.265570	9.503042
C	8.918464	18.230238	10.287415
C	10.489841	20.130779	10.017474
C	11.252081	21.101168	9.364395
C	12.062496	21.668332	10.357477
C	13.006346	22.757455	10.416556
C	13.569623	23.397233	9.308392
C	11.015463	9.610094	11.513470
C	10.456648	8.936482	10.429813
C	10.698705	9.403018	9.139105
C	11.508646	10.524913	8.969803
C	12.052276	11.144653	10.094482
C	12.952222	12.277043	10.068664
C	13.709325	12.924549	9.081671
C	14.486635	13.863106	9.760933
C	15.520345	14.759938	9.261471
C	17.123815	16.556624	9.637551
C	16.078855	15.741430	10.087236
C	17.631190	17.602808	10.545792
C	18.999691	17.841800	10.735763
C	17.112285	19.335071	12.179238
C	16.700657	18.360372	11.265212
C	16.133182	20.158812	12.875977
C	14.199880	24.132084	11.875836
C	15.041587	21.628539	14.141163
C	12.646462	24.027689	15.345027
C	14.512236	22.675408	14.980281
C	14.472511	24.436049	9.507635
C	16.016765	14.611031	7.953356
C	17.627023	16.377130	8.341477
C	19.419655	18.804109	11.656374
C	18.488570	19.545045	12.379391
C	16.309802	21.077591	13.912156
C	14.793025	24.809252	10.816011
C	13.262886	24.655947	16.421568

C	15.185539	23.266366	16.053607
C	17.062980	15.412293	7.504414
C	14.556429	24.269182	16.783434
H	12.566388	14.247383	14.963633
H	12.564823	19.390447	15.107255
H	10.821124	14.301523	11.839424
H	10.678607	19.438658	12.083988
H	14.399235	14.391522	11.869503
H	14.254007	19.506445	11.962877
H	13.887426	9.405427	11.199749
H	16.087584	8.273899	11.176743
H	17.870319	9.026235	12.797139
H	17.326301	10.899669	14.382535
H	16.263321	12.555799	16.201010
H	15.875122	13.481619	18.290818
H	15.624630	14.781784	20.377983
H	13.852718	16.519769	20.573208
H	12.569381	15.656880	16.564006
H	11.311879	16.772919	20.575190
H	9.536882	18.515484	20.511721
H	9.285475	19.972616	18.530761
H	12.615384	17.956189	16.659154
H	8.924012	21.081109	16.538563
H	7.823987	22.807649	14.793738
H	7.235510	24.709782	13.262561
H	8.970250	25.502140	11.611890
H	11.190687	24.382923	11.572255
H	13.450454	9.223443	14.437851
H	12.378819	7.921103	16.235682
H	10.122459	8.651902	17.104927
H	9.023401	10.643762	16.034700
H	7.954174	12.430925	14.355683
H	6.310801	13.464492	13.090801
H	4.604380	14.841727	11.950683
H	5.288854	16.670304	10.405735
H	9.419093	15.742876	11.144031
H	6.508039	17.055599	8.190333
H	7.421225	18.888375	6.776751
H	9.282225	20.293485	7.598688
H	9.321105	18.037411	11.281361
H	11.228875	21.339288	8.309153
H	13.304435	23.058065	8.308293
H	10.864306	9.229620	12.519134
H	9.869716	8.041286	10.625346
H	10.273748	8.895028	8.273598
H	15.717815	15.874404	11.107562
H	15.640311	18.182120	11.088458
H	11.640581	24.303893	15.035957
H	11.728254	10.925177	7.980981
H	13.699187	12.742860	8.015008
H	19.732547	17.247163	10.189282
H	14.426011	24.396264	12.906739
H	14.927198	24.943298	8.657362
H	15.595283	13.853104	7.293933
H	18.433112	17.016660	7.979952
H	20.484754	18.971188	11.818708
H	18.830529	20.296407	13.090615
H	17.232604	21.294625	14.433788
H	15.497287	25.613516	11.021140
H	12.729143	25.433294	16.965388
H	16.184835	22.918050	16.309836
H	17.440361	15.286724	6.489189
H	15.061724	24.738134	17.627105
B	12.089051	6.570266	13.108801
F	12.936904	7.542382	12.466998
F	11.958232	5.442441	12.285481
F	12.659696	6.232933	14.361862
F	10.806957	7.176739	13.319379

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[Cr(ox)_3]@[Fe_2L_3][BF_4] PBE(D3)+U@HS			
Cr	12.534727	16.916781	12.987141
Fe	12.674749	11.788154	12.802780
Fe	12.477265	21.962890	13.085899
O	11.542004	15.795248	14.313277
O	10.834134	17.990950	13.052438
O	9.653611	15.760096	15.557501

O	8.842813	18.110015	14.111565
O	11.874064	15.920374	11.382586
O	13.346455	18.092874	11.568418
O	11.752328	16.056422	9.127846
O	13.422808	18.387746	9.330763
O	14.246447	15.886281	13.131957
O	13.384472	17.979897	14.470564
O	16.278529	15.941935	14.122797
O	15.312450	18.192346	15.628413
N	14.395048	10.795733	12.717548
N	13.656114	12.757621	14.163840
N	13.313718	13.618897	15.136020
N	11.656392	19.970776	15.449535
N	11.381102	20.929107	14.555692
N	10.628632	23.122185	13.248877
N	11.919487	10.641959	14.246710
N	10.993244	12.710096	13.072609
N	10.294798	13.626283	12.379204
N	10.796401	20.062188	11.157001
N	11.746538	20.981643	11.373451
N	13.273777	23.174093	11.404931
N	11.824790	10.739546	11.343893
N	13.263208	12.842103	11.287022
N	14.203291	13.785296	11.106189
N	14.982766	20.086575	12.637053
N	14.305486	20.988365	13.362670
N	13.492963	23.181377	14.658158
C	10.358477	16.263035	14.692405
C	9.920905	17.562189	13.917949
C	12.146372	16.475638	10.208594
C	13.047424	17.763879	10.315957
C	15.144715	16.380021	13.974839
C	14.623126	17.622174	14.791528
C	14.716792	9.805934	11.862853
C	15.963821	9.187988	11.868131
C	16.927695	9.605743	12.785280
C	16.608745	10.627080	13.676731
C	15.338215	11.200820	13.625122
C	14.859444	12.242120	14.506109
C	15.289170	12.794261	15.721272
C	14.277960	13.672686	16.111295
C	14.141200	14.453293	17.334062
C	14.983954	14.195472	18.431168
C	14.805850	14.880877	19.629504
C	13.796094	15.836637	19.755175
C	12.965289	16.123807	18.662881
C	13.141240	15.423301	17.463346
C	11.929781	17.173206	18.717806
C	11.061797	17.324537	19.808968
C	10.069194	18.306088	19.781572
C	9.940065	19.151311	18.682312
C	10.818429	19.027034	17.591455
C	11.802512	18.033905	17.622806
C	10.733715	19.941950	16.460942
C	9.812687	20.954208	16.181519
C	10.255162	21.545867	14.987684
C	9.770217	22.666114	14.204410
C	8.509754	23.251167	14.391225
C	8.128658	24.317615	13.585928
C	9.011377	24.778949	12.602656
C	10.243154	24.148738	12.469218
C	12.503092	9.576641	14.827893
C	11.897595	8.854849	15.852377
C	10.641560	9.248700	16.308034
C	10.020008	10.341815	15.709560
C	10.674476	11.012934	14.677757
C	10.126019	12.122493	13.927956
C	8.850816	12.684572	13.776409
C	8.980605	13.645634	12.773370
C	7.962352	14.476186	12.144026
C	6.599682	14.214949	12.379510
C	5.618976	14.951989	11.722371
C	5.974005	15.964430	10.829434
C	7.326937	16.255062	10.604163
C	8.309931	15.502109	11.258264
C	7.754379	17.363338	9.729522
C	7.168933	17.612132	8.479272

C	7.645181	18.651582	7.677964
C	8.693326	19.458219	8.114628
C	9.275363	19.233982	9.374683
C	8.798496	18.184655	10.166290
C	10.334784	20.102496	9.869824
C	11.042351	21.124724	9.230379
C	11.909253	21.643943	10.203569
C	12.872952	22.731592	10.182665
C	13.386568	23.287497	9.002832
C	11.040022	9.653783	11.483104
C	10.483210	8.989904	10.392434
C	10.727525	9.467641	9.106227
C	11.538525	10.590412	8.947986
C	12.079933	11.200193	10.079120
C	12.982763	12.330685	10.065901
C	13.760291	12.970310	9.090063
C	14.541778	13.897038	9.780998
C	15.603325	14.767920	9.293807
C	17.261408	16.510861	9.684784
C	16.189380	15.726563	10.127437
C	17.790163	17.545853	10.593302
C	19.162329	17.759736	10.789551
C	17.297928	19.298528	12.213045
C	16.872391	18.326822	11.302157
C	16.321334	20.130852	12.902089
C	14.198340	24.145615	11.476670
C	15.220119	21.639683	14.119617
C	12.973320	24.178648	15.392299
C	14.740013	22.728212	14.958554
C	14.331751	24.303459	9.089514
C	16.101490	14.610226	7.987069
C	17.766121	16.320510	8.390960
C	19.596323	18.720436	11.705274
C	18.676092	19.484055	12.419563
C	16.500106	21.129404	13.867923
C	14.753076	24.742278	10.348984
C	13.661787	24.785367	16.438914
C	15.488306	23.280759	16.006099
C	17.175907	15.377908	7.546898
C	14.943993	24.322888	16.749563
H	12.513138	14.259435	14.981061
H	12.414683	19.283955	15.218966
H	10.807378	14.315972	11.802363
H	10.629542	19.344659	11.904633
H	14.427219	14.425809	11.891016
H	14.427349	19.387984	12.079646
H	13.934590	9.473155	11.188159
H	16.151851	8.373077	11.172231
H	17.911197	9.137358	12.812136
H	17.328361	10.988750	14.409671
H	16.208629	12.588604	16.253409
H	15.765524	13.440690	18.351426
H	15.463370	14.670935	20.473530
H	13.672712	16.387525	20.688279
H	12.469043	15.636276	16.631276
H	11.142901	16.649093	20.661289
H	9.381476	18.405260	20.621765
H	9.160043	19.912143	18.673893
H	12.502986	17.922507	16.795204
H	8.940703	21.213325	16.767954
H	7.840448	22.850042	15.150684
H	7.150517	24.780941	13.713628
H	8.750032	25.608484	11.947840
H	10.963086	24.468176	11.714498
H	13.459726	9.261202	14.421866
H	12.396133	7.965312	16.228947
H	10.140773	8.696070	17.102252
H	9.032878	10.678379	16.023223
H	7.948665	12.430007	14.316723
H	6.308829	13.419447	13.064471
H	4.566679	14.739222	11.912502
H	5.203737	16.556682	10.334185
H	9.358525	15.720961	11.051503
H	6.363927	16.968665	8.122597
H	7.200716	18.828211	6.698166
H	9.053636	20.268017	7.480642
H	9.224565	17.997721	11.151719

H	10.938595	21.434707	8.198518
H	13.059886	22.899778	8.039299
H	10.887583	9.265078	12.485572
H	9.895101	8.093460	10.578459
H	10.303314	8.967728	8.235655
H	15.829793	15.865096	11.147843
H	15.810367	18.171476	11.113107
H	11.966318	24.495962	15.117638
H	11.759915	10.999258	7.963079
H	13.765174	12.785772	8.023867
H	19.886580	17.147501	10.251043
H	14.488639	24.451404	12.482876
H	14.748178	24.743456	8.183388
H	15.658472	13.870482	7.321292
H	18.593286	16.936476	8.036267
H	20.663665	18.866484	11.872839
H	19.028810	20.227443	13.133922
H	17.437412	21.436016	14.314049
H	15.495503	25.531021	10.457355
H	13.199025	25.596409	16.998762
H	16.472788	22.876224	16.236132
H	17.554058	15.244356	6.533023
H	15.508129	24.764676	17.570838
B	12.147886	6.625472	13.079741
F	12.978241	7.600391	12.419883
F	12.024966	5.485983	12.271947
F	12.732871	6.310900	14.332527
F	10.859983	7.218465	13.293664

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[Fe(ox)_3]@[Fe_2L_3][BF_4] PBE(D3)+U@LS

Fe	12.538107	16.908755	12.978949
Fe	12.618417	11.702789	12.847948
Fe	12.448107	22.060151	13.116655
O	11.526182	15.786742	14.317896
O	10.843340	18.054359	13.157855
O	9.666686	15.765877	15.605648
O	8.839218	18.115742	14.199177
O	11.887494	15.866841	11.376423
O	13.224337	18.137276	11.483355
O	11.699797	15.963647	9.124365
O	13.318816	18.319613	9.233315
O	14.253721	15.860124	13.161417
O	13.486892	18.066679	14.384614
O	16.296598	15.909173	14.131307
O	15.385941	18.187279	15.602751
N	14.312401	10.662627	12.767446
N	13.636722	12.674767	14.177318
N	13.336591	13.574127	15.129780
N	11.796226	20.087445	15.327258
N	11.464208	21.024738	14.427533
N	10.742592	23.080559	13.110628
N	11.840501	10.589423	14.301860
N	10.957889	12.663200	13.112950
N	10.283100	13.596295	12.420098
N	10.868102	20.178676	11.336351
N	11.807705	21.110660	11.552733
N	13.302436	23.165918	11.703717
N	11.747757	10.662250	11.392954
N	13.218313	12.742019	11.328382
N	14.152907	13.688685	11.137650
N	14.782685	20.213576	12.528770
N	14.124641	21.102144	13.287513
N	13.243853	23.081569	14.624230
C	10.363290	16.266365	14.731870
C	9.927038	17.589507	13.993709
C	12.106964	16.410687	10.189103
C	12.957998	17.736514	10.249324
C	15.170290	16.363043	13.974323
C	14.688976	17.647986	14.750775
C	14.585292	9.621661	11.958010
C	15.814599	8.968286	11.967789
C	16.812404	9.407084	12.835218
C	16.541299	10.477845	13.684761
C	15.284717	11.080104	13.637670
C	14.846756	12.159738	14.494988
C	15.324622	12.752411	15.672631

C	14.336717	13.655538	16.065572
C	14.252900	14.488887	17.257334
C	15.134650	14.273725	18.332456
C	15.005162	15.012896	19.504835
C	14.004654	15.978999	19.626206
C	13.135840	16.223503	18.553485
C	13.265166	15.472026	17.379838
C	12.101378	17.274100	18.601232
C	11.256832	17.450433	19.706555
C	10.255527	18.422879	19.672927
C	10.097077	19.235295	18.553502
C	10.953812	19.087164	17.447883
C	11.945268	18.102022	17.484368
C	10.838135	19.983369	16.305232
C	9.845139	20.915022	15.997208
C	10.276893	21.544021	14.821726
C	9.804827	22.636727	14.007345
C	8.533955	23.213613	14.090038
C	8.205982	24.263858	13.239494
C	9.160478	24.711689	12.321703
C	10.406179	24.094687	12.287879
C	12.405737	9.519481	14.892564
C	11.782705	8.815382	15.919331
C	10.531836	9.231640	16.369439
C	9.930941	10.332246	15.761722
C	10.600112	10.985703	14.727760
C	10.076476	12.103117	13.973032
C	8.816761	12.700963	13.823841
C	8.971331	13.655063	12.817978
C	7.981288	14.517752	12.187518
C	6.608943	14.283670	12.391277
C	5.659443	15.053886	11.725736
C	6.056086	16.069631	10.853907
C	7.419686	16.332288	10.661503
C	8.370354	15.550062	11.327211
C	7.896760	17.431545	9.801131
C	7.370909	17.670519	8.523466
C	7.902275	18.687511	7.728013
C	8.943596	19.482080	8.199630
C	9.463426	19.270825	9.489396
C	8.934357	18.241891	10.274473
C	10.503586	20.146085	10.013003
C	11.262836	21.120010	9.361867
C	12.059537	21.698850	10.358818
C	12.995914	22.794128	10.419874
C	13.556173	23.438778	9.312933
C	10.954739	9.583002	11.532870
C	10.377257	8.932784	10.445694
C	10.611910	9.415302	9.160120
C	11.437523	10.526305	8.999472
C	11.998280	11.123751	10.127527
C	12.912515	12.244613	10.107980
C	13.667729	12.896938	9.122706
C	14.460644	13.818465	9.806887
C	15.497053	14.712360	9.308080
C	17.093138	16.516593	9.674621
C	16.046205	15.705133	10.126724
C	17.598875	17.572272	10.572469
C	18.968178	17.808143	10.760971
C	17.085479	19.327745	12.181644
C	16.670124	18.342285	11.280872
C	16.111463	20.163587	12.870861
C	14.178470	24.175563	11.881787
C	15.032601	21.644137	14.134044
C	12.649718	24.048336	15.352816
C	14.509930	22.690798	14.977554
C	14.451762	24.483505	9.514205
C	16.003187	14.548628	8.005525
C	17.604652	16.323749	8.383638
C	19.391455	18.781207	11.668339
C	18.462403	19.535623	12.379592
C	16.295217	21.079692	13.908122
C	14.768222	24.857759	10.823299
C	13.270420	24.668724	16.431444
C	15.187474	23.274013	16.052522
C	17.049383	15.348027	7.553737
C	14.563300	24.275272	16.788669

H	12.534171	14.210886	14.986240
H	12.574908	19.419147	15.097521
H	10.808775	14.264441	11.830765
H	10.679747	19.466605	12.086929
H	14.400332	14.317590	11.920771
H	14.227928	19.531704	11.951767
H	13.780789	9.259490	11.324562
H	15.950695	8.104309	11.321195
H	17.782795	8.912260	12.864729
H	17.286092	10.850864	14.386360
H	16.261880	12.559164	16.177647
H	15.909243	13.511406	18.256650
H	15.693334	14.836665	20.331966
H	13.917506	16.569987	20.538649
H	12.564844	15.655544	16.564057
H	11.362696	16.800279	20.575644
H	9.586000	18.542225	20.525108
H	9.315906	19.994847	18.543094
H	12.624840	17.971777	16.642462
H	8.929037	21.088631	16.546149
H	7.817102	22.817678	14.807618
H	7.218774	24.722691	13.283780
H	8.947957	25.527685	11.633318
H	11.172935	24.417305	11.586624
H	13.357170	9.177003	14.496212
H	12.275311	7.931793	16.318907
H	10.021126	8.697256	17.170052
H	8.950508	10.689935	16.073027
H	7.909651	12.478603	14.370254
H	6.286413	13.482762	13.055669
H	4.598723	14.862609	11.890281
H	5.310143	16.683869	10.348215
H	9.427428	15.749220	11.146946
H	6.571656	17.034549	8.141399
H	7.506511	18.855887	6.726135
H	9.345100	20.276030	7.570622
H	9.316225	18.062243	11.279240
H	11.246555	21.353008	8.305390
H	13.294114	23.099177	8.312149
H	10.823176	9.188802	12.536372
H	9.785827	8.038243	10.627524
H	10.174066	8.923996	8.291620
H	15.676402	15.849496	11.142592
H	15.608881	18.166389	11.106414
H	11.644116	24.329219	15.046783
H	11.657413	10.934688	8.014091
H	13.645719	12.730791	8.053704
H	19.698885	17.202814	10.223495
H	14.401515	24.440021	12.913323
H	14.903896	24.994694	8.664904
H	15.590060	13.779307	7.354088
H	18.411484	16.961412	8.020541
H	20.457064	18.946432	11.829308
H	18.806240	20.296310	13.079857
H	17.218386	21.283767	14.434263
H	15.466702	25.666642	11.029962
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H	16.185896	22.920664	16.305230
H	17.434448	15.211398	6.542865
H	15.071855	24.737816	17.633942
B	12.686980	6.612490	12.723518
F	12.904057	7.147552	11.413052
F	12.704928	5.213745	12.689756
F	13.714460	7.105275	13.590777
F	11.423033	7.085223	13.202944

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[Fe(ox)_3]@[Fe_2L_3][BF_4] PBE(D3)+U@HS

Fe	12.526594	16.885711	12.959165
Fe	12.617072	11.748952	12.866148
Fe	12.478259	21.989195	13.133099
O	11.476348	15.778012	14.285292
O	10.815936	18.016485	13.047796
O	9.642369	15.850032	15.607122
O	8.835495	18.159463	14.126193
O	11.923540	15.857029	11.331519
O	13.304105	18.103526	11.501047

O	11.746368	16.018566	9.082350
O	13.425133	18.327971	9.255971
O	14.255278	15.872401	13.202246
O	13.378623	18.043467	14.428585
O	16.296624	16.034732	14.163427
O	15.269823	18.254567	15.646266
N	14.314125	10.713281	12.808525
N	13.617668	12.730911	14.201937
N	13.294290	13.616420	15.159776
N	11.625584	19.979243	15.422925
N	11.334981	20.935349	14.528663
N	10.607190	23.194521	13.297828
N	11.825932	10.656146	14.327592
N	10.951783	12.709179	13.096602
N	10.279261	13.618467	12.370753
N	10.832191	20.094311	11.154254
N	11.745565	21.040628	11.404222
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N	13.234742	12.769755	11.341553
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N	14.984123	20.107791	12.547985
N	14.323717	20.995254	13.303804
N	13.538839	23.121994	14.720399
C	10.331837	16.298862	14.699562
C	9.907927	17.602907	13.917055
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C	13.040267	17.734729	10.257503
C	15.145889	16.425475	14.010891
C	14.599450	17.684464	14.792218
C	14.599581	9.672155	12.003771
C	15.835498	9.031425	12.019895
C	16.825943	9.483101	12.889161
C	16.541262	10.553653	13.734563
C	15.278925	11.143072	13.680930
C	14.825447	12.219926	14.533985
C	15.279363	12.802314	15.725943
C	14.277360	13.692182	16.114161
C	14.164275	14.496421	17.323758
C	15.036222	14.266691	18.404281
C	14.880143	14.969955	19.595153
C	13.863453	15.917058	19.729759
C	13.005003	16.177879	18.652636
C	13.158622	15.459425	17.460678
C	11.963051	17.220212	18.713044
C	11.106364	17.374733	19.812771
C	10.105420	18.347805	19.788363
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C	10.824905	19.054869	17.584375
C	11.817678	18.070659	17.612950
C	10.722373	19.958343	16.446697
C	9.793837	20.971462	16.175892
C	10.217904	21.556355	14.976054
C	9.726799	22.687585	14.202687
C	8.443161	23.227055	14.357789
C	8.065875	24.311551	13.572657
C	8.972813	24.829264	12.643105
C	10.225960	24.232953	12.536303
C	12.388899	9.598806	14.942460
C	11.760905	8.916026	15.980607
C	10.507624	9.340964	16.415726
C	9.908911	10.428157	15.782159
C	10.583062	11.060371	14.738320
C	10.063030	12.160951	13.956396
C	8.800466	12.743512	13.774608
C	8.960947	13.673759	12.747308
C	7.967992	14.503874	12.078104
C	6.597090	14.247401	12.265825
C	5.643288	14.982049	11.567421
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C	7.395143	16.271504	10.501697
C	8.351085	15.522459	11.198626
C	7.858562	17.369105	9.631783
C	7.332248	17.593528	8.351341
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C	10.413241	20.128320	9.850899
C	11.114930	21.169550	9.239007
C	11.931495	21.713190	10.243326
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C	13.322881	23.470475	9.108918
C	10.957118	9.620038	11.561751
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C	11.439383	10.553090	9.024013
C	12.005637	11.150759	10.149159
C	12.928371	12.264659	10.124681
C	13.698123	12.895676	9.137392
C	14.503171	13.810560	9.816294
C	15.561315	14.672887	9.307421
C	17.210379	16.434967	9.641465
C	16.146946	15.655454	10.113141
C	17.748936	17.494673	10.514518
C	19.124387	17.724043	10.665915
C	17.287797	19.285303	12.100551
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C	16.328007	20.124956	12.804035
C	14.125907	24.249987	11.609351
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C	17.703687	16.216166	8.347555
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C	18.669814	19.489470	12.259196
C	16.528589	21.096699	13.788830
C	14.626887	24.930934	10.505931
C	13.714416	24.593425	16.608881
C	15.556541	23.154328	16.032986
C	17.114742	15.248350	7.532288
C	15.011433	24.132473	16.857078
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H	12.388855	19.295658	15.180420
H	10.810360	14.280221	11.778505
H	10.654958	19.371857	11.894833
H	14.434621	14.332289	11.925830
H	14.417411	19.423642	11.988562
H	13.800207	9.300476	11.369208
H	15.983409	8.167338	11.375989
H	17.801389	8.998632	12.922949
H	17.280145	10.936915	14.436896
H	16.207154	12.605044	16.246601
H	15.824370	13.519637	18.317828
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H	12.463180	15.652410	16.642685
H	11.203146	16.707713	20.670117
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H	12.512009	17.959879	16.780156
H	8.934069	21.236840	16.777471
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H	10.965011	24.592420	11.818757
H	13.342392	9.249197	14.557037
H	12.251920	8.041694	16.401978
H	9.993516	8.823469	17.225204
H	8.927052	10.792050	16.081545
H	7.887015	12.523717	14.311386
H	6.279788	13.455816	12.943715
H	4.584054	14.773178	11.719673
H	5.284460	16.574613	10.149631
H	9.407108	15.737594	11.029606
H	6.547812	16.940156	7.967854
H	7.447766	18.777573	6.552136
H	9.255250	20.237870	7.397684
H	9.255991	18.033682	11.112753
H	11.040337	21.477518	8.204120
H	12.998070	23.115145	8.132249
H	10.826199	9.229891	12.567021

H	9.777501	8.079200	10.663138
H	10.164722	8.956185	8.324125
H	15.792684	15.818234	11.132201
H	15.778264	18.115878	11.079160
H	12.003255	24.380880	15.291594
H	11.658914	10.957571	8.036940
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H	19.838035	17.102708	10.123743
H	14.421639	24.521282	12.623746
H	14.593084	25.033888	8.341373
H	15.609033	13.722301	7.360123
H	18.522242	16.830097	7.970245
H	20.646636	18.874408	11.671882
H	19.035585	20.259751	12.937631
H	17.473024	21.376407	14.237483
H	15.327312	25.752746	10.644658
H	13.251342	25.353654	17.235550
H	16.550574	22.749900	16.216667
H	17.485718	15.091943	6.519047
H	15.586416	24.525532	17.695514
B	12.694786	6.679213	12.798508
F	12.904015	7.200827	11.481302
F	12.719160	5.280404	12.780194
F	13.723347	7.186587	13.656043
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