Electronic Supplementary Material (ESI) for Chemical Communications

Regioselective Heck Reaction of Aliphatic Olefins and Aryl Halides

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Supporting Information: DFT calculation

Contents

Method

All density functional theory (DFT) calculations were performed using the Gaussian 09 program [1]. The B3LYP DFT functional was used in conjunction with the Lanl2dz ECP basis set for Fe and Pd, the 6-31G* basis set for N, O, P, and Br, and the 6-31G basis set for H and C [2-4]. The solvent effect of methanol was taken into account by use of the IEFPCM method [5]. All optimized geometries were subjected to frequency calculations to verify their characters (local minima or saddle points) and to evaluate the zero-point energy (ZPE) corrections. The reported energy data are relative energy values with ZPE corrections. DFT-optimized structures were drawn with UCSF Chimera [6].

References

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Complete list of authors of Gaussian 09

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Table S1. Energy data.

(a) No MeOH

	E [hartree]	ZPE [hartree]	ΔE [kcal/mol]	Δ(E+ZPE) [kcal/mol]
RC	-5662.553894	0.803654	0.0	0.0
TS1	-5662.533415	0.803132	12.9	12.5
Int1	-5662.585961	0.805788	-20.1	-18.8

(b) 1 MeOH

	E [hartree]	ZPE [hartree]	ΔE [kcal/mol]	Δ(E+ZPE) [kcal/mol]
RC	-5778.266373	0.856520	0.0	0.0
TS1	-5778.244066	0.856132	14.0	13.8
Int1	-5778.297857	0.858974	-19.8	-18.2
TS2	-5778.276915	0.858279	-6.6	-5.5
Int2	-5778.292168	0.859819	-16.2	-14.1

(c) 2 MeOHs

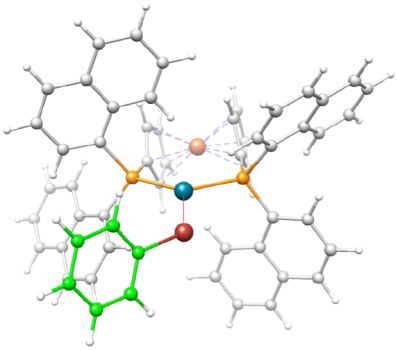
	E [hartree]	ZPE [hartree]	ΔE [kcal/mol]	Δ(E+ZPE) [kcal/mol]
RC	-5893.975871	0.909516	0.0	0.0
TS1	-5893.952981	0.908800	14.4	13.9
Int1	-5894.010839	0.911506	-21.9	-20.7
TS2	-5893.990528	0.911162	-9.2	-8.2
Int2	-5894.007567	0.913062	-19.9	-17.7

(d) 1 MeOHs and 1 Me_3NH^+

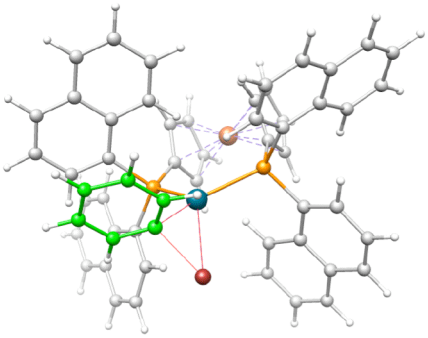
	E [hartree]	ZPE [hartree]	ΔE [kcal/mol]	Δ(E+ZPE) [kcal/mol]
RC	-5953.172634	0.995953	0.0	0.0
TS1	-5953.151159	0.994263	13.5	12.4
Int1	-5953.213003	0.997092	-25.3	-24.6
TS2	-5953.195646	0.996652	-14.4	-14.0
Int2	-5953.213638	0.997685	-25.7	-24.6

Figure S1. Optimized geometries for oxidative addition of PhBr onto (dnpf)Pd^0 (step 1) without explicit MeOH.

RC



TS1



Int1

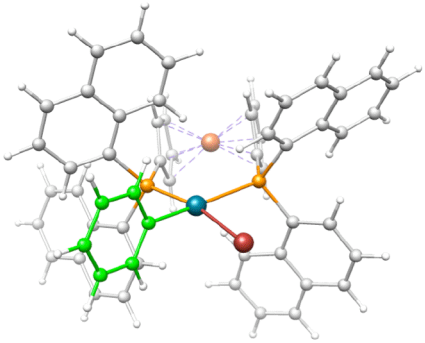
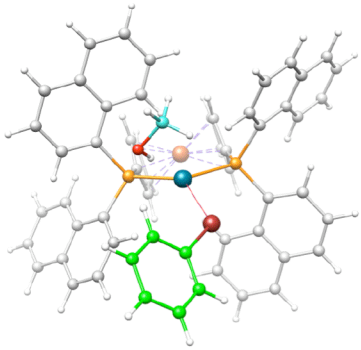
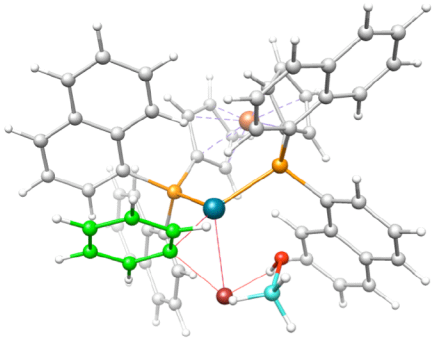


Figure S2. Optimized geometries for oxidative addition of PhBr onto (dnpf)Pd^0 (step 1) and bromide abstraction (step 2) with one explicit MeOH.

RC



TS1



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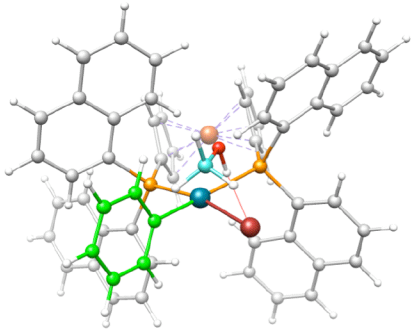
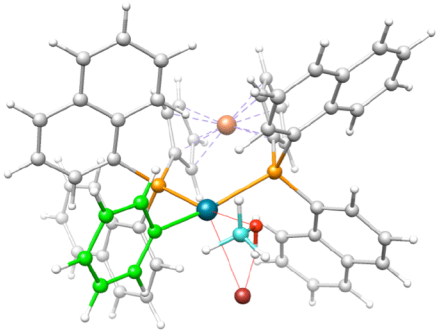


TS2



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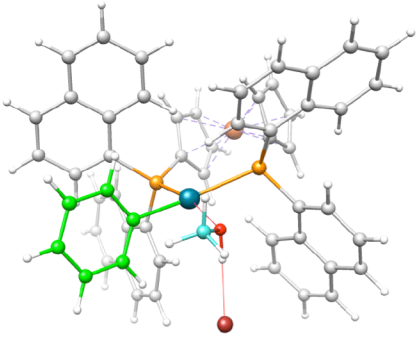
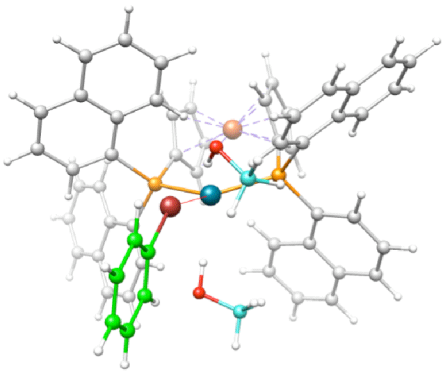
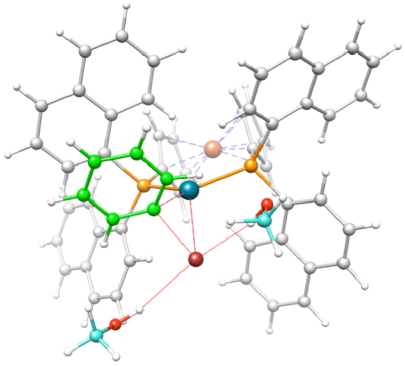


Figure S3. Optimized geometries for oxidative addition of PhBr onto (dnpf)Pd^0 (step 1) and bromide abstraction (step 2) with two explicit MeOHs.

RC



TS1



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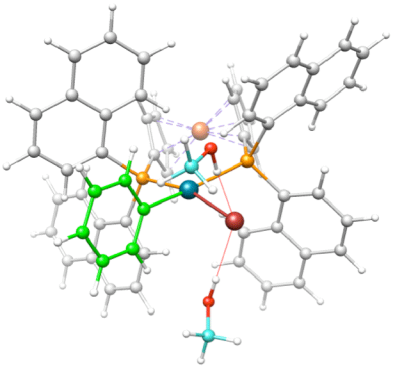
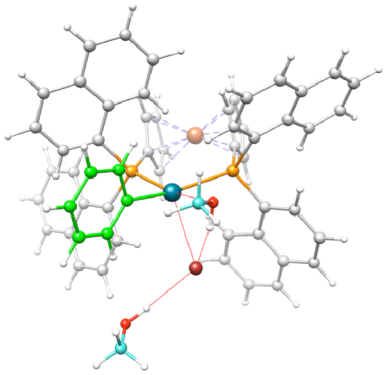


TS2



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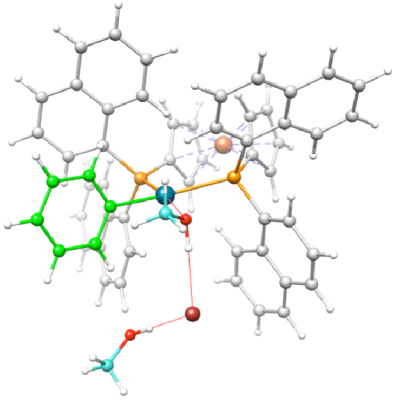
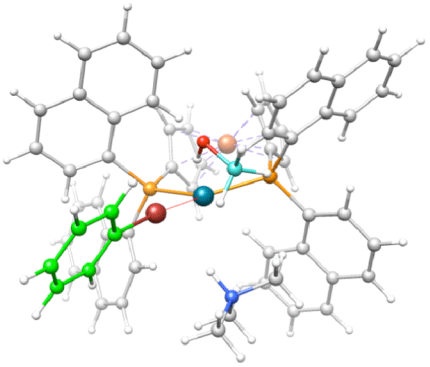
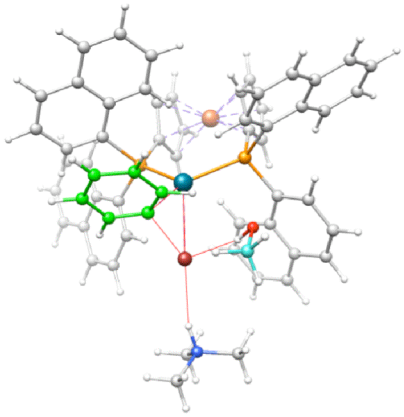


Figure S4. Optimized geometries for oxidative addition of PhBr onto (dnpf)Pd^0 (step 1) and bromide abstraction (step 2) with one explicit MeOH and one Me_3NH^+.

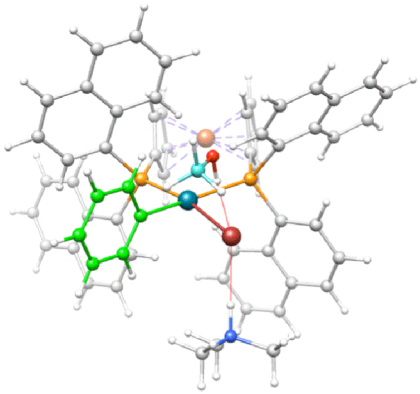
RC



TS1



Int1



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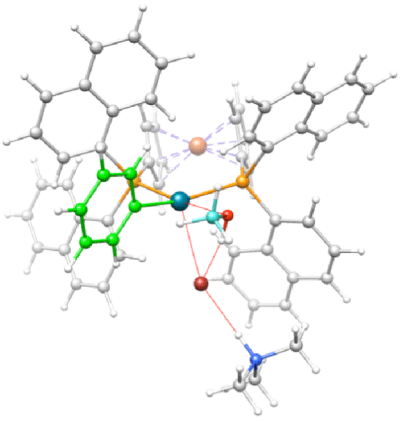

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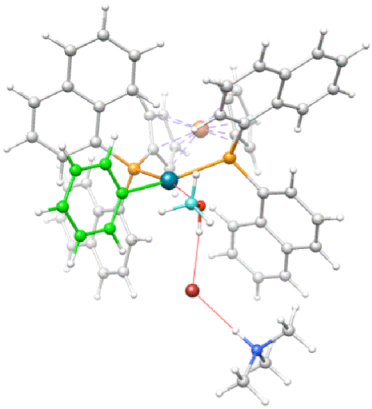


Figure S5. Energy diagrams for oxidative addition of PhBr onto (dnpf)Pd^0 (step 1) and bromide abstraction (step 2) with different numbers of explicit MeOHs. Energies in kcal/mol. No significant effect was seen in step 1 in the presence of hydrogen bonding.

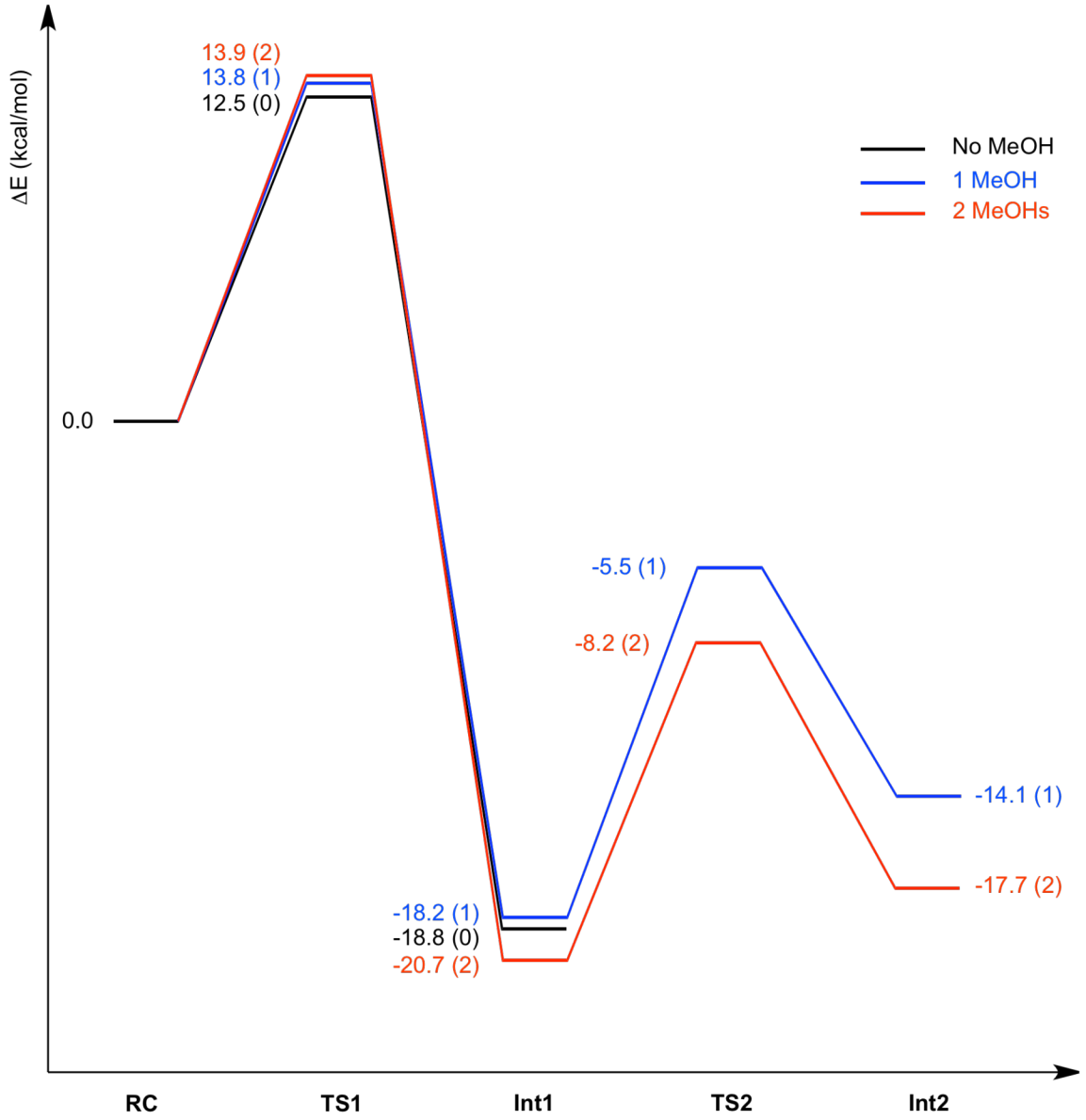


Figure S6. Energy diagrams for oxidative addition of PhBr (step 1) and bromide abstraction (step 2) with two explicit MeOH molecules and with one MeOH and one Me_3NH^+ cation. Energies in kcal/mol.

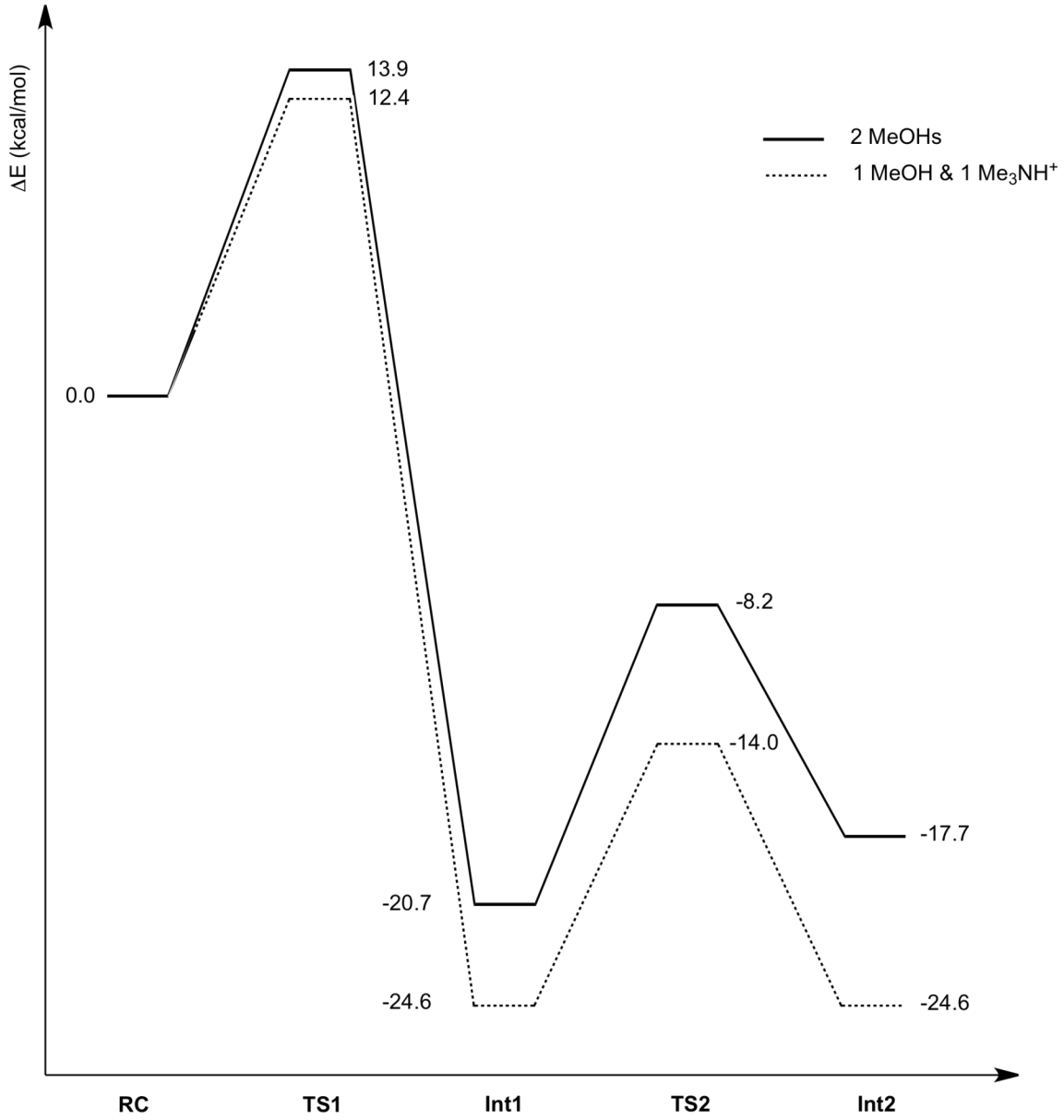


Figure S7. Energy scans for the dissociation of the bromide anion from complex **Int1** (step 2).

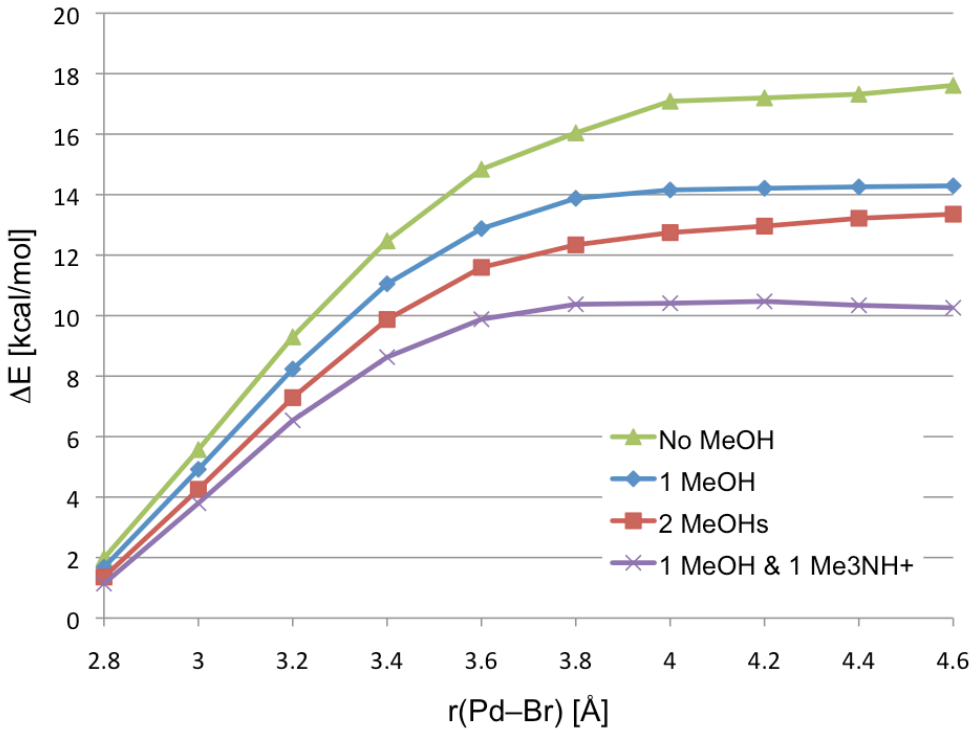


Figure S7*. For the dissociation of Br anion in the presence of 1 MeOH and 1 Me_3NH^+, an energy minimum was located in a stepwise pathway. Its overall barrier was slightly higher than that for the concerted pathway.

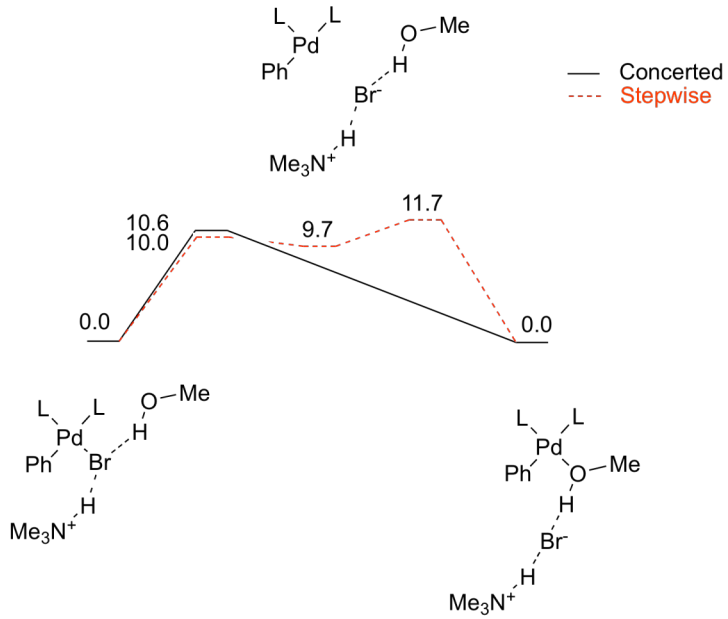


Figure S8. Energy scan calculations for the association of MeOH onto Pd from **Int1.** A stable pentacoordinate Pd species cannot be identified in the associative pathway.

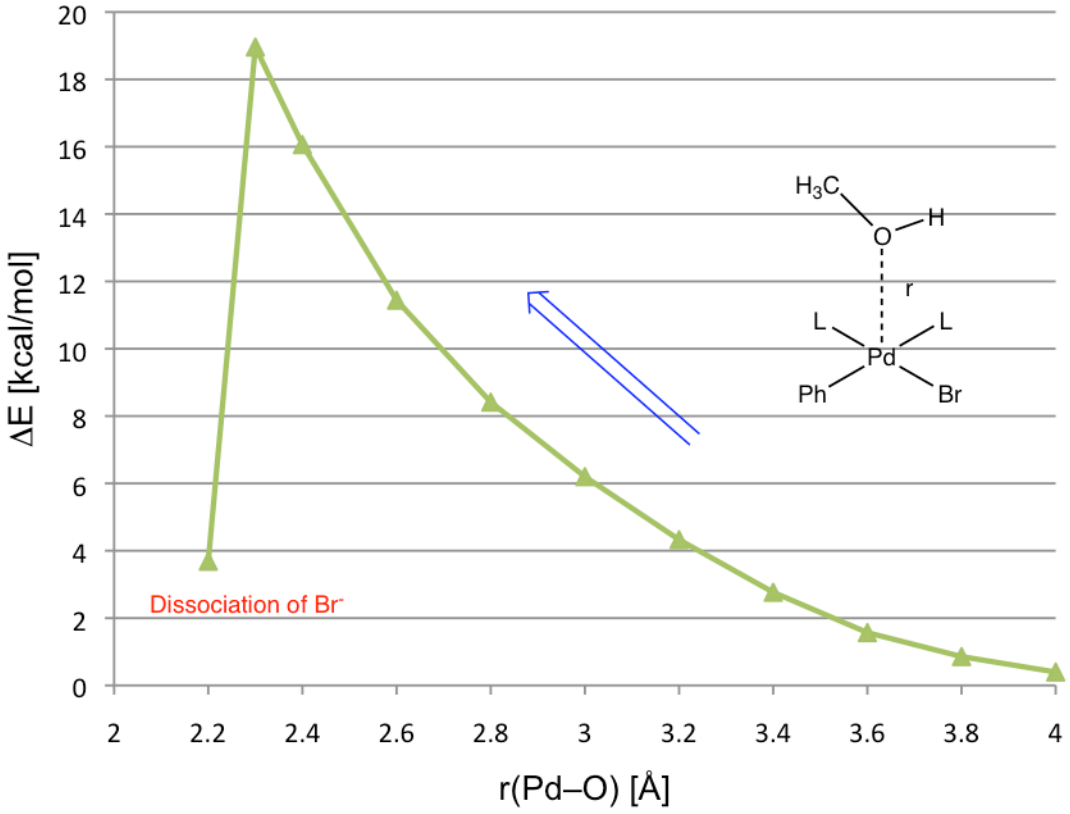
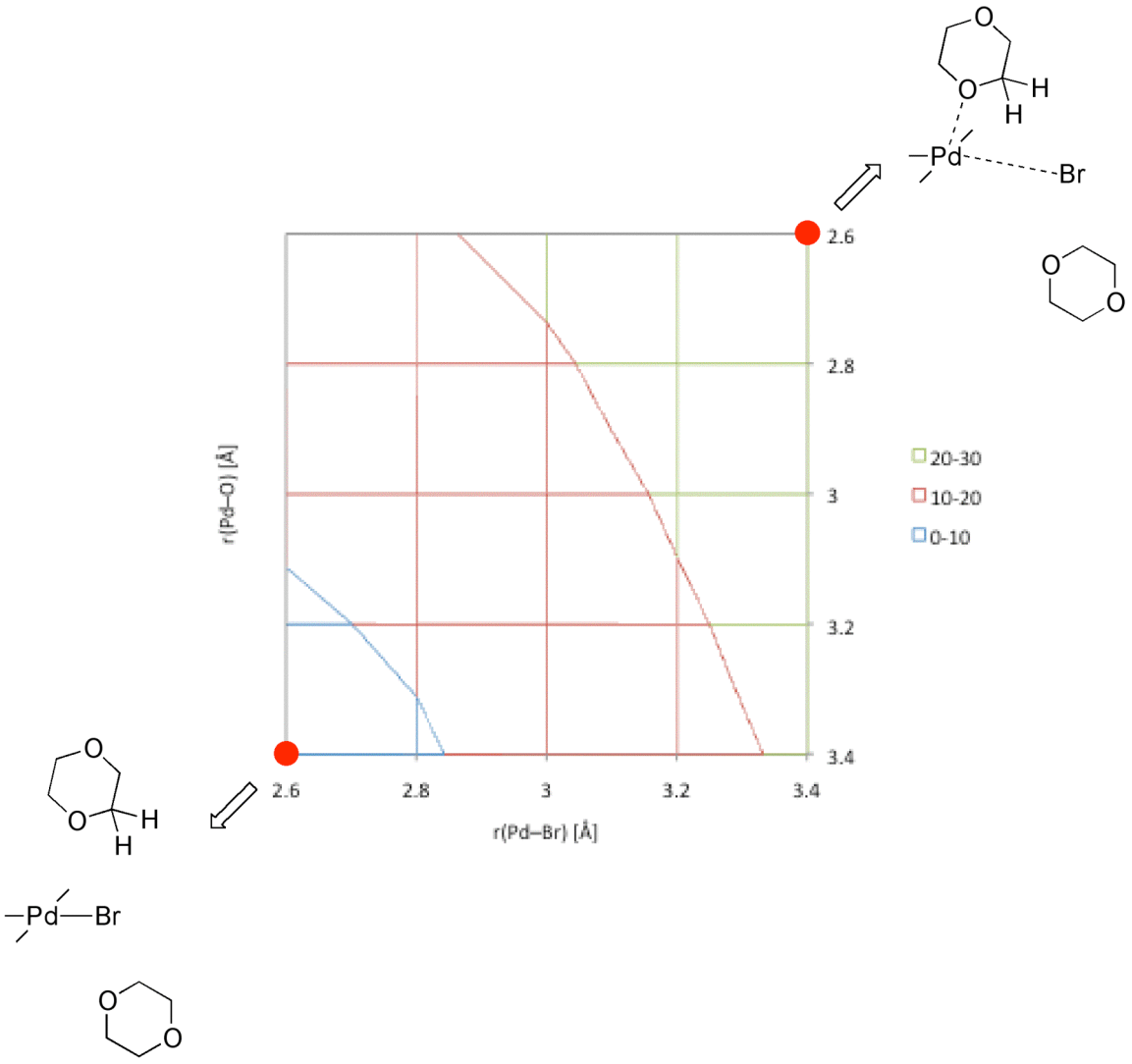


Figure S9. Two-dimensional energy scan for the association of 1,4-dioxane oxygen onto the (dnpf)(phenyl)Pd^{II} center and dissociation of Br anion using the B3LYP(SCRF) method. The solvent effect of dioxane was included by the SCRF method. Energy values are given in kcal/mol. No stable products and intermediates involving hydrogen bonding between α–CH of dioxane and the bromide were seen based on the energy scan.



XYZ coordinates of optimized geometries

No MeOH

=== RC ===

Fe	19.064995	14.941024	20.960160
Pd	20.137538	15.905833	17.166450
Br	20.450051	16.575435	14.401241
C	17.858822	16.239609	19.720612
C	18.474636	16.965243	20.808906
H	19.141587	17.806895	20.706614
C	18.015076	16.409134	22.047405
H	18.304779	16.736830	23.034425
C	17.140360	15.314835	21.741354
H	16.655050	14.667389	22.456336
C	17.050979	15.203072	20.313576
H	16.472472	14.469405	19.775302
C	20.890293	14.199853	20.070627
C	21.144055	14.743945	21.381132
H	21.808785	15.562793	21.605643
C	20.364446	14.011972	22.338060
H	20.331807	14.199937	23.400854
C	19.609352	13.019315	21.630283
H	18.909423	12.321468	22.064626
C	19.914773	13.145730	20.235539
H	19.513907	12.531298	19.444889
C	17.837405	18.531558	17.990862
C	18.786949	19.247305	17.267389
H	19.554833	18.698855	16.730007
C	18.793288	20.663460	17.221047
H	19.553933	21.175417	16.641215
C	17.844211	21.376318	17.919689
H	17.841866	22.462252	17.901416
C	16.844585	20.703861	18.679529
C	15.858345	21.444108	19.394181
H	15.895654	22.528842	19.352451
C	14.874424	20.803848	20.119095
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C	14.837918	19.387151	20.152691
H	14.057902	18.884429	20.715480
C	15.782368	18.639737	19.473942
H	15.728058	17.560579	19.512388
C	16.822974	19.260899	18.720387
C	16.549064	16.025399	17.111624
C	15.592865	16.898622	16.602900
H	15.701426	17.964914	16.750268
C	14.457933	16.438216	15.888964
H	13.737506	17.160671	15.519411
C	14.268422	15.090413	15.677641
H	13.395521	14.728079	15.142826
C	15.226668	14.148085	16.146712
C	15.056505	12.753407	15.907349
H	14.166072	12.425260	15.378796
C	16.000581	11.837408	16.324881
H	15.861479	10.778628	16.132596
C	17.165215	12.286250	16.997320
H	17.917789	11.566370	17.303295
C	17.353107	13.631536	17.258119
H	18.261073	13.958510	17.754190
C	16.394219	14.609366	16.857277
C	21.956279	16.180358	13.237468
C	23.157032	16.871308	13.421989
H	23.249566	17.618432	14.201407
C	24.238781	16.578288	12.580906
H	25.175992	17.108139	12.714758
C	24.111900	15.611565	11.574777
H	24.952803	15.389355	10.926688
C	22.898672	14.931745	11.406531
H	22.795232	14.182592	10.628604
C	21.807595	15.212843	12.239902
H	20.867219	14.689699	12.113834
C	23.277430	15.426083	18.900339
C	24.476783	14.777630	18.623630
H	24.468417	13.779166	18.207121
C	25.734021	15.382483	18.875476
H	26.640428	14.830589	18.648836
C	25.802131	16.649859	19.410602
H	26.760971	17.115629	19.617899
C	24.610613	17.377452	19.687967
C	24.669076	18.700860	20.213840
H	25.644693	19.132386	20.418396
C	23.518903	19.425991	20.450502
H	23.576807	20.434502	20.846583
C	22.255244	18.852005	20.161267
H	21.352987	19.432659	20.326054
C	22.163836	17.564684	19.663892
H	21.188730	17.151099	19.429725
C	23.327455	16.776197	19.418123
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H	21.692819	11.426204	14.743880
C	22.543080	10.472065	16.465705
H	22.709254	9.519327	15.971397
C	22.921749	10.607695	17.832041
C	23.513644	9.515764	18.531170
H	23.657706	8.579479	17.999801
C	23.901518	9.640629	19.849265
H	24.352420	8.803303	20.371513
C	23.713954	10.874628	20.521173
H	24.028114	10.975034	21.555145
C	23.138800	11.951806	19.872864
H	23.012944	12.882837	20.407951
C	22.713823	11.863355	18.513502
P	18.079567	16.685237	17.945916
P	21.650731	14.635101	18.449565

=== TS1 ===

Fe	19.243485	14.987578	20.771263
Pd	20.349505	15.990644	16.630273
Br	19.872663	15.409098	13.971519
C	18.093137	16.337698	19.576877
C	18.744446	17.029000	20.669531
H	19.445250	17.843103	20.570628
C	18.272848	16.477272	21.904273
H	18.587135	16.778358	22.892160
C	17.347280	15.427262	21.593565
H	16.840295	14.793343	22.305538
C	17.238786	15.335273	20.166723
H	16.620993	14.634435	19.629145
C	20.960261	14.169271	19.779337
C	21.328159	14.717982	21.062731
H	22.040662	15.509700	21.229290
C	20.591281	14.029193	22.081998
H	20.641451	14.231520	23.141392
C	19.750587	13.057944	21.444813
H	19.056086	12.394505	21.937787
C	19.961388	13.151917	20.030694
H	19.483630	12.539516	19.282305
C	18.183333	18.662236	17.954755
C	19.223112	19.381385	17.375829
H	20.018133	18.840502	16.874713
C	19.289381	20.795956	17.434550

H	20.121021	21.311045	16.965756
C	18.305106	21.501345	18.089775
H	18.343952	22.585207	18.146208
C	17.216900	20.823619	18.710908
C	16.201149	21.557017	19.390150
H	16.279240	22.639868	19.421432
C	15.140962	20.912625	19.993736
H	14.372866	21.480622	20.508003
C	15.056559	19.498922	19.937842
H	14.220639	18.992835	20.409948
C	16.025567	18.758222	19.286724
H	15.933477	17.681501	19.257068
C	17.139938	19.383561	18.652426
C	16.795507	16.263741	16.931975
C	15.956968	17.207823	16.347357
H	16.155004	18.263296	16.480268
C	14.828829	16.833807	15.575439
H	14.200830	17.608517	15.148080
C	14.530234	15.503372	15.379814
H	13.662011	15.207681	14.798581
C	15.368338	14.490702	15.925209
C	15.086290	13.111700	15.701597
H	14.203436	12.852511	15.124438
C	15.915200	12.124955	16.194940
H	15.692033	11.078654	16.014493
C	17.071361	12.483062	16.933074
H	17.732313	11.705793	17.303107
C	17.366070	13.811866	17.178278
H	18.261461	14.060819	17.735356
C	16.528405	14.862197	16.697764
C	21.660845	16.289667	14.896510
C	21.650702	17.700054	14.833239
H	20.712473	18.240179	14.802775
C	22.873786	18.390624	14.761347
H	22.868034	19.476126	14.737901
C	24.078920	17.688797	14.672701
H	25.018686	18.224883	14.593426
C	24.066430	16.281349	14.648073
H	24.998898	15.731561	14.565412
C	22.866368	15.573993	14.733131
H	22.863076	14.491406	14.706182
C	23.351811	15.194930	18.440907
C	24.478952	14.476074	18.058158
H	24.371062	13.487055	17.633600
C	25.788704	14.996577	18.209277
H	26.636343	14.390962	17.905792
C	25.981031	16.252104	18.741860
H	26.981330	16.654584	18.870816
C	24.865268	17.051850	19.118729
C	25.051086	18.365277	19.639632
H	26.065781	18.732329	19.764036
C	23.972989	19.161176	19.969970
H	24.127640	20.161416	20.360803
C	22.655858	18.670629	19.785738
H	21.808663	19.305887	20.023880
C	22.442495	17.394319	19.297242
H	21.426980	17.045651	19.150977
C	23.528772	16.534916	18.955650
C	21.923001	12.781065	17.500904
C	21.390530	12.515919	16.243151
H	20.892598	13.313705	15.702385
C	21.462229	11.231601	15.647402
H	21.034288	11.076559	14.662684
C	22.064513	10.193987	16.322968
H	22.122880	9.203828	15.880586
C	22.619261	10.397032	17.618976
C	23.236389	9.318895	18.317795
H	23.271895	8.345412	17.837380
C	23.777773	9.501502	19.573516
H	24.245021	8.673901	20.096825
C	23.722769	10.781187	20.180304
H	24.151239	10.925467	21.166928
C	23.131208	11.847541	19.528880
H	23.106935	12.812620	20.015136
C	22.556270	11.702812	18.231028
P	18.335426	16.813229	17.817646
P	21.650641	14.520760	18.110178

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Fe	19.159087	15.045171	20.890174
Pd	20.148022	15.952439	16.551115
Br	18.933884	16.902051	14.477612
C	17.858792	16.151524	19.656216
C	18.374719	16.976529	20.730406
H	18.946242	17.882894	20.610651
C	17.965898	16.403146	21.977272
H	18.214654	16.780600	22.957499
C	17.209249	15.219106	21.694613
H	16.789778	14.542383	22.423615
C	17.139623	15.060786	20.271783
H	16.640089	14.258726	19.753582
C	20.893828	14.448404	19.853382
C	21.260065	15.127797	21.077090
H	21.847312	16.027731	21.153014
C	20.709907	14.398721	22.180058
H	20.792703	14.676939	23.219768
C	19.998198	13.267633	21.661537
H	19.451899	12.538758	22.240613
C	20.100004	13.295424	20.234800
H	19.685427	12.564656	19.559152
C	17.865735	18.402651	17.948672
C	18.890229	19.135041	17.358161
H	19.689221	18.610181	16.849375
C	18.922247	20.550932	17.392604
H	19.742494	21.076485	16.915818
C	17.917468	21.244522	18.028827
H	17.928612	22.329890	18.062382
C	16.844902	20.553091	18.660623
C	15.811103	21.277239	19.322590
H	15.862344	22.362055	19.326036
C	14.768705	20.622319	19.944749
H	13.986825	21.183204	20.445673
C	14.722457	19.206040	19.926543
H	13.902348	18.689952	20.415111
C	15.708750	18.474196	19.291930
H	15.641851	17.395233	19.293570
C	16.804044	19.110505	18.634443
C	16.534090	15.891514	17.053255
C	15.594288	16.762543	16.516284
H	15.724142	17.831080	16.620478
C	14.452449	16.293578	15.820084
H	13.741405	17.012081	15.426543
C	14.249853	14.941958	15.649233
H	13.374038	14.573523	15.123706
C	15.197018	14.003024	16.145690
C	15.013913	12.604292	15.944663
H	14.121939	12.270321	15.422817
C	15.947723	11.691151	16.390337
H	15.799373	10.629020	16.227015
C	17.112994	12.146566	17.056648
H	17.856687	11.429484	17.388175
C	17.312038	13.496755	17.279580
H	18.212889	13.819494	17.786550
C	16.367030	14.472586	16.846025
C	21.789439	15.868892	15.295532
C	22.676437	16.958806	15.359679
H	22.546523	17.727536	16.114909
C	23.742383	17.071923	14.453461
H	24.414446	17.923292	14.519867
C	23.940111	16.093818	13.470553

H	24.766458	16.178077	12.771166
C	23.058062	15.009157	13.395823
H	23.193369	14.247379	12.632604
C	21.985947	14.900702	14.296891
H	21.305848	14.063471	14.193590
C	23.131274	15.549277	18.324044
C	24.270854	14.884630	17.889389
H	24.194866	13.886289	17.480131
C	25.553873	15.481195	17.960159
H	26.417397	14.919797	17.620313
C	25.698681	16.757697	18.457127
H	26.678969	17.219982	18.521806
C	24.560903	17.502763	18.875933
C	24.697413	18.841139	19.345567
H	25.694152	19.268238	19.403950
C	23.593611	19.586939	19.705650
H	23.709623	20.607430	20.054542
C	22.299340	19.017600	19.607324
H	21.429780	19.611265	19.869061
C	22.135265	17.715066	19.172764
H	21.133455	17.309124	19.100148
C	23.250077	16.906751	18.800653
C	21.732900	12.995817	17.602778
C	20.994592	12.585356	16.498928
H	20.354314	13.302145	15.999111
C	21.038639	11.255539	16.013103
H	20.446573	10.985739	15.145632
C	21.831339	10.322961	16.643216
H	21.882016	9.301686	16.277966
C	22.587243	10.672805	17.798197
C	23.379589	9.692910	18.463684
H	23.407377	8.687627	18.054043
C	24.089786	10.005807	19.603995
H	24.688107	9.251811	20.104147
C	24.028806	11.321449	20.126349
H	24.578714	11.566234	21.029183
C	23.276835	12.297641	19.499515
H	23.251891	13.290395	19.926171
C	22.537208	12.020881	18.311123
P	18.058416	16.558398	17.876125
P	21.471207	14.751732	18.134887

1 MeOH

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Fe	19.038265	15.014178	20.832835
Pd	20.176474	16.074066	17.141508
Br	19.745012	16.217401	14.212776
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C	18.369040	17.016864	20.732793
H	19.002050	17.887840	20.670363
C	17.908813	16.404244	21.943693
H	18.166402	16.711846	22.945948
C	17.084930	15.286420	21.586663
H	16.613328	14.597571	22.271378
C	17.025764	15.216478	20.155138
H	16.485244	14.478938	19.583883
C	20.930793	14.392891	19.983305
C	21.107411	14.884265	21.326969
H	21.727419	15.717777	21.616469
C	20.324454	14.074343	22.215556
H	20.241232	14.209408	23.283608
C	19.643303	13.085409	21.431678
H	18.959878	12.337076	21.803839
C	19.996606	13.292204	20.058300
H	19.657810	12.696731	19.225053
C	17.756726	18.639207	17.935766
C	18.709437	19.395862	17.259984
H	19.510165	18.880598	16.738155
C	18.677719	20.812192	17.245693
H	19.442187	21.358256	16.703388
C	17.686456	21.482124	17.928511
H	17.654382	22.567691	17.934258
C	16.682136	20.765577	18.640330
C	15.652833	21.461080	19.339031
H	15.659890	22.547076	19.322771
C	14.665359	20.776562	20.017177
H	13.885588	21.316056	20.544438
C	14.668597	19.358960	20.018553
H	13.886128	18.821809	20.544845
C	15.655098	18.654187	19.354237
H	15.631087	17.573184	19.367024
C	16.699636	19.322213	18.648190
C	16.566619	16.120801	16.958985
C	15.605598	16.977466	16.431901
H	15.675796	18.042728	16.607525
C	14.515671	16.500126	15.661273
H	13.788629	17.208948	15.278669
C	14.377984	15.152719	15.410683
H	13.540032	14.777607	14.830753
C	15.344033	14.228211	15.898879
C	15.226766	12.835080	15.621865
H	14.370767	12.493164	15.047190
C	16.178224	11.937577	16.062186
H	16.079474	10.879826	15.841651
C	17.296966	12.404220	16.797453
H	18.053771	11.698808	17.125818
C	17.433305	13.748346	17.093683
H	18.305701	14.087015	17.642748
C	16.465302	14.707008	16.669353
C	20.939506	15.768015	12.746090
C	22.291121	16.106684	12.851131
H	22.663330	16.611229	13.737807
C	23.145020	15.777483	11.789064
H	24.197627	16.033351	11.854425
C	22.648570	15.125946	10.652297
H	23.316318	14.875274	9.834880
C	21.289035	14.797311	10.571720
H	20.899441	14.292143	9.694059
C	20.420157	15.117409	11.623773
H	19.367990	14.864892	11.567447
C	23.300784	15.793720	19.000279
C	24.545995	15.214467	18.779832
H	24.614681	14.235123	18.325557
C	25.752559	15.867695	19.136104
H	26.698164	15.369194	18.949778
C	25.722079	17.114739	19.720044
H	26.640957	17.617359	20.006950
C	24.480168	17.773198	19.943929
C	24.438319	19.076296	20.519521
H	25.375755	19.545223	20.804413
C	23.240566	19.736516	20.704264
H	23.222369	20.730574	21.138773
C	22.028403	19.115063	20.310973
H	21.089733	19.646099	20.435056
C	22.033868	17.844609	19.764178
H	21.099110	17.392804	19.450420
C	23.248672	17.122754	19.568675
C	22.346814	13.312613	17.719985
C	22.111369	13.163559	16.356170
H	21.641699	13.979322	15.814745
C	22.448567	11.978960	15.655630
H	22.246942	11.912583	14.591794
C	23.014894	10.920478	16.330807
H	23.267766	10.001673	15.809785
C	23.283685	11.010066	17.726555
C	23.879947	9.916927	18.420036
H	24.110263	9.014640	17.860954
C	24.165959	9.999283	19.767182
H	24.621306	9.161622	20.285006

C	23.868660	11.190828	20.475008
H	24.104609	11.259343	21.532127
C	23.285185	12.267262	19.832980
H	23.074869	13.165426	20.396641
C	22.960669	12.220562	18.444072
P	18.047595	16.806109	17.857394
P	21.751945	14.932383	18.423904
O	22.868825	17.702810	15.798718
H	22.116194	17.231808	16.215906
C	22.476532	19.082830	15.627836
H	23.332384	19.602906	15.190683
H	21.621394	19.181114	14.946779
H	22.230454	19.557550	16.586015

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Fe	19.242122	14.982708	20.761068
Pd	20.350099	15.992500	16.626751
Br	19.912395	15.270648	13.946317
C	18.098671	16.339031	19.567806
C	18.748675	17.025403	20.664288
H	19.451548	17.838196	20.569706
C	18.272273	16.471132	21.896042
H	18.584664	16.768284	22.885719
C	17.344930	15.424395	21.579596
H	16.834464	14.789544	22.288242
C	17.240062	15.337077	20.152179
H	16.621798	14.639616	19.610753
C	20.955837	14.158565	19.770023
C	21.325762	14.707772	21.052613
H	22.040874	15.497410	21.217941
C	20.587203	14.022224	22.072830
H	20.638003	14.225758	23.131960
C	19.743639	13.052527	21.437009
H	19.047231	12.391824	21.930961
C	19.954204	13.144252	20.022739
H	19.474452	12.532483	19.275088
C	18.199924	18.669153	17.956793
C	19.245043	19.385876	17.384470
H	20.035482	18.844542	16.876495
C	19.320163	20.799456	17.455146
H	20.155635	21.312937	16.991388
C	18.339393	21.506021	18.114340
H	18.385093	22.589150	18.179374
C	17.245740	20.830485	18.728195
C	16.233393	21.565011	19.411288
H	16.318028	22.647120	19.450605
C	15.168328	20.922718	20.008499
H	14.402817	21.491587	20.525662
C	15.075591	19.509993	19.942221
H	14.235994	19.005458	20.409463
C	16.041152	18.768275	19.287122
H	15.942705	17.692350	19.249669
C	17.160008	19.391466	18.658591
C	16.802250	16.275182	16.924116
C	15.959383	17.221728	16.350180
H	16.157264	18.276421	16.488139
C	14.828997	16.850953	15.580071
H	14.197994	17.627439	15.160481
C	14.532832	15.521396	15.375345
H	13.663380	15.228099	14.794711
C	15.374348	14.506423	15.911231
C	15.092752	13.128499	15.680436
H	14.208974	12.872058	15.103449
C	15.922624	12.139464	16.167509
H	15.699568	11.094029	15.981950
C	17.079209	12.494219	16.906560
H	17.740423	11.715276	17.272624
C	17.374116	13.821859	17.157881
H	18.269835	14.067910	17.715598
C	16.535982	14.874616	16.683130
C	21.641115	16.264971	14.887144
C	21.554892	17.670802	14.787119
H	20.591541	18.159436	14.695273
C	22.746436	18.418941	14.732789
H	22.687628	19.501875	14.679613
C	23.986455	17.776985	14.693454
H	24.900191	18.358029	14.627440
C	24.046471	16.370022	14.698667
H	25.007594	15.867250	14.655468
C	22.882025	15.604036	14.767430
H	22.933070	14.522345	14.768460
C	23.350065	15.179583	18.431618
C	24.477765	14.459525	18.052647
H	24.370491	13.469209	17.630983
C	25.787515	14.979957	18.204269
H	26.635365	14.373073	17.903944
C	25.979367	16.236871	18.733631
H	26.979550	16.639423	18.863226
C	24.863174	17.037993	19.106199
C	25.048706	18.352872	19.623510
H	26.063362	18.719749	19.748717
C	23.970419	19.150339	19.949361
H	24.124828	20.151693	20.337420
C	22.653420	18.659933	19.763976
H	21.806101	19.296539	19.997958
C	22.440327	17.382139	19.279212
H	21.424974	17.033818	19.131218
C	23.526709	16.521080	18.942323
C	21.931579	12.757627	17.505786
C	21.410638	12.481775	16.245646
H	20.916120	13.273068	15.693250
C	21.489650	11.193119	15.660182
H	21.070346	11.030055	14.673057
C	22.087564	10.161685	16.348705
H	22.151030	9.168171	15.914630
C	22.631937	10.375905	17.647336
C	23.246076	9.304314	18.358666
H	23.286085	8.327133	17.886204
C	23.779466	9.497760	19.616172
H	24.244619	8.675088	20.149020
C	23.719374	10.782352	20.211886
H	24.142279	10.935523	21.199572
C	23.129990	11.842489	19.548363
H	23.102332	12.811435	20.026543
C	22.562359	11.686328	18.248675
P	18.343163	16.820534	17.810331
P	21.649968	14.501015	18.100753
O	18.413375	18.393529	13.631686
H	18.671611	17.456148	13.695942
C	18.714387	18.820104	12.284873
H	18.433564	19.873920	12.215648
H	19.784018	18.726627	12.056063
H	18.140300	18.254801	11.539185

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Fe	19.173841	15.061109	20.895243
Pd	20.167283	15.980986	16.558063
Br	18.974882	16.981104	14.478707
C	17.873921	16.168988	19.664389
C	18.392108	16.993309	20.738120
H	18.964993	17.898784	20.617275
C	17.984277	16.420001	21.985246
H	18.235235	16.796446	22.965295
C	17.225635	15.237069	21.703163
H	16.806487	14.560560	22.432550
C	17.153709	15.079241	20.280362
H	16.652087	14.278213	19.762585
C	20.903685	14.460971	19.854331
C	21.275050	15.141698	21.075919
H	21.863864	16.040821	21.148552

C	20.727889	14.414837	22.181717
H	20.814550	14.694550	23.220704
C	20.013129	13.283806	21.667389
H	19.467893	12.556487	22.249413
C	20.109936	13.309272	20.240377
H	19.692726	12.577482	19.567570
C	17.842501	18.426641	17.969474
C	18.844571	19.184693	17.375017
H	19.663291	18.686509	16.873297
C	18.835319	20.601246	17.395953
H	19.629752	21.135628	16.888676
C	17.816509	21.269532	18.036066
H	17.794734	22.355098	18.060874
C	16.767534	20.551570	18.678919
C	15.718014	21.250031	19.343529
H	15.742764	22.335824	19.346770
C	14.692485	20.570146	19.967207
H	13.898460	21.112048	20.469988
C	14.679099	19.153388	19.946540
H	13.871340	18.617398	20.434309
C	15.682014	18.445843	19.310072
H	15.639569	17.365699	19.309365
C	16.762442	19.108343	18.654284
C	16.559169	15.909781	17.048914
C	15.626822	16.778322	16.494632
H	15.753510	17.847220	16.598737
C	14.496946	16.306499	15.781213
H	13.791642	17.023341	15.374555
C	14.298534	14.954289	15.610523
H	13.431763	14.583567	15.071790
C	15.238184	14.017699	16.125249
C	15.058640	12.618273	15.926215
H	14.175431	12.282296	15.390934
C	15.984811	11.706936	16.391067
H	15.839139	10.644156	16.229655
C	17.138621	12.165056	17.075112
H	17.876159	11.449071	17.422233
C	17.334156	13.516191	17.295718
H	18.225648	13.840992	17.817508
C	16.396505	14.490213	16.843039
C	21.801626	15.860057	15.295213
C	22.716257	16.925865	15.354854
H	22.607347	17.700685	16.105076
C	23.778877	17.010457	14.440913
H	24.475118	17.842247	14.504792
C	23.942632	16.029429	13.454537
H	24.766481	16.092040	12.749974
C	23.029744	14.970539	13.382744
H	23.137942	14.207007	12.617041
C	21.962354	14.889400	14.292541
H	21.258991	14.071254	14.192780
C	23.144593	15.545389	18.322258
C	24.279242	14.871146	17.889550
H	24.195476	13.873616	17.479899
C	25.567024	15.456833	17.962851
H	26.426512	14.888187	17.624865
C	25.721315	16.732223	18.459853
H	26.705309	17.186258	18.526564
C	24.589026	17.486974	18.876209
C	24.736137	18.824053	19.346279
H	25.736374	19.242679	19.406152
C	23.638235	19.578990	19.705274
H	23.762373	20.598326	20.054680
C	22.339380	19.020476	19.605404
H	21.474454	19.620782	19.867406
C	22.164795	17.719703	19.169660
H	21.159415	17.322755	19.096541
C	23.273279	16.902112	18.798620
C	21.724486	13.001761	17.601690
C	20.977703	12.596581	16.501667
H	20.339472	13.317230	16.005261
C	21.009680	11.266556	16.015538
H	20.411484	11.001219	15.150914
C	21.798282	10.328134	16.641977
H	21.839826	9.306559	16.276433
C	22.561245	10.672108	17.794051
C	23.347664	9.685674	18.456845
H	23.365912	8.680308	18.046889
C	24.063579	9.992393	19.595237
H	24.657089	9.233387	20.093525
C	24.014547	11.308248	20.118220
H	24.568615	11.548219	21.019792
C	23.268807	12.290759	19.493781
H	23.252818	13.283354	19.921203
C	22.523722	12.020485	18.307297
P	18.070993	16.587628	17.887089
P	21.479205	14.759736	18.134586
O	20.869588	19.838223	14.773144
H	20.369146	19.010031	14.633635
C	21.501615	20.165280	13.520612
H	22.046338	21.101725	13.670539
H	22.216096	19.392481	13.207774
H	20.768600	20.316185	12.715711

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Fe	19.186070	15.036064	20.750590
Pd	20.275780	15.947595	16.464508
Br	18.924489	14.816054	14.097422
C	17.923866	16.207990	19.541192
C	18.502082	17.005534	20.606141
H	19.117213	17.881032	20.475448
C	18.089112	16.456347	21.861555
H	18.379466	16.819674	22.835627
C	17.263456	15.316221	21.595608
H	16.821884	14.663254	22.333198
C	17.156788	15.161001	20.175027
H	16.603942	14.384909	19.673491
C	20.920465	14.426492	19.720176
C	21.279891	15.002685	20.998368
H	21.904475	15.866702	21.152300
C	20.666326	14.225039	22.032004
H	20.730933	14.426238	23.090625
C	19.919390	13.167895	21.416527
H	19.323081	12.428114	21.928475
C	20.064378	13.288770	19.998795
H	19.642321	12.623190	19.263254
C	18.028886	18.479809	17.908010
C	19.112216	19.197485	17.414855
H	19.907260	18.672254	16.904109
C	19.202867	20.606615	17.536894
H	20.069568	21.120308	17.135093
C	18.196697	21.308261	18.161158
H	18.252309	22.388290	18.260206
C	17.063904	20.630809	18.695882
C	16.029978	21.362408	19.349268
H	16.126539	22.442032	19.417378
C	14.932675	20.720894	19.885009
H	14.151364	21.287141	20.380808
C	14.830631	19.311054	19.785916
H	13.969115	18.804754	20.209145
C	15.815028	18.572730	19.155397
H	15.704501	17.499324	19.095490
C	16.964512	19.195331	18.583553
C	16.582346	16.090417	16.912777
C	15.786413	17.038576	16.279975
H	16.052494	18.086707	16.325104
C	14.611491	16.675609	15.575969
H	14.015743	17.450862	15.106023
C	14.224990	15.355124	15.505569
H	13.316076	15.069834	14.984466

C	15.023479	14.337420	16.098825
C	14.653513	12.964886	15.995918
H	13.729927	12.716117	15.481442
C	15.451216	11.970410	16.523451
H	15.161190	10.928680	16.436129
C	16.667034	12.312767	17.167972
H	17.307902	11.527468	17.555454
C	17.045629	13.636009	17.295769
H	17.991382	13.868481	17.770675
C	16.236435	14.695339	16.790698
C	22.015580	16.046861	15.381075
C	22.689098	17.269810	15.542765
H	22.366139	17.980864	16.296102
C	23.794666	17.584943	14.737251
H	24.299825	18.537530	14.869505
C	24.248576	16.671698	13.777371
H	25.108945	16.909871	13.159457
C	23.586334	15.447799	13.623805
H	23.927820	14.732298	12.880831
C	22.472393	15.133441	14.420496
H	21.963929	14.191915	14.266031
C	23.235622	15.582875	18.340191
C	24.389352	14.944404	17.901738
H	24.327173	13.970906	17.434020
C	25.667966	15.536347	18.046263
H	26.542496	14.996647	17.699534
C	25.795333	16.779945	18.625177
H	26.772476	17.237039	18.747966
C	24.644201	17.497787	19.054410
C	24.763921	18.803934	19.611272
H	25.757789	19.225477	19.728752
C	23.648029	19.526709	19.980751
H	23.751234	20.523223	20.396526
C	22.358178	18.966137	19.803262
H	21.480408	19.545188	20.070498
C	22.209843	17.693325	19.283525
H	21.212727	17.291927	19.150674
C	23.337228	16.908584	18.900730
C	21.899412	13.044606	17.485997
C	21.231367	12.650109	16.332790
H	20.612138	13.363411	15.799024
C	21.316991	11.327671	15.830717
H	20.779509	11.069494	14.924781
C	22.075338	10.388784	16.491898
H	22.153637	9.373361	16.115121
C	22.760315	10.724915	17.694293
C	23.519479	9.738915	18.388515
H	23.575232	8.740063	17.966025
C	24.164083	10.037612	19.570859
H	24.737413	9.278780	20.092541
C	24.069006	11.345703	20.106319
H	24.568895	11.580772	21.040323
C	23.347185	12.327581	19.453003
H	23.297382	13.314119	19.891174
C	22.672378	12.064802	18.223733
P	18.140087	16.629854	17.761927
P	21.591863	14.784708	18.049849
O	19.307026	17.908991	14.690919
H	19.116321	17.053320	14.244751
C	20.056529	18.739596	13.775047
H	20.318938	19.654345	14.312524
H	20.978002	18.250519	13.442157
H	19.449555	19.008495	12.901358

=== Int2 ===

Fe	19.189341	15.118295	20.834690
Pd	20.348963	16.178400	16.627452
Br	18.644782	14.417571	13.112614
C	17.940645	16.310679	19.633275
C	18.497377	17.091176	20.720521
H	19.111079	17.971681	20.616482
C	18.066651	16.512701	21.957007
H	18.337663	16.857664	22.943198
C	17.252102	15.372996	21.654829
H	16.803225	14.703230	22.372537
C	17.169128	15.245757	20.229996
H	16.631957	14.477143	19.699273
C	20.928154	14.510084	19.807700
C	21.284723	15.081883	21.089127
H	21.908574	15.945184	21.248425
C	20.667082	14.302986	22.118750
H	20.728660	14.501891	23.177916
C	19.921160	13.248316	21.498615
H	19.322818	12.507415	22.006439
C	20.070885	13.371811	20.081704
H	19.650457	12.704850	19.346835
C	18.031280	18.576294	17.933280
C	19.088988	19.293667	17.384350
H	19.915457	18.757139	16.932929
C	19.134731	20.709265	17.407034
H	19.980914	21.222814	16.963886
C	18.110084	21.417239	17.994307
H	18.131358	22.502550	18.020473
C	17.004813	20.741540	18.585595
C	15.952175	21.479828	19.200251
H	16.014052	22.563997	19.200455
C	14.878682	20.838131	19.782123
H	14.082760	21.409559	20.247641
C	14.817892	19.422239	19.769452
H	13.972803	18.917930	20.226510
C	15.821461	18.676542	19.179626
H	15.743483	17.598140	19.182816
C	16.949141	19.299565	18.566793
C	16.708071	16.105226	16.960467
C	15.843507	17.003139	16.344895
H	16.014330	18.067744	16.432218
C	14.721642	16.565463	15.598249
H	14.069199	17.303024	15.143453
C	14.460726	15.219653	15.461714
H	13.596035	14.876167	14.902115
C	15.332776	14.253699	16.037030
C	15.092153	12.859347	15.870752
H	14.211158	12.549952	15.316284
C	15.959910	11.919579	16.388508
H	15.768802	10.860658	16.251308
C	17.116366	12.342336	17.090805
H	17.810594	11.601938	17.474423
C	17.368734	13.688083	17.281578
H	18.263130	13.987326	17.813886
C	16.488239	14.690221	16.780421
C	22.026443	16.218253	15.434688
C	22.922852	17.280109	15.648978
H	22.827533	17.911791	16.525812
C	23.958986	17.533663	14.736206
H	24.641525	18.359814	14.915153
C	24.114764	16.722755	13.604918
H	24.919600	16.913727	12.901565
C	23.221557	15.666876	13.385742
H	23.325442	15.039108	12.504945
C	22.178162	15.414970	14.292746
H	21.471458	14.623802	14.072090
C	23.270081	15.617585	18.450509
C	24.400412	14.940618	18.010140
H	24.302889	13.981607	17.519107
C	25.700612	15.475370	18.182133
H	26.556180	14.907850	17.832892
C	25.871698	16.699750	18.790017
H	26.865336	17.112912	18.933725
C	24.746433	17.456223	19.222077
C	24.913691	18.744073	19.808317

H	25.922669	19.120922	19.946552
C	23.824438	19.504853	20.181104
H	23.964176	20.486597	20.620491
C	22.514430	19.003246	19.976863
H	21.658396	19.611028	20.250731
C	22.318858	17.749434	19.427128
H	21.306124	17.394493	19.276355
C	23.417811	16.925980	19.040832
C	21.820181	13.176763	17.485509
C	21.143182	12.884728	16.306715
H	20.563890	13.658144	15.817722
C	21.166908	11.594145	15.724580
H	20.623481	11.421368	14.802396
C	21.872229	10.581013	16.333377
H	21.902475	9.587226	15.896945
C	22.563781	10.809914	17.557219
C	23.267940	9.748068	18.195184
H	23.275974	8.773829	17.715653
C	23.920176	9.945299	19.394598
H	24.451203	9.129423	19.873104
C	23.890010	11.223572	20.004647
H	24.397117	11.378227	20.951382
C	23.222084	12.277004	19.408129
H	23.219576	13.238325	19.902418
C	22.540172	12.118682	18.164979
P	18.196653	16.731962	17.869174
P	21.598740	14.892463	18.141634
O	19.196795	17.015167	14.899249
H	19.006022	16.188463	14.364888
C	19.689379	18.024245	13.967727
H	19.762577	18.962950	14.517243
H	20.666490	17.748881	13.565930
H	18.965611	18.134041	13.155110

2 MeOHs

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Fe	18.983472	14.928229	20.936485
Pd	20.082074	15.542759	17.302699
Br	21.969041	17.413891	15.015021
C	17.800501	16.173649	19.598710
C	18.455651	16.959170	20.620434
H	19.146372	17.769085	20.444629
C	17.992469	16.517610	21.902245
H	18.303749	16.912013	22.857712
C	17.081278	15.430549	21.691112
H	16.584849	14.856820	22.459214
C	16.970659	15.210917	20.277650
H	16.361682	14.457285	19.804580
C	20.796431	14.013514	20.149049
C	21.054499	14.670489	21.405300
H	21.758595	15.470723	21.567432
C	20.224796	14.072167	22.411149
H	20.186775	14.361169	23.450723
C	19.433015	13.052782	21.786397
H	18.694220	12.432465	22.271048
C	19.763456	13.031687	20.392753
H	19.344315	12.364500	19.655718
C	17.820576	18.330639	17.701999
C	18.805126	18.965469	16.951917
H	19.558732	18.358264	16.461695
C	18.867699	20.375077	16.818623
H	19.666153	20.817531	16.230654
C	17.930324	21.160723	17.452839
H	17.967942	22.243108	17.370320
C	16.892827	20.572306	18.232256
C	15.920930	21.388629	18.880407
H	15.994406	22.466545	18.769060
C	14.906561	20.828604	19.629676
H	14.171289	21.459522	20.117994
C	14.824123	19.419150	19.757408
H	14.021633	18.980106	20.341417
C	15.752760	18.598908	19.143979
H	15.664126	17.526602	19.254031
C	16.820885	19.136903	18.366134
C	16.474499	15.797252	16.995319
C	15.563086	16.656713	16.390556
H	15.712164	17.727064	16.443243
C	14.422992	16.176329	15.698658
H	13.737907	16.888328	15.250393
C	14.184848	14.822859	15.607458
H	13.307538	14.446118	15.090166
C	15.095912	13.891556	16.180982
C	14.871561	12.488669	16.068563
H	13.977825	12.148626	15.553453
C	15.767771	11.578921	16.591730
H	15.587405	10.513239	16.496946
C	16.937286	12.042031	17.245568
H	17.652085	11.324529	17.635977
C	17.178232	13.397068	17.382963
H	18.090588	13.729310	17.867722
C	16.268995	14.370671	16.870850
C	22.665042	17.366150	13.203219
C	23.335000	18.484567	12.700253
H	23.446124	19.379913	13.300555
C	23.841710	18.427791	11.394522
H	24.363806	19.287938	10.988879
C	23.675333	17.272553	10.619762
H	24.071512	17.235161	9.610647
C	22.992851	16.168027	11.146243
H	22.856406	15.274401	10.546130
C	22.477501	16.205264	12.449321
H	21.932808	15.364399	12.865347
C	23.278003	14.969291	18.870694
C	24.428354	14.235905	18.598722
H	24.349239	13.214991	18.249323
C	25.725229	14.782765	18.766633
H	26.590952	14.166516	18.547495
C	25.881623	16.077140	19.210465
H	26.871347	16.500999	19.351890
C	24.742871	16.888024	19.478439
C	24.894713	18.237650	19.910471
H	25.899861	18.624630	20.050781
C	23.796558	19.041698	20.138670
H	23.925289	20.068737	20.463916
C	22.493004	18.523314	19.934857
H	21.630780	19.162909	20.095366
C	22.311454	17.213792	19.528225
H	21.305059	16.844580	19.359478
C	23.419226	16.345042	19.294837
C	21.939103	12.484912	18.004889
C	21.546992	12.167424	16.707920
H	21.107507	12.934302	16.078332
C	21.685938	10.858891	16.180394
H	21.367465	10.659344	15.162721
C	22.210757	9.853592	16.961701
H	22.315006	8.845142	16.572162
C	22.629209	10.115760	18.297655
C	23.178135	9.075499	19.102443
H	23.260462	8.080447	18.674902
C	23.600940	9.321691	20.392465
H	24.018514	8.522779	20.996188
C	23.492561	10.629606	20.928205
H	23.832859	10.824086	21.940230
C	22.960903	11.659909	20.174906
H	22.895035	12.648825	20.607449
C	22.504173	11.447183	18.840054
P	18.007726	16.484765	17.795185
P	21.604012	14.240504	18.507864
O	20.196515	14.287103	14.229578

H	20.203249	14.840751	15.041096
C	18.913721	14.475992	13.588083
H	18.895213	13.812446	12.720107
H	18.083708	14.211675	14.253518
H	18.781443	15.509232	13.242266
O	21.551206	20.929737	14.545442
H	21.521536	19.978101	14.746085
C	20.720520	21.145596	13.380447
H	20.782657	22.210659	13.144572
H	21.076141	20.571660	12.515918
H	19.671238	20.889726	13.574395

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Fe	19.201896	15.051953	20.858044
Pd	20.135612	15.985189	16.658247
Br	19.439375	15.311359	14.011366
C	18.053851	16.442290	19.711895
C	18.764997	17.107613	20.783238
H	19.485474	17.901285	20.662981
C	18.320066	16.565172	22.031994
H	18.678239	16.851764	23.009248
C	17.351732	15.546025	21.750515
H	16.850704	14.924751	22.477681
C	17.189480	15.464599	20.328217
H	16.531813	14.785636	19.810482
C	20.840429	14.171660	19.792665
C	21.287641	14.713900	21.053296
H	22.035912	15.479513	21.180616
C	20.576823	14.056286	22.110927
H	20.683964	14.262691	23.165268
C	19.674653	13.110549	21.521002
H	18.982246	12.474109	22.051089
C	19.820447	13.190385	20.097812
H	19.285558	12.592757	19.376197
C	18.185667	18.767586	18.095763
C	19.233255	19.433987	17.469444
H	19.968888	18.855397	16.922004
C	19.380640	20.842032	17.534371
H	20.214618	21.315040	17.026952
C	18.471378	21.594188	18.243656
H	18.572987	22.673692	18.305493
C	17.379931	20.971400	18.914594
C	16.442410	21.753080	19.650038
H	16.582153	22.829626	19.684734
C	15.380075	21.162362	20.302773
H	14.672015	21.766802	20.859892
C	15.214001	19.756126	20.240956
H	14.376012	19.292502	20.751475
C	16.105880	18.969425	19.535787
H	15.952612	17.899716	19.502611
C	17.219977	19.538502	18.849886
C	16.627436	16.438418	17.141271
C	15.791863	17.421486	16.620968
H	16.039993	18.466382	16.751379
C	14.604432	17.100881	15.916807
H	13.981509	17.904557	15.538308
C	14.244046	15.785539	15.723262
H	13.331229	15.531235	15.192938
C	15.074276	14.734180	16.203858
C	14.726482	13.369951	15.981686
H	13.801849	13.152484	15.454925
C	15.543625	12.345579	16.414412
H	15.269706	11.311110	16.235686
C	16.753277	12.649476	17.088340
H	17.404024	11.843245	17.411599
C	17.112991	13.962729	17.330146
H	18.047945	14.169563	17.836990
C	16.291760	15.051140	16.909532
C	21.301266	16.164042	14.801961
C	21.309622	17.574281	14.751620
H	20.381357	18.134010	14.739355
C	22.548757	18.234357	14.638838
H	22.568921	19.319830	14.626629
C	23.730336	17.504670	14.489727
H	24.678798	18.019421	14.379058
C	23.683439	16.098015	14.433787
H	24.597175	15.529505	14.291817
C	22.472304	15.416042	14.559508
H	22.433636	14.336356	14.486775
C	23.193176	15.123377	18.324007
C	24.281475	14.378032	17.882892
H	24.128851	13.388594	17.473365
C	25.608574	14.870741	17.954573
H	26.423907	14.245154	17.606410
C	25.858235	16.124314	18.467334
H	26.872600	16.505886	18.535551
C	24.783432	16.949239	18.904029
C	25.027326	18.260013	19.407124
H	26.055179	18.605380	19.470747
C	23.987560	19.080031	19.796084
H	24.186014	20.078010	20.172674
C	22.651742	18.617365	19.691635
H	21.834085	19.271863	19.976131
C	22.383044	17.344538	19.221665
H	21.353998	17.016111	19.137111
C	23.428816	16.460970	18.820985
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C	21.113972	12.447934	16.266903
H	20.608828	13.244310	15.732407
C	21.158973	11.157585	15.681563
H	20.728323	11.009310	14.698105
C	21.762996	10.121273	16.357106
H	21.802357	9.125730	15.924602
C	22.352422	10.333175	17.636745
C	22.975383	9.256933	18.333093
H	22.981372	8.275592	17.867527
C	23.560849	9.451157	19.567301
H	24.032617	8.624734	20.088496
C	23.547005	10.741347	20.153610
H	24.012211	10.895190	21.122018
C	22.949607	11.806012	19.504507
H	22.956853	12.779593	19.973877
C	22.327286	11.648489	18.230469
P	18.236548	16.914362	17.944225
P	21.463886	14.478687	18.088688
O	21.271375	12.678738	12.638890
H	20.661369	13.385607	12.913682
C	21.891084	13.111469	11.409280
H	22.588067	12.323934	11.111356
H	21.156387	13.250048	10.604862
H	22.453723	14.045163	11.540150
O	18.137687	18.537944	13.821817
H	18.316420	17.582140	13.870866
C	18.334265	18.932245	12.445996
H	18.141234	20.006544	12.394076
H	19.362036	18.744106	12.109321
H	17.638393	18.418113	11.770374

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Fe	19.126271	14.974686	21.038202
Pd	20.159825	16.071331	16.763631
Br	18.945247	17.037549	14.665086
C	17.851189	16.157863	19.852338
C	18.397579	16.932848	20.948385
H	18.993136	17.826791	20.853776
C	17.981736	16.330310	22.179064
H	18.249182	16.667439	23.168969
C	17.188992	15.178367	21.864144
H	16.756214	14.490045	22.574203
C	17.104752	15.068756	20.437549

H	16.579900	14.298160	19.897152
C	20.850535	14.386325	19.980548
C	21.226457	14.984235	21.243546
H	21.838205	15.860993	21.374528
C	20.648318	14.209508	22.299743
H	20.731727	14.425269	23.354158
C	19.908744	13.131075	21.713500
H	19.337606	12.386381	22.246625
C	20.022073	13.236607	20.291471
H	19.593333	12.554916	19.575008
C	17.840476	18.462953	18.207916
C	18.836093	19.219823	17.600526
H	19.633509	18.719917	17.065825
C	18.846753	20.635557	17.649112
H	19.634406	21.170348	17.131842
C	17.854507	21.304036	18.329592
H	17.848985	22.389025	18.377316
C	16.811474	20.587433	18.983325
C	15.787318	21.286449	19.685884
H	15.828080	22.371461	19.711421
C	14.765434	20.608021	20.317103
H	13.990567	21.150310	20.848525
C	14.729858	19.192412	20.265512
H	13.923893	18.657808	20.757720
C	15.708608	18.484365	19.593051
H	15.649541	17.405323	19.569250
C	16.785340	19.145210	18.929678
C	16.521879	15.983531	17.244861
C	15.585114	16.873435	16.733532
H	15.721118	17.938308	16.864894
C	14.437186	16.428360	16.031623
H	13.729161	17.160556	15.658407
C	14.223864	15.082278	15.831873
H	13.342417	14.731954	15.303384
C	15.166918	14.125753	16.301772
C	14.972941	12.733056	16.071788
H	14.075239	12.416278	15.549064
C	15.904145	11.804551	16.490400
H	15.747799	10.747266	16.304676
C	17.078254	12.237728	17.156097
H	17.821512	11.508867	17.461839
C	17.287244	13.581022	17.407965
H	18.195168	13.889041	17.911534
C	16.344733	14.571431	17.004486
C	21.834510	16.062553	15.548212
C	22.730271	17.131113	15.724677
H	22.594206	17.833249	16.540173
C	23.820591	17.301117	14.855890
H	24.503429	18.132259	15.009574
C	24.030548	16.401897	13.802614
H	24.876805	16.528815	13.134129
C	23.135562	15.341195	13.617199
H	23.280213	14.642900	12.797026
C	22.038518	15.175001	14.479001
H	21.338683	14.370797	14.286858
C	23.130612	15.506375	18.541320
C	24.255237	14.831957	18.083339
H	24.153331	13.864231	17.610841
C	25.555080	15.380034	18.212253
H	26.406242	14.813370	17.850705
C	25.731716	16.616401	18.793619
H	26.725181	17.040251	18.904085
C	24.611250	17.371328	19.240897
C	24.782162	18.671325	19.798790
H	25.791016	19.059430	19.903192
C	23.696310	19.429755	20.186169
H	23.838758	20.420941	20.603056
C	22.385959	18.913100	20.026258
H	21.531469	19.518291	20.310629
C	22.187652	17.647606	19.505045
H	21.174385	17.282409	19.386287
C	23.283305	16.826503	19.104327
C	21.667183	13.045974	17.645851
C	20.943330	12.735388	16.500717
H	20.339138	13.496732	16.024493
C	20.953989	11.439516	15.929424
H	20.374407	11.257572	15.031644
C	21.694057	10.438411	16.516152
H	21.716693	9.440893	16.087585
C	22.433985	10.685266	17.708067
C	23.173567	9.635602	18.325911
H	23.171101	8.657137	17.854829
C	23.871845	9.849071	19.496305
H	24.429625	9.042253	19.959608
C	23.853290	11.132076	20.096915
H	24.395830	11.299409	21.021653
C	23.151865	12.173993	19.518849
H	23.158527	13.139517	20.004733
C	22.423297	11.999584	18.304489
P	18.046696	16.623501	18.087375
P	21.452668	14.770539	18.287671
O	18.963375	13.702690	13.796045
H	18.966476	14.650131	14.037369
C	19.054215	13.636380	12.357172
H	19.035957	12.578172	12.083992
H	18.207552	14.137681	11.870039
H	19.988474	14.077746	11.985114
O	20.642262	20.040799	14.831818
H	20.197779	19.178774	14.718053
C	21.429661	20.271510	13.647281
H	21.910578	21.246363	13.767867
H	22.210733	19.511119	13.517895
H	20.809979	20.301397	12.740063

=== TS2 ===

Fe	19.124415	14.976998	20.966432
Pd	20.127720	16.069346	16.698919
Br	18.583801	15.109705	14.359370
C	17.868153	16.245623	19.856187
C	18.499687	16.972432	20.940784
H	19.140673	17.832794	20.835587
C	18.105125	16.374118	22.179477
H	18.433865	16.680242	23.161006
C	17.236523	15.274132	21.883015
H	16.795681	14.599041	22.600815
C	17.085380	15.192427	20.460452
H	16.496669	14.457439	19.938263
C	20.812049	14.381153	19.857356
C	21.218820	14.863541	21.160428
H	21.871215	15.698981	21.352282
C	20.604442	14.040266	22.157537
H	20.698844	14.171273	23.224848
C	19.810692	13.047433	21.494677
H	19.202541	12.295128	21.973441
C	19.926601	13.254452	20.084146
H	19.461932	12.653947	19.318382
C	17.984838	18.584149	18.309132
C	19.067788	19.290898	17.799097
H	19.830633	18.763641	17.242567
C	19.198265	20.692559	17.963314
H	20.061575	21.198885	17.545271
C	18.234409	21.396554	18.648765
H	18.321096	22.470989	18.780850
C	17.105796	20.729168	19.204814
C	16.116237	21.462515	19.921689
H	16.242225	22.536595	20.021874
C	15.024171	20.829392	20.477913
H	14.276724	21.396969	21.022031
C	14.882771	19.426612	20.336325
H	14.025439	18.927007	20.775690

C	15.823698	18.686849	19.644068
H	15.685052	17.618845	19.553312
C	16.965623	19.301302	19.049046
C	16.451528	16.261671	17.276276
C	15.637357	17.244776	16.726076
H	15.913331	18.287825	16.811640
C	14.430094	16.923278	16.057152
H	13.820448	17.723944	15.652133
C	14.030987	15.609882	15.938480
H	13.098268	15.356091	15.443773
C	14.846645	14.559376	16.444967
C	14.464472	13.195218	16.288508
H	13.518236	12.976289	15.802430
C	15.278588	12.172256	16.729701
H	14.979244	11.137391	16.601703
C	16.522961	12.476710	17.337891
H	17.175556	11.670213	17.656212
C	16.914096	13.790227	17.516631
H	17.881220	13.995847	17.960177
C	16.090197	14.876346	17.100845
C	21.826314	16.177986	15.553001
C	22.581862	17.333274	15.816501
H	22.349287	17.958461	16.672081
C	23.652804	17.690090	14.982833
H	24.222066	18.590222	15.196714
C	23.989927	16.883149	13.889284
H	24.823656	17.151284	13.247559
C	23.244880	15.726123	13.632067
H	23.495540	15.094252	12.784421
C	22.163587	15.369479	14.456988
H	21.594932	14.482448	14.211461
C	23.126668	15.572269	18.511926
C	24.263966	14.938683	18.025356
H	24.178503	13.995195	17.502926
C	25.555031	15.496676	18.190973
H	26.415531	14.962252	17.803472
C	25.712004	16.700400	18.842408
H	26.699018	17.130412	18.982623
C	24.579223	17.412899	19.325970
C	24.730024	18.679147	19.961692
H	25.733241	19.072127	20.097087
C	23.632047	19.399915	20.384811
H	23.758914	20.365887	20.861585
C	22.329454	18.878805	20.181689
H	21.466101	19.458836	20.490475
C	22.150717	17.644105	19.585291
H	21.144458	17.273576	19.432837
C	23.259097	16.860481	19.148161
C	21.760223	13.103911	17.542769
C	21.109980	12.785940	16.357070
H	20.501345	13.535783	15.865814
C	21.197828	11.499246	15.769241
H	20.695453	11.320831	14.825476
C	21.932987	10.514456	16.388172
H	22.013664	9.524329	15.949202
C	22.597897	10.768282	17.622115
C	23.337694	9.734661	18.265922
H	23.386833	8.761520	17.786354
C	23.974456	9.956805	19.469394
H	24.533439	9.162061	19.951778
C	23.892474	11.233840	20.076700
H	24.389009	11.409794	21.025430
C	23.188043	12.260272	19.474635
H	23.148691	13.221299	19.966971
C	22.517883	12.075361	18.228877
P	18.045625	16.740299	18.092699
P	21.468787	14.812778	18.199152
O	20.286616	12.686896	12.776569
H	19.759599	13.385194	13.218424
C	20.451932	13.090687	11.403203
H	21.062356	12.326647	10.913809
H	19.490738	13.158426	10.875261
H	20.967938	14.056450	11.316732
O	19.213937	18.169941	14.973217
H	18.951256	17.337735	14.524089
C	20.008641	18.944937	14.046400
H	20.359989	19.827821	14.586113
H	20.877119	18.383503	13.686744
H	19.406013	19.273843	13.190279

=== Int2 ===

Fe	19.117879	15.000237	21.024997
Pd	20.227256	16.266071	16.849686
Br	17.837273	15.559456	12.940171
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C	18.406424	16.968616	21.064689
H	19.013962	17.859135	21.038945
C	17.970885	16.286958	22.245692
H	18.229013	16.553560	23.259240
C	17.172396	15.166780	21.843890
H	16.724547	14.436330	22.500393
C	17.104077	15.154327	20.412580
H	16.580986	14.424739	19.816630
C	20.843336	14.457823	19.943192
C	21.216433	14.969180	21.245394
H	21.837368	15.827954	21.437493
C	20.620581	14.135796	22.245091
H	20.697894	14.282622	23.311699
C	19.872272	13.106665	21.585699
H	19.287139	12.337430	22.066123
C	19.997530	13.301159	20.174402
H	19.565149	12.671928	19.413566
C	18.037528	18.664632	18.400036
C	19.121970	19.383477	17.907768
H	19.927016	18.854543	17.410616
C	19.221821	20.789511	18.047132
H	20.086689	21.305435	17.644748
C	18.225625	21.485391	18.694857
H	18.288663	22.563258	18.809957
C	17.096528	20.806023	19.234472
C	16.074747	21.530650	19.914182
H	16.177539	22.608137	20.001954
C	14.980131	20.884291	20.449599
H	14.208032	21.445199	20.965318
C	14.866563	19.477165	20.323633
H	14.005699	18.968942	20.745549
C	15.839021	18.745085	19.668426
H	15.722472	17.673195	19.587465
C	16.986018	19.373600	19.098213
C	16.623137	16.317032	17.249408
C	15.756419	17.277915	16.741845
H	15.944699	18.328149	16.920334
C	14.607517	16.923481	15.992021
H	13.953941	17.707172	15.624434
C	14.323022	15.598957	15.742422
H	13.438208	15.317985	15.179468
C	15.198355	14.574367	16.199379
C	14.936372	13.204952	15.906817
H	14.035217	12.958684	15.353159
C	15.810425	12.212133	16.299889
H	15.604241	11.173546	16.064443
C	16.992830	12.554602	17.002799
H	17.691937	11.775189	17.287399
C	17.265079	13.872898	17.319029
H	18.178997	14.109904	17.850937
C	16.380865	14.926881	16.944556
C	21.844617	16.279188	15.577969
C	22.791739	17.296699	15.790130
H	22.767984	17.888517	16.699206
C	23.783603	17.560743	14.832757

H	24.505840	18.352295	15.012299
C	23.843311	16.805183	13.655185
H	24.612345	17.004688	12.915130
C	22.902418	15.790931	13.439798
H	22.935892	15.201782	12.527422
C	21.903617	15.526371	14.392983
H	21.184223	14.744447	14.176449
C	23.166084	15.633569	18.598762
C	24.292323	14.982029	18.111367
H	24.191160	14.043917	17.582110
C	25.593034	15.514642	18.285519
H	26.444841	14.966890	17.897683
C	25.769378	16.711328	18.944740
H	26.763663	17.121913	19.091349
C	24.648419	17.442121	19.428850
C	24.821003	18.700706	20.073916
H	25.830918	19.074109	20.214380
C	23.735569	19.437889	20.501227
H	23.879262	20.397193	20.986505
C	22.424157	18.941874	20.293103
H	21.570366	19.531890	20.609319
C	22.223877	17.715731	19.685677
H	21.210182	17.365312	19.533924
C	23.318588	16.915362	19.243639
C	21.734510	13.209645	17.584712
C	21.055675	12.937945	16.403194
H	20.472202	13.719989	15.935870
C	21.086434	11.662730	15.786953
H	20.551406	11.527323	14.854245
C	21.800207	10.641960	16.372326
H	21.838100	9.658494	15.913127
C	22.497082	10.847877	17.597681
C	23.214670	9.777628	18.205861
H	23.225021	8.814238	17.704776
C	23.877856	9.953181	19.402731
H	24.419390	9.130820	19.857894
C	23.845674	11.217816	20.040194
H	24.362101	11.356040	20.984464
C	23.163933	12.278904	19.473297
H	23.160148	13.229251	19.988114
C	22.469691	12.142593	18.234517
P	18.135593	16.828028	18.186888
P	21.496297	14.904573	18.285353
O	19.834755	12.904806	12.995235
H	19.208066	13.662563	13.025813
C	20.193980	12.720324	11.612996
H	20.936140	11.918051	11.575006
H	19.331134	12.424790	10.999676
H	20.636388	13.625786	11.176163
O	19.096231	17.388704	15.270907
H	18.705334	16.716766	14.644616
C	19.676220	18.436074	14.435247
H	20.013062	19.230923	15.100057
H	20.518160	18.055937	13.853672
H	18.899804	18.819138	13.767698

1 MeOH & 1 Me3NH+

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Fe	19.041707	14.962761	21.078285
Pd	19.896649	15.595365	17.364698
Br	21.605045	16.698556	14.840749
C	17.777228	16.213947	19.824085
C	18.485677	16.993007	20.815303
H	19.159601	17.809958	20.609640
C	18.098274	16.535877	22.116482
H	18.462331	16.921933	23.056542
C	17.180751	15.447225	21.946163
H	16.729900	14.864164	22.735112
C	16.991171	15.240631	20.539490
H	16.358298	14.489398	20.095044
C	20.812336	14.077991	20.177445
C	21.137147	14.717495	21.427281
H	21.841477	15.523116	21.559805
C	20.371244	14.096470	22.469011
H	20.390309	14.369173	23.513463
C	19.553161	13.079917	21.874521
H	18.848128	12.446223	22.391011
C	19.803724	13.082051	20.464092
H	19.347961	12.421631	19.743030
C	17.703792	18.394402	17.954821
C	18.647507	19.029582	17.154242
H	19.371526	18.420014	16.622539
C	18.708733	20.439267	17.025739
H	19.469361	20.874775	16.386613
C	17.814916	21.225383	17.719296
H	17.852314	22.307967	17.639881
C	16.823299	20.637164	18.556234
C	15.896195	21.453994	19.266490
H	15.968908	22.532245	19.158302
C	14.924885	20.893946	20.070686
H	14.223392	21.525222	20.605892
C	14.842700	19.484135	20.194243
H	14.074579	19.045248	20.822790
C	15.728552	18.663335	19.521334
H	15.641698	17.590857	19.631060
C	16.750923	19.201178	18.684232
C	16.286813	15.887116	17.303142
C	15.350753	16.764027	16.762687
H	15.509765	17.832331	16.826716
C	14.170967	16.304618	16.124732
H	13.468442	17.029761	15.727571
C	13.917540	14.954855	16.021472
H	13.011400	14.594023	15.544220
C	14.848888	14.006835	16.531601
C	14.606202	12.608070	16.407636
H	13.684903	12.284200	15.932316
C	15.517567	11.681744	16.872492
H	15.321962	10.619498	16.770496
C	16.719943	12.123490	17.479615
H	17.442542	11.393579	17.830722
C	16.980202	13.474282	17.625821
H	17.911688	13.789790	18.083472
C	16.059186	14.464405	17.169600
C	22.814058	16.897711	13.311286
C	23.158460	18.178270	12.873704
H	22.754830	19.060784	13.357651
C	24.037830	18.294956	11.787585
H	24.315943	19.282218	11.434146
C	24.553469	17.151696	11.164253
H	25.233312	17.251484	10.325080
C	24.192446	15.878942	11.624913
H	24.590925	14.990529	11.146712
C	23.315887	15.741444	12.709818
H	23.038238	14.759811	13.074686
C	23.197667	15.106208	18.778387
C	24.345328	14.397910	18.436848
H	24.267248	13.377099	18.087006
C	25.638026	14.971454	18.531863
H	26.502353	14.374125	18.261081
C	25.792302	16.268442	18.968687
H	26.779244	16.713585	19.051889
C	24.654548	17.053758	19.307383
C	24.802699	18.405361	19.734175
H	25.805620	18.815009	19.811934
C	23.703255	19.182961	20.035841
H	23.829046	20.211877	20.356151
C	22.401689	18.633975	19.917801
H	21.537335	19.251433	20.141108
C	22.224406	17.321987	19.517139

H	21.218653	16.927113	19.421720
C	23.334425	16.481964	19.203991
C	21.864186	12.612688	17.936016
C	21.419217	12.331278	16.647792
H	20.941958	13.121701	16.076420
C	21.554287	11.045880	16.067451
H	21.193790	10.873824	15.058866
C	22.130553	10.024606	16.790561
H	22.232824	9.031954	16.362079
C	22.605358	10.248783	18.114499
C	23.207954	9.192521	18.857680
H	23.287139	8.213775	18.393652
C	23.685687	9.403963	20.134616
H	24.143874	8.593252	20.691206
C	23.581031	10.691255	20.719146
H	23.964873	10.857834	21.720437
C	22.998196	11.736332	20.026718
H	22.936264	12.709507	20.494673
C	22.483609	11.558737	18.707959
P	17.876032	16.547001	18.015296
P	21.521789	14.347639	18.500390
O	20.987073	20.261876	14.477744
H	20.944548	19.329470	14.751134
C	20.027962	20.435120	13.406155
H	20.107762	21.474537	13.080638
H	20.250360	19.780901	12.554126
H	19.002175	20.250798	13.747925
H	19.549023	15.879400	13.645136
N	18.729795	15.515104	13.131864
C	17.584975	16.462397	13.395889
H	17.387623	16.481645	14.467436
H	17.865059	17.455581	13.045401
H	16.706933	16.106124	12.857101
C	19.101893	15.477324	11.669599
H	19.330644	16.490302	11.340125
H	19.974375	14.836261	11.547327
H	18.257714	15.078967	11.106412
C	18.449681	14.135461	13.676127
H	19.316825	13.503295	13.486940
H	18.270782	14.215656	14.748735
H	17.571023	13.732859	13.171442

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Fe	19.257590	15.127861	20.991704
Pd	20.114409	15.977804	16.779510
Br	19.377677	15.189702	14.112419
C	18.088332	16.495704	19.836264
C	18.813786	17.181887	20.884317
H	19.529832	17.975458	20.739186
C	18.388515	16.660968	22.149048
H	18.760089	16.966365	23.115524
C	17.419123	15.634280	21.900519
H	16.930624	15.025244	22.646291
C	17.236368	15.526612	20.482457
H	16.572179	14.837739	19.986434
C	20.873553	14.214325	19.917759
C	21.348950	14.798673	21.148918
H	22.097444	15.569797	21.233644
C	20.664102	14.175736	22.243956
H	20.795560	14.417171	23.288037
C	19.750468	13.209876	21.707135
H	19.071955	12.590666	22.274233
C	19.862923	13.242485	20.279137
H	19.312783	12.619979	19.590928
C	18.167242	18.791243	18.164268
C	19.186504	19.453565	17.488463
H	19.914308	18.869643	16.936090
C	19.314724	20.864761	17.509219
H	20.126698	21.334722	16.964647
C	18.415275	21.624234	18.223357
H	18.503091	22.706327	18.252030
C	17.351787	21.006095	18.941813
C	16.422659	21.795529	19.679591
H	16.548131	22.874362	19.680984
C	15.385373	21.209209	20.375213
H	14.683287	21.819537	20.933444
C	15.236864	19.799786	20.355843
H	14.417949	19.339752	20.899470
C	16.121721	19.005470	19.650378
H	15.982267	17.933316	19.650227
C	17.210723	19.569900	18.921729
C	16.625200	16.424360	17.285660
C	15.768028	17.388149	16.764353
H	15.999968	18.438275	16.881538
C	14.579475	17.041791	16.074180
H	13.939450	17.831868	15.695739
C	14.240581	15.719263	15.892223
H	13.328466	15.445263	15.370696
C	15.092300	14.686317	16.375492
C	14.766901	13.314091	16.165439
H	13.840866	13.076254	15.649929
C	15.602543	12.306552	16.605938
H	15.341745	11.265979	16.443296
C	16.806799	12.636947	17.277755
H	17.468738	11.844866	17.612751
C	17.144626	13.958532	17.506307
H	18.074551	14.186105	18.013504
C	16.307315	15.029551	17.073491
C	21.211105	16.066745	14.866093
C	21.194315	17.476313	14.787672
H	20.258382	18.021392	14.744825
C	22.425888	18.153424	14.680715
H	22.428543	19.238424	14.644243
C	23.620432	17.440327	14.566080
H	24.562013	17.968088	14.459044
C	23.599217	16.031415	14.546416
H	24.525770	15.475754	14.444209
C	22.398495	15.332270	14.665356
H	22.383659	14.249883	14.650561
C	23.195212	15.097199	18.351952
C	24.258096	14.328650	17.889196
H	24.079258	13.332724	17.506760
C	25.592987	14.805151	17.904296
H	26.387930	14.161494	17.542204
C	25.875693	16.066005	18.380522
H	26.896425	16.435666	18.405434
C	24.827088	16.913964	18.836305
C	25.105190	18.231768	19.301736
H	26.138916	18.564553	19.321460
C	24.090346	19.073735	19.709082
H	24.314471	20.076793	20.056603
C	22.746116	18.626367	19.662603
H	21.947411	19.296870	19.963133
C	22.444835	17.347397	19.230465
H	21.409165	17.031313	19.191756
C	23.464400	16.441758	18.811512
C	21.628640	12.696692	17.644463
C	21.000271	12.391081	16.441761
H	20.483782	13.177309	15.902138
C	20.998904	11.080350	15.902286
H	20.498668	10.892829	14.958324
C	21.623556	10.057394	16.579702
H	21.626513	9.047745	16.179665
C	22.275249	10.302350	17.822159
C	22.916467	9.240391	18.523895
H	22.894054	8.245685	18.088377
C	23.552775	9.464968	19.727216
H	24.037845	8.649602	20.253448
C	23.572702	10.771616	20.276090
H	24.076244	10.948239	21.221073

C	22.960103	11.823178	19.620167
H	22.993116	12.809588	20.060736
C	22.287900	11.635157	18.375857
P	18.239415	16.936177	18.058062
P	21.451159	14.469807	18.189054
O	18.058899	18.424023	13.840195
H	18.234459	17.467765	13.888915
C	18.271362	18.821941	12.467255
H	18.087487	19.897792	12.417839
H	19.300721	18.626476	12.139981
H	17.577270	18.316040	11.783695
H	18.300311	13.226962	12.775059
N	17.659613	12.623482	12.238864
C	16.298083	13.278338	12.274116
H	15.976363	13.362277	13.312260
H	16.373049	14.266435	11.820931
H	15.601927	12.656059	11.711514
C	18.205047	12.537959	10.833398
H	18.241061	13.541287	10.410374
H	19.205933	12.109087	10.872347
H	17.544023	11.902635	10.243964
C	17.641893	11.274391	12.916470
H	18.650621	10.862878	12.905052
H	17.296265	11.403541	13.941815
H	16.962974	10.621564	12.367557

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Fe	19.137121	14.953984	21.002278
Pd	20.162896	15.985581	16.707559
Br	18.984869	17.084947	14.637236
C	17.841227	16.088191	19.793249
C	18.347455	16.886356	20.892455
H	18.918465	17.796451	20.800153
C	17.933238	16.277554	22.120274
H	18.175947	16.628138	23.111874
C	17.182027	15.099508	21.800980
H	16.760882	14.401789	22.508833
C	17.120866	14.979275	20.374186
H	16.626043	14.189966	19.832449
C	20.877389	14.387622	19.960735
C	21.236593	15.041053	21.201091
H	21.819317	15.941443	21.300598
C	20.685976	14.284696	22.284855
H	20.763970	14.539960	23.330761
C	19.980952	13.162676	21.738873
H	19.435743	12.418795	22.299533
C	20.087262	13.222388	20.313924
H	19.679765	12.503188	19.622099
C	17.823150	18.392450	18.159230
C	18.832822	19.169950	17.603626
H	19.665818	18.690233	17.106821
C	18.817036	20.585318	17.663060
H	19.618238	21.136314	17.185170
C	17.784147	21.231626	18.303378
H	17.757740	22.315941	18.357961
C	16.727094	20.492525	18.907819
C	15.663433	21.168144	19.573488
H	15.683468	22.253443	19.607745
C	14.630426	20.466954	20.160194
H	13.825766	20.991409	20.664473
C	14.623330	19.051301	20.099747
H	13.809889	18.498869	20.558776
C	15.639937	18.365623	19.461081
H	15.602282	17.285677	19.430336
C	16.728316	19.050713	18.843071
C	16.562641	15.902512	17.143970
C	15.647468	16.786198	16.584854
H	15.769353	17.851795	16.723052
C	14.541103	16.334715	15.822703
H	13.847741	17.062678	15.415496
C	14.348426	14.987438	15.608684
H	13.497378	14.631784	15.035866
C	15.270302	14.036354	16.130810
C	15.096085	12.642022	15.891393
H	14.229733	12.320330	15.321070
C	16.005377	11.717855	16.365650
H	15.862974	10.659519	16.175397
C	17.135231	12.157046	17.100176
H	17.857957	11.431105	17.457139
C	17.324951	13.502219	17.359215
H	18.196961	13.812561	17.921096
C	16.404899	14.488844	16.898171
C	21.812067	15.899667	15.462580
C	22.687670	16.997184	15.533776
H	22.545864	17.765399	16.285557
C	23.753562	17.121476	14.628529
H	24.420327	17.976166	14.701257
C	23.959262	16.150094	13.640209
H	24.786211	16.243933	12.942974
C	23.087235	15.058377	13.559833
H	23.231823	14.298641	12.796441
C	22.016810	14.935908	14.462331
H	21.354429	14.084432	14.364400
C	23.128145	15.506120	18.459267
C	24.261081	14.843459	18.004455
H	24.175775	13.858183	17.566355
C	25.549160	15.426180	18.092360
H	26.407637	14.867536	17.735809
C	25.705087	16.685666	18.628001
H	26.689619	17.136464	18.706981
C	24.574343	17.428310	19.069628
C	24.723851	18.749455	19.582011
H	25.724754	19.164370	19.654600
C	23.627446	19.494039	19.966389
H	23.753519	20.501062	20.349091
C	22.327615	18.941245	19.849027
H	21.463727	19.533629	20.131634
C	22.150620	17.655631	19.371176
H	21.144010	17.264190	19.285902
C	23.257691	16.848055	18.975115
C	21.698023	12.982171	17.674678
C	20.937855	12.605468	16.573757
H	20.294332	13.339610	16.103661
C	20.962065	11.288133	16.054493
H	20.353811	11.044776	15.190301
C	21.756740	10.333636	16.648337
H	21.793573	9.321716	16.256464
C	22.531198	10.647365	17.801259
C	23.321193	9.643122	18.432172
H	23.334430	8.648559	17.996626
C	24.045852	9.919531	19.572764
H	24.641793	9.147157	20.046914
C	24.002092	11.221241	20.130528
H	24.562190	11.436532	21.034530
C	23.253639	12.220817	19.537255
H	23.241391	13.201641	19.991330
C	22.500612	11.982277	18.349080
P	18.055686	16.557848	18.032144
P	21.464003	14.725968	18.253270
O	20.916504	19.955493	15.068745
H	20.420926	19.140473	14.865131
C	21.579235	20.362212	13.854749
H	22.127625	21.280194	14.082744
H	22.294076	19.605965	13.505123
H	20.864913	20.575803	13.047647
H	18.281900	15.477484	13.108847
N	17.983232	14.828545	12.348645
C	16.641237	15.307929	11.857224
H	15.938099	15.290569	12.689862
H	16.748179	16.325099	11.481066

H	16.301563	14.645000	11.060650
C	19.035725	14.911943	11.272945
H	19.091296	15.941242	10.919034
H	19.994275	14.613890	11.697122
H	18.758637	14.245444	10.455552
C	17.895975	13.446788	12.943526
H	18.872926	13.173966	13.341739
H	17.154264	13.453398	13.741956
H	17.600294	12.746274	12.161774

=== TS2 ===

Fe	19.241686	14.926575	21.023989
Pd	20.415692	15.779233	16.785863
Br	19.186120	14.430291	14.339307
C	17.955873	16.009618	19.758215
C	18.484392	16.863110	20.804594
H	19.066487	17.757981	20.655692
C	18.069024	16.338462	22.069648
H	18.325992	16.744193	23.036332
C	17.294250	15.157945	21.827469
H	16.866155	14.511781	22.578781
C	17.218925	14.953369	20.411330
H	16.707470	14.140285	19.924011
C	21.029596	14.366790	20.061724
C	21.325751	14.977342	21.340706
H	21.912039	15.866845	21.499749
C	20.708711	14.193192	22.366610
H	20.729865	14.414523	23.422889
C	20.022334	13.098401	21.746047
H	19.437474	12.345314	22.251636
C	20.207622	13.201854	20.331962
H	19.834660	12.509206	19.594529
C	17.968317	18.212719	17.994766
C	18.986482	18.943060	17.393017
H	19.781755	18.421459	16.877776
C	19.005507	20.360008	17.403322
H	19.822207	20.884689	16.919517
C	17.994442	21.055181	18.026948
H	17.998126	22.140963	18.045794
C	16.921193	20.365210	18.660076
C	15.874737	21.091715	19.298640
H	15.919569	22.176761	19.288648
C	14.826868	20.438534	19.913706
H	14.034771	21.001121	20.396279
C	14.787807	19.022180	19.910600
H	13.962007	18.507499	20.390958
C	15.788129	18.287952	19.300536
H	15.724773	17.208940	19.312054
C	16.890765	18.922424	18.654865
C	16.661230	15.703179	17.130248
C	15.791865	16.581316	16.492869
H	15.981864	17.646146	16.518028
C	14.634933	16.124691	15.813505
H	13.976521	16.848459	15.345272
C	14.342610	14.778549	15.768698
H	13.444842	14.421449	15.272953
C	15.221774	13.829955	16.363889
C	14.950330	12.432652	16.285830
H	14.039616	12.109418	15.790044
C	15.822272	11.506967	16.823068
H	15.606351	10.445978	16.756605
C	17.012659	11.946392	17.455621
H	17.708540	11.215836	17.854962
C	17.296051	13.295470	17.558459
H	18.222153	13.604982	18.027774
C	16.412696	14.284846	17.036873
C	22.174151	15.965573	15.753010
C	22.776502	17.224888	15.913237
H	22.417651	17.919594	16.665288
C	23.859523	17.598876	15.102661
H	24.310731	18.578491	15.230944
C	24.360946	16.709878	14.143558
H	25.205458	16.994297	13.523553
C	23.768905	15.450270	13.993709
H	24.148483	14.753336	13.251831
C	22.678017	15.074410	14.795803
H	22.224931	14.104262	14.646481
C	23.328299	15.619190	18.742115
C	24.533819	15.039574	18.365260
H	24.547823	14.054408	17.918101
C	25.768670	15.708288	18.549459
H	26.686889	15.213983	18.251850
C	25.798572	16.968728	19.105103
H	26.741632	17.484480	19.257884
C	24.590950	17.626693	19.470124
C	24.611355	18.948366	20.002080
H	25.573101	19.429698	20.151685
C	23.440703	19.611729	20.307997
H	23.468230	20.620734	20.704945
C	22.193965	18.973272	20.089976
H	21.274355	19.505752	20.309298
C	22.141214	17.683483	19.594167
H	21.174922	17.221566	19.431546
C	23.327856	16.959285	19.276331
C	22.165555	12.988409	17.895118
C	21.558719	12.534953	16.729909
H	20.921760	13.201134	16.159134
C	21.727829	11.208278	16.262496
H	21.235542	10.902944	15.345724
C	22.509468	10.324503	16.970989
H	22.652028	9.306493	16.621252
C	23.134945	10.721791	18.186826
C	23.919491	9.792008	18.928669
H	24.040862	8.788445	18.532093
C	24.507728	10.149882	20.123821
H	25.101338	9.433635	20.681641
C	24.327551	11.462470	20.625205
H	24.782440	11.743370	21.569387
C	23.578691	12.390974	19.925949
H	23.462667	13.382559	20.339457
C	22.961221	12.066549	18.681664
P	18.177245	16.368789	17.970378
P	21.750413	14.716807	18.413975
O	19.443112	17.654115	14.580728
H	19.313765	16.724372	14.297060
C	20.286200	18.299637	13.599918
H	20.474169	19.314837	13.958245
H	21.245934	17.784694	13.486029
H	19.787076	18.360275	12.624071
H	17.693511	14.001539	12.713615
N	16.977625	13.767624	11.983485
C	15.909232	14.824531	12.068534
H	15.484387	14.812296	13.072059
H	16.363124	15.795325	11.869573
H	15.138821	14.610678	11.326693
C	17.674859	13.782946	10.649251
H	18.082295	14.779287	10.478338
H	18.480745	13.049447	10.666510
H	16.953267	13.532373	9.870720
C	16.445344	12.399930	12.320211
H	17.260533	11.680514	12.241699
H	16.063616	12.410910	13.341461
H	15.650717	12.145000	11.617974

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Fe	19.196762	15.001868	21.048674
Pd	20.469776	16.087888	16.891421
Br	19.161301	14.071326	13.347206
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C	18.417993	16.940087	20.905113

H	18.992693	17.849032	20.826675
C	17.962290	16.340666	22.122468
H	18.173807	16.697397	23.119012
C	17.217080	15.163584	21.787087
H	16.770998	14.472245	22.485783
C	17.200519	15.034019	20.360178
H	16.724162	14.240769	19.808102
C	21.000182	14.472636	20.095655
C	21.279819	15.060201	21.388991
H	21.858434	15.950130	21.571103
C	20.655725	14.255481	22.394377
H	20.664770	14.458162	23.454530
C	19.983226	13.167914	21.747190
H	19.398084	12.401733	22.232345
C	20.183701	13.297530	20.337077
H	19.821361	12.613909	19.586427
C	18.012251	18.402411	18.089251
C	19.050372	19.160005	17.556352
H	19.909803	18.659233	17.126070
C	19.037000	20.576346	17.570068
H	19.870128	21.121620	17.140407
C	17.973154	21.245066	18.132933
H	17.949867	22.330416	18.153169
C	16.884417	20.528065	18.705551
C	15.790139	21.226782	19.293217
H	15.809300	22.312515	19.289119
C	14.729970	20.545750	19.854271
H	13.902073	21.087130	20.299411
C	14.725061	19.128615	19.846307
H	13.890125	18.592975	20.286014
C	15.770468	18.420776	19.283151
H	15.734111	17.340322	19.289743
C	16.887212	19.084927	18.693810
C	16.813274	15.881631	17.089326
C	15.924304	16.746265	16.461069
H	16.054259	17.816401	16.549195
C	14.825111	16.267056	15.706257
H	14.148743	16.979642	15.246769
C	14.610146	14.912066	15.576233
H	13.753874	14.536667	15.023796
C	15.514556	13.979391	16.157621
C	15.323298	12.576345	15.996139
H	14.449484	12.233481	15.449591
C	16.223941	11.669416	16.517599
H	16.069765	10.603949	16.385323
C	17.363012	12.135434	17.220785
H	18.083209	11.421639	17.606664
C	17.564689	13.489775	17.411465
H	18.447163	13.821560	17.944124
C	16.649720	14.459022	16.905962
C	22.201926	16.236036	15.788040
C	22.978841	17.380641	16.040845
H	22.772912	18.005952	16.902959
C	24.039098	17.725365	15.188343
H	24.627608	18.614509	15.396289
C	24.340479	16.923514	14.080208
H	25.164379	17.185256	13.423404
C	23.569568	15.783088	13.824710
H	23.788814	15.158685	12.962996
C	22.502066	15.438802	14.671763
H	21.898781	14.573222	14.426420
C	23.340230	15.697516	18.836311
C	24.523075	15.077564	18.452950
H	24.498349	14.111034	17.967641
C	25.784852	15.680612	18.677944
H	26.683406	15.155855	18.372644
C	25.864677	16.916741	19.280914
H	26.827981	17.382638	19.464367
C	24.683543	17.615792	19.656122
C	24.757608	18.915090	20.236309
H	25.738541	19.345856	20.413094
C	23.614999	19.619891	20.555150
H	23.683747	20.611223	20.989785
C	22.343332	19.047176	20.302068
H	21.445726	19.610271	20.534907
C	22.237929	17.780690	19.756984
H	21.252788	17.370979	19.569294
C	23.393772	17.014702	19.422910
C	22.066212	13.178964	17.822801
C	21.464356	12.848327	16.613574
H	20.870408	13.588023	16.090345
C	21.583608	11.558893	16.040945
H	21.096234	11.355323	15.094046
C	22.310416	10.586167	16.689111
H	22.414235	9.594093	16.260150
C	22.929313	10.855067	17.943240
C	23.657907	9.834032	18.619148
H	23.740362	8.860355	18.145622
C	24.241884	10.069179	19.846498
H	24.792720	9.284316	20.353536
C	24.115335	11.345902	20.447289
H	24.568854	11.530436	21.415582
C	23.421109	12.360607	19.814708
H	23.346195	13.321794	20.303712
C	22.807596	12.162661	18.542022
P	18.251027	16.565217	18.042318
P	21.725153	14.881041	18.460119
O	19.339450	16.825218	15.084779
H	19.241639	15.981963	14.568535
C	19.814748	17.846999	14.154709
H	19.804470	18.795823	14.690896
H	20.825348	17.623960	13.807475
H	19.125376	17.899761	13.307546
H	17.448616	13.659539	12.016833
N	16.610210	13.444970	11.414419
C	15.641874	14.581919	11.596036
H	15.386277	14.658662	12.652887
H	16.119874	15.503761	11.264506
H	14.747523	14.386206	11.002919
C	17.094674	13.343906	9.993661
H	17.558233	14.290299	9.714628
H	17.827191	12.539163	9.930576
H	16.245968	13.133669	9.341282
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H	16.804081	11.366571	11.791790
H	15.792642	12.249897	12.965190
H	15.157390	11.891504	11.330280