

Electronic supplementary information (ESI)

Structures and properties of large supramolecular coordination complexes predicted with the generalized energy-based fragmentation method

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Contents

Table S1 Comparison of relative energies calculated with the GEBF-M06-2X and conventional M06-2X methods for six conformers of $M_7(\text{timb})_2(\text{tim})_2$	2
Table S2 Comparison of Pd-N bond lengths around seven Pd^{2+} ions in $M_7(\text{timb})_2(\text{tim})_2$ optimized with the GEBF-M06-2X and conventional M06-2X methods.	3
Table S3 The average lengths of coordinate bonds between different metal ions and (terminal, central) pyridinyl groups in $\text{Fe}_2\text{Zn}_2(\text{RuL}_2)_2$ optimized with the GEBF-M06-2X method.	4
Fig. S1 The superposition of optimized structure obtained with the GEBF-M06-2X method and crystal structure for $\text{Pd}_4\text{L}_8(\text{BF}_4^-)_3$	5
Table S4 Comparison of Pd-N bond lengths optimized with the GEBF-M06-2X method and corresponding bond lengths in the crystal structure for $\text{Pd}_4\text{L}_8(\text{BF}_4^-)_3$	6
Cartesian coordinates of $M_7(\text{timb})_2(\text{tim})_2$	6
Cartesian coordinates of $\text{Fe}_2\text{Zn}_2(\text{RuL}_2)_2$	11
Cartesian coordinates of $\text{Pd}_4\text{L}_8(\text{BF}_4^-)_3$	19

Table S1 Comparison of relative energies (in millihartree) calculated with the GEBF-M06-2X and conventional M06-2X methods for six conformers of $M_7(\text{timb})_2(\text{tim})_2$. The LANL2DZ basis set is used for metal atoms and the 6-31G(d,p) basis set is used for H, C, N atoms.

	GEBF-M06-2X	Convent. M06-2X	Deviation
1	0	0	0.00
2	5.79	5.71	0.08
3	26.53	26.38	0.15
4	53.57	53.47	0.10
5	98.59	98.86	-0.27

Table S2 Comparison of Pd-N bond lengths (in Å) around seven Pd²⁺ ions in M₇(timb)₂(tim)₂ optimized with the GEBF-M06-2X and conventional M06-2X methods. The 6-31G(d,p) basis set is used for H, C, N atoms and the LANL2DZ basis set is used for metal atoms.

Pd ²⁺ center	GEBF-M06-2X	Convent. M06-2X
1	2.10, 2.12, 2.29, 2.28	2.11, 2.12, 2.26, 2.26
2	2.09, 2.09, 2.28, 2.28	2.09, 2.09, 2.29, 2.29
3	2.11, 2.13, 2.23, 2.32	2.11, 2.12, 2.24, 2.34
4	2.11, 2.12, 2.26, 2.34	2.11, 2.12, 2.25, 2.32
5	2.12, 2.11, 2.24, 2.30	2.12, 2.11, 2.25, 2.32
6	2.11, 2.13, 2.23, 2.33	2.11, 2.12, 2.24, 2.34
7	2.09, 2.09, 2.28, 2.28	2.09, 2.09, 2.30, 2.29

Table S3 The average lengths of coordinate bonds (in Å) between different metal ions and (terminal, central) pyridinyl groups in $\text{Fe}_2\text{Zn}_2(\text{RuL}_2)_2$ optimized with the GEBF-M06-2X method. The LANL2DZ basis set for metal atoms and 6-31G** basis set for non-metal atoms are employed.

Metal ion	terminal	central	terminal
Ru^{2+}	2.16	2.05	2.16
Fe^{2+}	2.24	2.17	2.24
Zn^{2+}	2.23	2.16	2.23

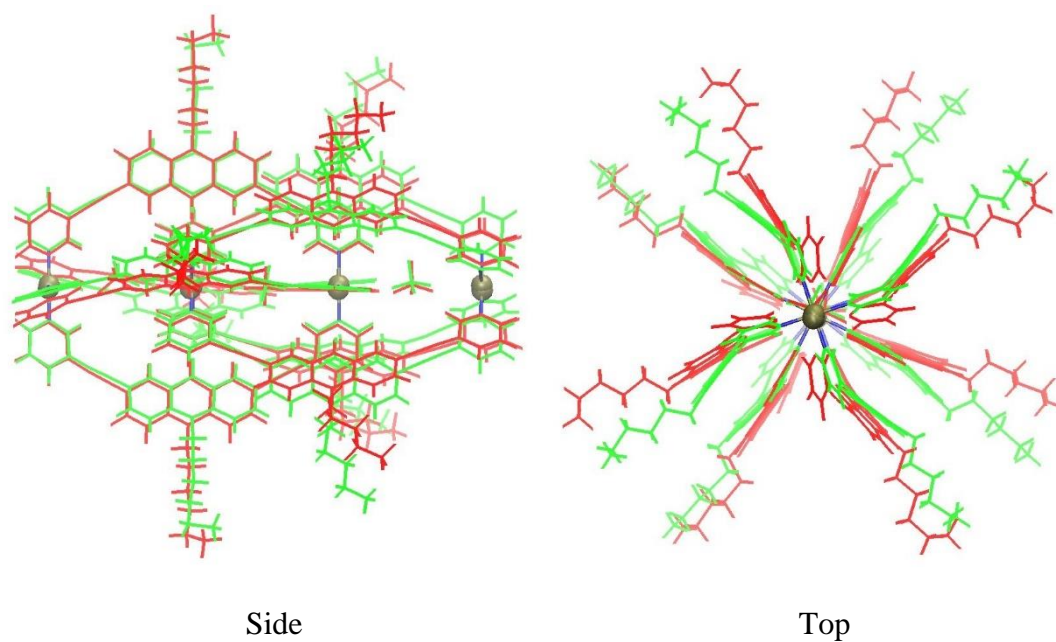


Fig. S1 The superposition of optimized structure obtained with the GEBF-M06-2X method and crystal structure for $\text{Pd}_4\text{L}_8(\text{BF}_4)_3$.

Table S4 Comparison of Pd-N bond lengths (in Å) optimized with the GEBF-M06-2X method and corresponding bond lengths in the crystal structure for Pd₄L₈(BF₄)₃. The LANL2DZ basis set is used for Pd atoms and the 6-31G** basis set is used for H, C, N atoms in the GEBF-M06-2X calculations.

Pd ²⁺ center	GEBF-M06-2X	Crystal
1	2.08, 2.07, 2.08, 2.07	2.03, 2.03, 2.03, 2.03
2	2.06, 2.06, 2.06, 2.06	2.02, 2.02, 2.02, 2.02
3	2.06, 2.06, 2.06, 2.06	2.03, 2.03, 2.03, 2.03
4	2.09, 2.07, 2.07, 2.08	2.01, 2.01, 2.01, 2.01

Cartesian coordinates of $M_7(\text{timb})_2(\text{tim})_2$			
Pd	9.035869	3.028885	-0.016511
Pd	-6.376541	-2.721148	4.573871
Pd	3.513254	-5.522422	5.147976
Pd	-1.774475	6.455604	-5.177649
Pd	-1.717041	6.345369	5.332263
Pd	3.429270	-5.424774	-5.307663
Pd	-6.450442	-2.628172	-4.540850
C	0.790329	3.210755	-6.531106
H	1.156786	2.535441	-7.289156
N	3.546584	-1.095746	5.304600
C	2.568846	2.450429	4.888214
N	-0.060927	-5.421797	2.387946
N	-4.925849	0.920031	2.443896
N	3.478872	-0.996039	-5.370683
C	2.542004	1.091806	5.205370
H	1.698124	0.674221	5.743990
N	-4.969129	0.979105	-2.381288
N	1.488908	3.267263	5.366285
C	6.188041	4.080688	-3.216923
H	5.802370	4.748054	-3.972579
N	3.396559	-3.305288	5.365667
N	-0.239645	4.833106	-5.379325
C	3.576581	3.045709	-4.124451
H	3.610577	4.097326	-3.859682
N	-4.124726	3.840177	-2.380588
N	-4.087419	3.778274	2.503030
C	-4.309718	3.059678	1.285648
N	7.422779	3.065006	-1.641943
N	-4.484066	-3.436749	-3.706275
C	4.643003	0.852144	-4.166286
H	5.517316	0.230982	-3.997271
N	-4.420595	-3.514876	3.718846
C	-0.175207	-5.352723	-0.051527
H	0.757719	-5.908378	-0.064801
N	7.408542	3.063319	1.581752
N	-0.172026	4.728368	5.491919
N	-0.102478	-5.361168	-2.494913
N	1.418823	3.365542	-5.305068
N	1.557918	-5.569073	3.902952
N	-5.658440	-0.729369	3.735484
N	5.785356	2.721182	3.056531
C	-4.124061	3.711605	0.059424
H	-3.877265	4.769317	0.069449
C	-4.609498	-0.091590	4.371352
H	-4.277194	-0.381638	5.357253
C	3.546468	0.355860	-4.879041
C	3.608357	0.266713	4.841956
N	5.749689	2.769728	-3.071564
C	0.879922	3.088964	6.598893
H	1.259631	2.401342	7.339176
C	-4.976140	3.884775	3.563922
H	-5.972934	3.470294	3.528512
N	-3.135388	5.074122	-3.938706
C	2.474043	1.187494	-5.207680
H	1.623028	0.781160	-5.743706
C	-0.759541	-5.068289	1.190458
N	-2.727806	-4.075187	2.397122
N	3.324831	-3.203308	-5.476913
N	-3.078703	4.980744	4.073526
N	-2.767960	-4.017238	-2.424031
C	-3.232482	-3.193025	4.348517
H	-3.207543	-2.773341	5.343473
C	2.505427	2.538538	-4.860048
C	-0.779460	-5.039227	-1.276741
C	-4.329105	3.089293	-1.179260
C	-3.308674	-3.055267	-4.326671
H	-3.302137	-2.585650	-5.299356
C	-2.032816	-4.456401	1.205624
C	4.693979	0.778593	4.123154
H	5.565110	0.161794	3.924465
C	-5.833741	-0.098843	2.592698
H	-6.613835	-0.300899	1.871603
C	3.102958	-1.440279	6.571375
H	2.951257	-0.706440	7.348802
C	-4.759048	1.743959	-1.190536
N	-5.719633	-0.646422	-3.693632
C	3.716393	-2.261734	4.615385
H	4.065443	-2.293139	3.593698
C	-0.140798	3.986698	6.657941
H	-0.825294	4.163172	7.475303
C	-5.865527	-0.050615	-2.528663
H	-6.616607	-0.286359	-1.787541
C	4.687846	2.135500	3.761738
C	4.641921	2.200197	-3.772788
C	-2.244187	-3.397893	-3.550542
H	-1.184426	-3.261331	-3.695257

C	-4.142724	0.920932	3.590247	H	-4.802982	-4.483661	-1.868654
H	-3.343263	1.627722	3.744392	C	-0.648662	-6.009545	-3.595099
C	0.337401	-6.063540	-4.532324	H	-1.655136	-6.400451	-3.596698
H	0.286316	-6.495943	-5.520809	C	-5.038402	3.994619	-3.414008
C	0.818060	4.276748	4.737407	H	-6.040752	3.594893	-3.365796
H	1.082355	4.634217	3.752453	C	7.205798	4.245697	-2.330496
C	0.760784	4.365378	-4.648193	H	7.803028	5.131222	-2.165672
H	1.041082	4.704636	-3.661245	C	-4.090583	-4.049882	2.561639
C	2.925234	-2.669578	-6.687902	H	-4.777753	-4.464355	1.837050
H	2.603492	-3.283470	-7.516421	C	3.022540	-1.312852	-6.640161
C	-4.738454	1.714242	1.268608	H	2.864273	-0.562488	-7.400356
C	-4.411794	4.744295	-4.363340	C	7.226022	4.216185	2.324906
H	-4.804456	5.060408	-5.318195	H	7.810978	5.110176	2.163356
C	-4.338084	4.615776	4.519925	C	-4.935820	1.093189	0.033128
H	-4.711523	4.895687	5.493710	H	-5.171250	0.035046	0.023781
C	-2.052904	-4.428135	-1.254179	C	1.200463	-5.070043	-2.818955
C	3.629612	2.973918	4.149005	H	1.867954	-4.558735	-2.140078
H	3.661467	4.031362	3.907916	C	-4.704304	0.026859	-4.347172
C	6.238782	4.021432	3.240132	H	-4.404300	-0.228685	-5.352870
H	5.881341	4.660498	4.033541	N	5.223208	-5.614134	6.374897
C	-2.991189	4.521512	-2.750820	N	5.117977	-5.504072	-6.563875
H	-2.110987	4.569298	-2.125851	N	10.597136	3.124791	1.391308
C	-4.226048	1.024176	-3.553670	N	10.631960	3.048316	-1.407311
H	-3.441426	1.745496	-3.715433	N	-8.179976	-1.858833	-5.428641
C	6.538204	2.186368	2.042115	N	3.784509	-7.627315	5.047417
H	6.407170	1.176141	1.683299	N	-0.564481	7.664964	6.517991
C	6.541412	2.200757	-2.106590	N	-3.155421	8.051706	-5.177261
H	6.429095	1.176416	-1.782693	N	-6.967362	-4.516043	5.471631
C	-0.580604	-6.118946	3.470790	N	-7.073824	-4.421627	-5.412147
H	-1.580217	-6.527492	3.471325	N	3.671859	-7.534594	-5.272712
C	1.240811	-5.118555	2.705087	N	-0.617814	7.791862	-6.340996
H	1.888632	-4.569309	2.036896	C	-0.115208	7.068495	7.807050
C	-2.956150	4.467884	2.865719	H	-0.973109	6.666004	8.350550
H	-2.093847	4.551321	2.219748	H	0.347797	7.850019	8.421142
C	-0.228584	4.112045	-6.558535	H	0.622693	6.289774	7.617831
H	-0.924846	4.304852	-7.362192	C	3.007901	-2.797848	6.591324
C	0.419256	-6.188575	4.392498	H	2.694814	-3.429538	7.409707
H	0.389229	-6.656671	5.365440	N	-3.107940	7.931657	5.369364
C	3.653315	-2.176432	-4.707870	C	-2.304502	9.166175	5.666666
H	4.012398	-2.229786	-3.690593	H	-2.981882	10.000884	5.885407
C	-2.633615	-4.144892	-0.016195	H	-1.741481	9.422863	4.764851
H	-3.565199	-3.590214	-0.003947	C	10.500803	4.092537	-2.460280
N	1.493344	-5.482322	-4.036460	H	9.672128	3.844563	-3.123117
C	-4.132111	-4.017756	-2.577663	H	11.423173	4.123828	-3.052681

H	10.356614	5.072397	-1.999069	H	5.529530	-5.684529	-8.643791
N	-8.138774	-1.981247	5.417884	C	-1.440411	9.023768	-6.622843
C	-5.846875	-5.152639	6.214630	H	-0.770501	9.870909	-6.810768
H	-5.437286	-4.446524	6.939823	H	-2.006475	8.856196	-7.541566
H	-5.077406	-5.466825	5.508848	C	-4.168914	7.857736	-6.258694
H	-6.222153	-6.031359	6.752412	H	-3.694289	7.584513	-7.201370
C	-4.117096	7.705139	6.448247	H	-4.735617	8.785239	-6.402137
H	-4.809392	6.924919	6.135681	H	-4.868333	7.077613	-5.962386
H	-4.692311	8.623812	6.613148	C	10.783872	4.541301	1.832837
H	-3.637771	7.416191	7.383885	H	10.825255	5.219551	0.980037
C	-1.394797	8.884406	6.829764	H	11.718694	4.627741	2.399450
H	-1.956355	8.692582	7.746598	H	9.962418	4.822979	2.490390
H	-0.730300	9.732105	7.033668	C	6.190979	-4.508483	6.148614
C	2.582611	-8.435952	5.387761	H	6.452390	-4.462567	5.089686
H	2.179544	-8.116726	6.351889	H	7.097440	-4.703361	6.733205
H	2.867129	-9.492021	5.465369	H	5.756079	-3.565728	6.479204
H	1.837276	-8.338476	4.599200	C	-2.343216	9.286354	-5.450077
C	2.452845	-8.311384	-5.626545	H	-3.014791	10.131095	-5.647148
H	1.716425	-8.225673	-4.828207	H	-1.774653	9.518259	-4.544983
H	2.717850	-9.369348	-5.739988	C	11.917773	3.295323	-0.659038
H	2.046504	-7.955154	-6.576174	H	12.758934	2.905339	-1.244785
C	-7.781088	-1.143020	6.599204	H	12.062323	4.374653	-0.571701
H	-7.239079	-1.730797	7.340923	C	5.906802	-6.911332	6.046291
H	-8.696331	-0.753600	7.059496	H	6.409538	-6.786899	5.083213
H	-7.164819	-0.305400	6.267386	H	6.677755	-7.117149	6.798948
C	0.631068	8.062412	5.724244	C	10.672332	1.709091	-2.057733
H	0.327982	8.589634	4.818179	H	9.716233	1.526085	-2.551536
H	1.199510	7.168280	5.464224	H	10.867109	0.931324	-1.317809
H	1.261659	8.725941	6.326290	H	11.471660	1.692202	-2.807445
C	11.831198	2.632920	0.687057	C	10.371051	2.274089	2.588575
H	12.714176	2.857116	1.298249	H	10.199074	1.242062	2.277107
H	11.754739	1.545565	0.601491	H	9.518265	2.653197	3.151955
C	-2.182027	-3.522657	3.548027	H	11.260627	2.308909	3.228491
H	-1.118621	-3.416030	3.691130	C	-3.817884	8.138235	4.081236
C	4.804553	-5.600024	7.810730	H	-3.087538	8.273464	3.281276
H	4.014885	-6.328059	7.998999	H	-4.441769	9.036794	4.151617
H	4.457218	-4.601733	8.073038	H	-4.459205	7.282005	3.871931
H	5.666416	-5.840912	8.443797	C	-3.860643	8.237135	-3.883194
C	4.880859	-8.009624	6.006427	H	-3.127324	8.350187	-3.082533
H	4.433198	-8.178903	6.988233	H	-4.508529	7.382270	-3.689369
H	5.325542	-8.960442	5.689688	H	-4.477571	9.141762	-3.933557
C	4.679853	-5.447999	-7.992819	C	-8.679883	-2.872252	-6.426570
H	4.343057	-4.438669	-8.225209	H	-9.731794	-2.666559	-6.659463
H	3.877729	-6.160463	-8.188063	H	-8.112052	-2.741568	-7.351049

C	4.198215	-7.945413	3.653799	C	-6.195068	-4.700367	-6.585033
H	5.132914	-7.437816	3.410055	H	-5.163664	-4.796911	-6.240765
H	3.410946	-7.624767	2.968443	H	-6.267094	-3.897464	-7.319539
H	4.344652	-9.026650	3.551558	H	-6.505040	-5.639278	-7.057950
C	-0.178490	7.219076	-7.644144	C	-8.505047	-4.252975	-5.852202
H	-1.041497	6.834542	-8.192541	H	-8.753662	-5.026452	-6.589338
H	0.553965	6.430869	-7.474102	H	-9.145863	-4.415760	-4.981848
H	0.288184	8.009631	-8.243671	C	-7.446615	-5.447051	4.411770
C	-6.995984	-5.561962	-4.462370	H	-8.300400	-5.019795	3.884373
H	-5.951437	-5.753832	-4.214667	H	-7.750940	-6.396660	4.866844
H	-7.418911	-6.457544	-4.933077	H	-6.631505	-5.636100	3.710611
H	-7.573309	-5.333313	-3.564258	C	6.101370	-4.415531	-6.322465
C	-9.199504	-1.624803	-4.367170	H	5.672204	-3.459686	-6.621480
H	-9.446978	-2.557445	-3.858819	H	6.997233	-4.604541	-6.925073
H	-10.111254	-1.216219	-4.817917	H	6.378236	-4.400567	-5.266594
H	-8.805142	-0.902161	-3.650329	C	-8.916958	-1.157734	4.456377
C	4.093404	-7.903719	-3.894199	H	-9.139800	-1.744720	3.563097
H	3.318395	-7.591918	-3.191031	H	-8.344399	-0.265397	4.201287
H	5.038987	-7.419682	-3.644423	H	-9.862610	-0.852966	4.920290
H	4.222374	-8.989917	-3.827767	C	4.752692	-7.904471	-6.254276
C	-7.914532	-0.579877	-6.140964	H	5.190302	-8.867934	-5.967143
H	-7.116944	-0.722859	-6.872972	H	4.291787	-8.044208	-7.234490
H	-7.638534	0.187306	-5.416948	C	5.790700	-6.817132	-6.278383
H	-8.822452	-0.265321	-6.669065	H	6.550050	-7.011294	-7.045736
C	-8.078597	-4.206848	6.442356	H	6.306500	-6.724140	-5.318543
H	-8.631690	-5.126496	6.668882	C	-8.977064	-3.160229	5.839572
H	-7.624542	-3.864171	7.375254	H	-9.740708	-2.828883	6.554054
C	0.584028	8.164653	-5.544949	H	-9.498095	-3.533778	4.954435
H	1.147167	7.261497	-5.305259				
H	0.288447	8.675983	-4.627352				
H	1.216767	8.835540	-6.136534				

Cartesian coordinates of Fe ₂ Zn ₂ (RuL ₂) ₂			
N	-1.873693	0.053628	-8.317410
C	-2.611013	-0.784257	-9.047538
C	-2.057556	-1.840217	-9.765608
C	-0.681479	-2.027598	-9.717344
C	0.094771	-1.160013	-8.953209
C	-0.532901	-0.127414	-8.266741
C	0.197042	0.887389	-7.461509
C	1.475543	0.754008	-6.929158
C	1.989918	1.780700	-6.120271
C	1.198432	2.922832	-5.910112
C	-0.077423	2.980430	-6.459651
N	-0.542514	1.974729	-7.210255
C	-1.094420	4.036791	-6.211295
C	-0.783538	5.304940	-5.736771
C	-1.812520	6.226039	-5.554147
C	-3.117242	5.847968	-5.846333
C	-3.347081	4.559054	-6.319257
N	-2.366635	3.672879	-6.501115
C	3.293305	1.654215	-5.430706
C	4.139206	2.765066	-5.340138
C	5.324748	2.675145	-4.620888
C	5.653261	1.494559	-3.963153
C	4.820491	0.370296	-4.037442
C	3.649243	0.456776	-4.796443
C	5.178671	-0.864585	-3.291126
C	5.561658	-0.783574	-1.947180
C	5.937690	-1.919937	-1.242865
C	5.971145	-3.176702	-1.859988
C	5.580723	-3.253432	-3.203851
C	5.179348	-2.120770	-3.903910
H	-3.679821	-0.588861	-9.063236
H	-2.694668	-2.483131	-10.361051
H	-0.211538	-2.826594	-10.280713
H	1.173666	-1.262534	-8.922336
H	2.068110	-0.136297	-7.110822
H	1.557355	3.708469	-5.254377
H	0.246172	5.579962	-5.537824
H	-1.593694	7.227548	-5.199300
H	-3.944310	6.537202	-5.724140
H	-4.348735	4.220671	-6.570808
H	3.887250	3.685514	-5.858717
H	5.995537	3.526128	-4.576104
H	6.578779	1.429047	-3.399331
H	2.979041	-0.399460	-4.830902
H	5.548452	0.179997	-1.445525
H	6.203463	-1.829272	-0.194179
H	5.642382	-4.202916	-3.726243
H	4.923192	-2.202686	-4.956715
N	-2.675732	0.859469	-5.510109
C	-1.711360	0.572775	-4.632679
C	-1.965501	-0.017593	-3.399368
C	-3.279754	-0.320665	-3.068587
C	-4.290089	-0.027029	-3.977499
C	-3.957682	0.564540	-5.192034
C	-4.967510	0.930912	-6.219814
C	-6.338656	0.750022	-6.110726
C	-7.179391	1.187861	-7.146378
C	-6.587194	1.785826	-8.271696
C	-5.202766	1.937725	-8.317838
N	-4.438704	1.510745	-7.303718
C	-4.407600	2.567101	-9.409546
C	-4.966167	3.073686	-10.576439
C	-4.130777	3.654395	-11.529374
C	-2.764360	3.710428	-11.286517
C	-2.278321	3.179105	-10.094239
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C	-8.646285	1.065895	-7.001099
C	-9.475689	2.099499	-7.448169
C	-10.845120	2.026676	-7.222713
C	-11.389540	0.933211	-6.560136
C	-10.586150	-0.133379	-6.128761
C	-9.209540	-0.045954	-6.360718
C	-11.189772	-1.306584	-5.441068
C	-12.519404	-1.673351	-5.687090
C	-13.102763	-2.746536	-5.025565
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C	-11.036103	-3.164313	-3.880132
C	-10.462535	-2.071462	-4.520375
H	-0.697079	0.829380	-4.925624
H	-1.146763	-0.224019	-2.720646
H	-3.519450	-0.775652	-2.113596
H	-5.323197	-0.249709	-3.739858
H	-6.779832	0.320096	-5.219563
H	-7.212058	2.114667	-9.094512
H	-6.035122	3.020245	-10.747599
H	-4.545664	4.056690	-12.447423

H	-2.081133	4.154153	-12.001123	N	-3.526214	-16.272577	-3.552929
H	-1.218275	3.197872	-9.857755	C	-9.188334	-14.039127	-4.350284
H	-9.052353	2.979564	-7.922743	C	-10.077403	-15.094110	-4.115470
H	-11.489133	2.838169	-7.543279	C	-11.387390	-14.825156	-3.738588
H	-12.454778	0.918752	-6.356497	C	-11.808032	-13.510671	-3.568929
H	-8.571158	-0.879448	-6.079967	C	-10.936898	-12.437551	-3.798676
H	-13.103206	-1.136366	-6.427524	C	-9.629714	-12.716622	-4.208704
H	-14.131070	-3.017864	-5.245083	C	-11.410769	-11.045479	-3.580805
H	-10.456168	-3.737381	-3.162091	C	-12.123572	-10.720466	-2.420751
H	-9.442054	-1.792718	-4.273213	C	-12.615275	-9.437196	-2.221029
C	-12.996733	-4.685706	-3.443922	C	-12.434732	-8.434480	-3.182450
C	-12.407353	-5.948154	-3.544201	C	-11.712549	-8.761339	-4.337948
C	-14.201665	-4.547670	-2.749022	C	-11.200089	-10.040120	-4.529469
C	-13.024424	-7.080241	-3.001092	H	-1.525440	-12.699061	-6.960605
H	-11.465530	-6.047096	-4.077196	H	-2.210799	-11.280685	-8.897435
C	-14.823333	-5.656134	-2.164254	H	-4.657525	-11.025312	-9.389404
H	-14.668708	-3.568748	-2.677472	H	-6.301272	-12.200097	-7.934173
C	-14.231889	-6.914854	-2.313112	H	-7.549781	-12.767076	-6.139351
H	-14.733630	-7.782886	-1.895070	H	-7.621969	-15.933113	-3.236091
C	6.451281	-4.382517	-1.131705	H	-6.434742	-17.777690	-2.738243
C	5.980425	-5.657465	-1.463941	H	-4.859043	-19.316468	-1.579655
C	7.432064	-4.272774	-0.138990	H	-2.397484	-18.862262	-1.731170
C	6.512032	-6.802970	-0.867636	H	-1.628406	-16.876661	-3.035592
H	5.206673	-5.771593	-2.218032	H	-9.755217	-16.121069	-4.260991
H	7.849105	-3.297996	0.097267	H	-12.084844	-15.641117	-3.584172
C	7.503216	-6.666605	0.108866	H	-12.833540	-13.304509	-3.278123
H	7.897402	-7.555687	0.594064	H	-8.934963	-11.891828	-4.351298
N	-3.450938	-13.177583	-6.416647	H	-12.278822	-11.479420	-1.659318
C	-2.573466	-12.547425	-7.202306	H	-13.139548	-9.208594	-1.298406
C	-2.962075	-11.756073	-8.278122	H	-11.594097	-8.020796	-5.122691
C	-4.318183	-11.615865	-8.545331	H	-10.683262	-10.278014	-5.455136
C	-5.238932	-12.265365	-7.728426	N	-3.192783	-13.192586	-3.274336
C	-4.779641	-13.042251	-6.670848	C	-4.300152	-12.700784	-2.710576
C	-5.693650	-13.810142	-5.782460	C	-4.268400	-11.800911	-1.652216
C	-7.049656	-13.561232	-5.595830	C	-3.032418	-11.398020	-1.163342
C	-7.772403	-14.329683	-4.669268	C	-1.876660	-11.903377	-1.747387
C	-7.095518	-15.355114	-3.987513	C	-1.978976	-12.803315	-2.804563
C	-5.736437	-15.550922	-4.208418	C	-0.788828	-13.401590	-3.467745
N	-5.075555	-14.776179	-5.083402	C	0.532550	-13.137943	-3.135660
C	-4.863613	-16.506902	-3.473539	C	1.568803	-13.797268	-3.814259
C	-5.367198	-17.591700	-2.765478	C	1.223007	-14.706376	-4.826614
C	-4.484285	-18.456232	-2.123982	C	-0.120407	-14.934419	-5.121989
C	-3.119810	-18.209378	-2.206748	N	-1.077881	-14.281900	-4.441526
C	-2.685187	-17.105396	-2.933292	C	-0.655781	-15.868639	-6.153548

C	0.164178	-16.641631	-6.968079	H	-19.167525	-6.976115	-1.158824
C	-0.410784	-17.498382	-7.904080	C	-19.925877	-4.996762	0.518942
C	-1.794599	-17.559420	-8.001004	C	-21.064000	-5.136135	-0.287718
C	-2.556840	-16.757521	-7.155964	C	-20.100315	-4.657979	1.865781
N	-2.012892	-15.932932	-6.256187	C	-22.338981	-4.937299	0.226710
C	2.974315	-13.561346	-3.414136	H	-20.940538	-5.379698	-1.338320
C	3.873532	-14.631319	-3.370435	C	-21.383477	-4.450430	2.392297
C	5.166854	-14.422522	-2.906134	H	-19.225430	-4.544844	2.502600
C	5.567464	-13.158496	-2.489882	H	-23.206847	-5.052085	-0.413528
C	4.697290	-12.059828	-2.553163	C	-21.606581	-4.127905	3.821758
C	3.398022	-12.284958	-3.020760	C	-22.604042	-3.215557	4.197400
C	5.150830	-10.707870	-2.126416	C	-20.883147	-4.760986	4.842609
C	6.505143	-10.353808	-2.188543	C	-22.857551	-2.985289	5.546313
C	6.942360	-9.105617	-1.762227	H	-23.159006	-2.695627	3.425958
C	6.037720	-8.150348	-1.287831	C	-21.195272	-4.489241	6.171893
C	4.682183	-8.491647	-1.242143	H	-20.124333	-5.488022	4.578226
C	4.250191	-9.752217	-1.639169	N	-22.157065	-3.617511	6.495822
H	-5.243593	-13.047849	-3.123300	C	-23.913866	-2.059594	6.058782
H	-5.195325	-11.436264	-1.226190	C	-24.783465	-1.366917	5.221703
H	-2.964394	-10.702671	-0.333947	C	-25.756559	-0.546011	5.786372
H	-0.904330	-11.604544	-1.375858	H	-24.719367	-1.464368	4.144931
H	0.783788	-12.460355	-2.328700	H	-26.446542	-0.001510	5.150320
H	2.008356	-15.212972	-5.376092	C	-20.547332	-5.158356	7.340976
H	1.242450	-16.582494	-6.878010	C	-19.599209	-6.169354	7.204192
H	0.216962	-18.108909	-8.544178	C	-19.076679	-6.764096	8.348044
H	-2.283660	-18.213661	-8.713285	H	-19.280135	-6.504526	6.225225
H	-3.641577	-16.770260	-7.192477	C	-20.457085	-5.318487	9.647871
H	3.553945	-15.630904	-3.649227	H	-18.345361	-7.560335	8.260255
H	5.859809	-15.254520	-2.845080	H	-20.834642	-4.949198	10.598275
H	6.567108	-13.029002	-2.089599	C	-19.509713	-6.334724	9.596713
H	2.717717	-11.443679	-3.125008	H	-19.133649	-6.777292	10.511175
H	7.229373	-11.048126	-2.601701	N	-23.992579	-1.950401	7.399641
H	7.996273	-8.852967	-1.831242	N	-20.961918	-4.746300	8.553354
H	3.967002	-7.770131	-0.857195	C	7.955808	-5.401616	0.500097
H	3.198654	-10.004465	-1.536886	C	8.997095	-5.252457	1.553094
C	-16.108602	-5.506909	-1.427896	C	10.106677	-6.104843	1.594281
C	-16.316249	-4.452354	-0.531017	C	8.907771	-4.242358	2.518866
C	-17.153358	-6.416848	-1.628654	C	11.106506	-5.928847	2.542429
C	-17.531701	-4.302541	0.130792	H	10.208937	-6.889987	0.851190
H	-15.516053	-3.740036	-0.351130	C	9.904074	-4.071055	3.475769
C	-18.370154	-6.261497	-0.977169	H	8.046269	-3.580694	2.518048
H	-17.024164	-7.234799	-2.331224	H	11.964300	-6.594847	2.542803
C	-18.583997	-5.196415	-0.093220	H	9.827960	-3.257088	4.191602
H	-17.679692	-3.457523	0.797823	C	11.029859	-4.900870	3.490867

C	12.169792	-4.666941	4.419428	C	-4.581421	-5.528275	31.252960
C	12.001376	-4.400029	5.782932	C	-5.097459	-6.547085	30.460301
C	13.472615	-4.698985	3.901466	C	-4.239836	-7.592379	29.839006
C	13.109879	-4.158035	6.607960	C	-2.877620	-7.482754	29.578376
H	10.996079	-4.370161	6.198061	C	-2.214521	-8.528801	28.915883
C	14.575848	-4.463836	4.711635	C	-2.953924	-9.675417	28.580000
H	13.615302	-4.887651	2.842082	C	-4.316236	-9.723125	28.855911
C	14.398519	-4.186410	6.060859	N	-4.919643	-8.687220	29.461080
H	15.575060	-4.496436	4.291290	C	-5.251349	-10.802428	28.436271
H	15.265107	-4.035174	6.697451	C	-4.821216	-12.078258	28.090801
C	12.970543	-3.919134	8.063679	C	-5.761171	-13.038925	27.727369
C	13.788945	-2.983639	8.714854	C	-7.106949	-12.694747	27.715220
C	12.071655	-4.656703	8.848127	C	-7.466976	-11.399683	28.074173
C	13.702036	-2.831447	10.095423	N	-6.571141	-10.474136	28.428045
H	14.474065	-2.384703	8.127123	C	-0.798591	-8.413790	28.498960
C	12.044165	-4.459328	10.225720	C	0.040898	-9.531624	28.563906
H	11.447099	-5.403886	8.372924	C	1.345037	-9.446727	28.091899
N	12.841555	-3.561433	10.815680	C	1.808995	-8.261385	27.531962
C	11.187658	-5.239162	11.170678	C	0.988297	-7.128148	27.457469
C	10.375501	-6.294069	10.761843	C	-0.312438	-7.213602	27.963006
C	9.642104	-6.990895	11.716912	C	1.505867	-5.882251	26.833776
H	10.324917	-6.585871	9.720206	C	2.194206	-5.936591	25.616215
C	10.566502	-5.551697	13.378097	C	2.727921	-4.788198	25.045750
H	9.014987	-7.824346	11.419320	C	2.615252	-3.544782	25.680702
H	10.681004	-5.221813	14.407867	C	1.917592	-3.493785	26.894874
C	14.544258	-1.888793	10.893792	C	1.362546	-4.638489	27.456234
C	15.539710	-1.098284	10.327171	H	-8.321402	-5.938241	30.611462
C	15.025447	-1.068294	13.004646	H	-7.532808	-4.066334	32.063654
C	16.296022	-0.268222	11.150945	H	-5.070214	-3.831744	32.484471
H	15.738258	-1.127057	9.262919	H	-3.515001	-5.471067	31.439351
H	14.786961	-1.092498	14.064918	H	-2.327780	-6.590018	29.855582
H	17.079871	0.351406	10.728161	H	-2.473062	-10.478539	28.032636
C	9.734898	-6.616964	13.052016	H	-3.767133	-12.328100	28.131763
H	9.188463	-7.140257	13.827278	H	-5.444863	-14.043763	27.469172
C	16.038560	-0.250006	12.516395	H	-7.871767	-13.413650	27.445852
H	16.609097	0.377292	13.190953	H	-8.506458	-11.085188	28.089138
N	14.297096	-1.865161	12.218158	H	-0.313556	-10.455020	29.012616
N	11.272827	-4.881882	12.465512	H	2.004237	-10.304638	28.166874
C	-22.501630	-4.588788	1.561230	H	2.830044	-8.198435	27.168475
H	-23.501004	-4.465003	1.967147	H	-0.969176	-6.350945	27.873670
N	-6.434313	-6.670401	30.245821	H	2.299318	-6.889232	25.104751
C	-7.264135	-5.787711	30.808932	H	3.234670	-4.858409	24.088159
C	-6.817898	-4.745605	31.614863	H	1.854881	-2.555536	27.437052
C	-5.453382	-4.617314	31.842246	H	0.867969	-4.576718	28.421767

N	-6.715275	-7.606558	27.241687	H	-17.018008	-5.333611	25.735997
C	-5.582875	-7.363303	26.574562	H	-17.690076	-3.501144	24.255697
C	-5.566292	-6.822613	25.294769	H	-13.622741	-2.997045	23.006174
C	-6.778852	-6.523870	24.687022	H	-12.950842	-4.894726	24.419441
C	-7.960187	-6.772750	25.376081	C	-16.131961	-1.986096	22.650861
C	-7.906423	-7.317839	26.655865	C	-15.539953	-0.729033	22.789266
C	-9.127077	-7.631147	27.447273	C	-17.148245	-2.159714	21.707584
C	-10.432741	-7.424587	27.025267	C	-15.976930	0.363326	22.031765
C	-11.502550	-7.800909	27.851675	H	-14.747324	-0.599200	23.520900
C	-11.204713	-8.370648	29.099707	C	-17.575071	-1.097534	20.902609
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C	-9.391069	-9.158763	30.750908	H	-17.379219	1.007724	20.529596
C	-10.250987	-9.604052	31.748323	C	3.255591	-2.326733	25.114437
C	-9.722660	-10.167917	32.907451	C	2.712487	-1.058325	25.347130
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C	-7.540136	-9.803250	32.003758	C	3.370532	0.098267	24.923895
N	-8.039289	-9.261025	30.889173	H	1.776029	-0.960656	25.889623
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C	-15.459751	-7.449198	26.313287	N	-7.609550	6.534013	27.586742
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C	-16.649427	-3.810018	24.285670	C	-8.954187	6.404119	27.494565
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H	-11.324464	-9.516646	31.628552	C	-5.860529	11.202434	23.536336
H	-10.382443	-10.521473	33.692553	C	-5.741688	10.127507	24.412751
H	-7.891138	-10.705151	33.922691	N	-6.784369	9.383331	24.785697
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H	-16.450112	-7.410514	25.872512	C	-14.807862	6.818809	22.523549
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C	-15.428031	1.724687	22.275620	C	-0.196080	5.546221	26.308833
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C	-14.550251	3.401384	23.803352	C	3.030065	3.621149	26.275466
H	-5.895242	6.082793	28.630522	C	3.560950	2.380562	25.944142
H	-7.073983	4.733727	30.372559	C	2.803616	1.437584	25.241943
H	-9.564631	4.494242	30.219672	C	1.500538	1.783744	24.870069
H	-10.765646	5.608547	28.340753	C	0.982522	3.037216	25.173509
H	-11.483309	6.151536	26.216302	H	-8.511819	6.261281	24.038728
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H	-9.206218	10.974399	23.055271	H	-5.608607	3.787266	22.062728
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H	-15.018336	8.950573	22.354887	H	-4.975294	11.531625	30.476445
H	-15.718611	6.609840	21.970751	H	-7.395176	11.575584	29.823946
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H	-14.842018	4.678562	20.679713	H	-0.230401	8.889831	26.968515
H	-15.625482	2.392629	20.236514	H	2.208532	8.519054	26.832139
H	-15.116445	1.420830	24.385551	H	3.102921	6.303770	26.278380
H	-14.282778	3.690523	24.815996	H	-0.875512	4.702835	26.222133
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C	-7.198167	4.949394	22.938561	H	0.903903	1.072569	24.305734
C	-5.884030	4.517006	22.816593	H	-0.010528	3.295321	24.817266
C	-4.919121	5.037522	23.671782	C	-18.657640	-1.298988	19.901474
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C	-4.336154	6.607188	25.570188	C	-19.754314	-2.117321	20.197156
C	-2.974881	6.350776	25.633115	C	-19.653917	-0.854188	17.727719
C	-2.179128	7.047747	26.556731	H	-17.774826	-0.051664	18.385505
C	-2.806655	7.985520	27.394296	C	-20.783898	-2.290798	19.282879
C	-4.179309	8.199062	27.276650	H	-19.819340	-2.599055	21.167999
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C	-5.005559	9.166242	28.053453	H	-19.616212	-0.335031	16.773837
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C	-5.353925	10.874599	29.700675	C	-21.919735	-1.804668	17.115444
C	-6.695673	10.902048	29.342787	C	-23.213150	-1.778508	17.657018
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H	-20.782836	-2.042685	15.302349	C	11.602726	-2.341237	19.230701
H	-25.325725	-1.911178	17.293745	H	9.448610	-2.164175	19.140260
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C	-23.614738	-3.360597	12.831631	H	11.203836	-1.678809	23.022912
C	-21.929158	-1.658460	12.655096	C	12.727617	-2.302992	20.063834
C	-23.554084	-3.519238	11.450559	H	13.454696	-2.012923	22.063135
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C	-21.930423	-1.860182	11.277327	C	11.811490	-2.566744	17.780801
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N	-22.722675	-2.776767	10.709655	C	11.103871	-1.842467	16.810519
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C	-24.863453	-5.363765	8.586529	N	12.337344	-2.904498	15.073733
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H	-24.623696	-5.365531	7.526282	C	9.869576	-0.222585	14.559289
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C	-19.651290	0.736568	9.708497	C	10.667206	-0.952488	12.056514
H	-20.308437	0.352468	11.718872	H	8.666463	1.284103	13.607293
C	-20.519974	-0.783501	8.089333	H	11.020375	-1.276296	11.080522
H	-19.061008	1.604725	9.981037	C	14.049121	-4.539142	15.390291
H	-20.626685	-1.142927	7.068750	C	14.901454	-5.315767	16.170067
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C	-25.873400	-6.173936	9.094555	H	14.844857	-5.294245	17.251388
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C	5.112115	-1.276289	23.925696	H	9.400456	0.613813	11.303285
C	6.384537	-1.399872	23.163253	C	15.917776	-6.129389	14.153627
C	7.461977	-0.545617	23.425499	H	16.644110	-6.737061	13.627102
C	6.548550	-2.381572	22.178105	N	14.119591	-4.553648	14.044778
C	8.667735	-0.688925	22.751213	N	11.157107	-1.613720	13.106856
H	7.367107	0.216817	24.192772	C	-24.184249	-2.170045	15.493183
C	7.753313	-2.520262	21.495190	H	-25.062969	-2.283478	14.865315
H	5.720888	-3.045666	21.945370	Ru	-6.945488	-8.491811	29.189787
H	9.491161	-0.019660	22.982550	Zn	-22.567975	-3.176320	8.580949
H	7.866407	-3.312033	20.759667	Zn	12.707851	-3.228324	12.957600
C	8.838879	-1.686363	21.782446	Ru	-3.039463	-14.629572	-4.867079
C	10.170499	-1.884979	21.147678	Fe	-2.500097	1.792694	-7.370405
C	10.328984	-2.128901	19.778391	Fe	-6.819263	7.866701	26.201910

C	-25.834365	-0.438740	7.169597
H	-26.580114	0.185368	7.647632
C	-24.927696	-1.162436	7.936888
H	-24.949666	-1.115012	9.022599

Cartesian coordinates of Pd ₄ L ₈ (BF ₄) ₃							
				C	-0.245850	1.726875	-3.777108
				H	-1.199523	2.015752	-4.202922
				C	-0.204905	1.097122	-2.541793
				H	-1.110899	0.879933	-1.985053
				N	0.958008	0.727255	-1.980417
				C	9.449375	2.576582	-9.163185
				H	10.296065	2.034603	-9.588307
				H	8.566009	2.101054	-9.588567
				C	9.515582	4.061914	-9.512530
				H	10.435459	4.480904	-9.088074
				H	8.684911	4.581322	-9.017675
				C	9.460013	4.315350	-11.020209
				H	9.660255	5.377061	-11.200822
				H	10.269152	3.764905	-11.519450
				C	8.121116	3.951333	-11.663584
				H	7.309675	4.455200	-11.118017
				H	7.931022	2.871952	-11.579049
				C	8.050171	4.341601	-13.139396
				H	8.222198	5.420485	-13.231270
				H	8.869524	3.851927	-13.679599
				C	6.715351	3.974011	-13.779814
				H	6.685014	4.266604	-14.831244
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				H	5.886043	4.474185	-13.270325
				N	9.380114	-3.981754	7.119213
				O	9.391505	-2.179682	3.431962
				C	9.397810	-2.725713	4.530660
				C	10.635116	-3.015120	5.265708
				C	10.591853	-3.655139	6.525159
				C	11.817121	-3.954249	7.161451
				H	11.842127	-4.492896	8.098937
				C	13.011981	-3.593215	6.580256
				H	13.943681	-3.836049	7.080336
				C	13.055170	-2.923069	5.340762
				C	11.857646	-2.650432	4.691694
				H	11.857392	-2.146178	3.729298
				C	14.312269	-2.557800	4.774330
				C	15.398581	-2.258356	4.331539
				C	16.664157	-1.919701	3.772161
				C	16.723937	-1.387092	2.480405
				H	15.814155	-1.216721	1.908286
				C	17.866784	-2.119291	4.460440
				H	17.845582	-2.527377	5.465820
				C	19.066838	-1.790104	3.845524
Pd	0.997517	-0.272584	-0.154041				
Pd	17.895704	-0.342620	-0.009167				
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C	10.628876	2.184746	-7.026296				
C	11.872413	2.338613	-7.680031				
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C	13.051190	2.132899	-6.998285				
H	13.996120	2.251891	-7.517655				
C	13.061277	1.777374	-5.633423				
C	11.846145	1.673338	-4.971942				
H	11.799084	1.424550	-3.916021				
C	14.301900	1.521306	-4.976217				
C	15.382328	1.343384	-4.457980				
C	16.648168	1.090909	-3.852438				
C	16.715745	0.632285	-2.532505				
H	15.817675	0.453882	-1.944846				
C	17.849664	1.278855	-4.546528				
H	17.824962	1.630230	-5.572650				
C	19.053602	1.012187	-3.910651				
H	19.999889	1.144601	-4.421819				
C	19.036693	0.565689	-2.597117				
H	19.943587	0.340862	-2.042310				
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C	7.002201	2.556434	-7.722806				
H	6.991185	2.866079	-8.759512				
C	5.800083	2.450596	-7.063159				
H	4.878322	2.653847	-7.597677				
C	5.741876	2.086024	-5.699905				
C	6.934422	1.874246	-5.020204				
H	6.950401	1.619953	-3.964481				
C	4.484763	1.930688	-5.046465				
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H	3.021218	0.649665	-2.099217				
C	0.944460	1.972159	-4.448329				
H	0.947219	2.457844	-5.418195				

H	20.017202	-1.926948	4.348301	N	9.421634	-8.023175	-2.403214
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N	17.888862	-1.086508	1.907623	C	10.672404	-5.959349	-2.065319
C	8.157811	-3.161138	5.188632	C	10.632187	-7.352833	-2.294676
C	8.184963	-3.801356	6.446878	C	11.861179	-8.039795	-2.417293
C	6.957545	-4.248226	6.994347	H	11.889551	-9.093225	-2.660161
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C	5.771345	-4.002105	6.342323	H	13.988589	-7.914962	-2.360766
H	4.840070	-4.344189	6.781127	C	13.095029	-5.988886	-1.986181
C	5.741231	-3.312968	5.110711	C	11.893525	-5.298607	-1.907220
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H	6.972030	-2.399841	3.586161	C	14.349102	-5.335912	-1.794272
C	4.495498	-3.008928	4.488656	C	15.431777	-4.818915	-1.628344
C	3.429859	-2.718183	3.992852	C	16.698005	-4.200105	-1.414074
C	2.180294	-2.325945	3.441106	C	16.755491	-2.878907	-0.960197
C	2.138120	-1.690146	2.193079	H	15.850860	-2.306127	-0.766888
H	3.049103	-1.538431	1.621373	C	17.905670	-4.875250	-1.629828
C	0.971478	-2.528036	4.120959	H	17.889439	-5.902739	-1.977953
H	0.976043	-3.021820	5.086712	C	19.105127	-4.219318	-1.390171
C	-0.214939	-2.087773	3.550301	H	20.059150	-4.711524	-1.539325
H	-1.165745	-2.228642	4.050414	C	19.078841	-2.906707	-0.940206
C	-0.173103	-1.449961	2.320052	H	19.989461	-2.351393	-0.732271
H	-1.073211	-1.078421	1.841320	N	17.918558	-2.269358	-0.737486
N	0.985872	-1.265140	1.665072	C	8.196087	-5.939116	-2.170471
C	9.358049	-4.532967	8.479930	C	8.224542	-7.333508	-2.398074
H	10.179220	-4.086190	9.043402	C	6.992392	-7.995136	-2.626484
H	8.451113	-4.174259	8.966101	H	6.960301	-9.047396	-2.876096
C	9.440686	-6.058330	8.502691	C	5.804435	-7.304977	-2.563165
H	10.391703	-6.365582	8.052220	H	4.871563	-7.830494	-2.736988
H	8.650284	-6.465632	7.858918	C	5.775230	-5.921955	-2.279772
C	9.304358	-6.637424	9.912558	C	6.981033	-5.255818	-2.105396
H	9.518668	-7.710974	9.870948	H	7.017590	-4.187362	-1.915301
H	10.067942	-6.199866	10.570033	C	4.531940	-5.233527	-2.176677
C	7.920145	-6.435098	10.531083	C	3.468919	-4.662510	-2.070787
H	7.156114	-6.813582	9.835754	C	2.220701	-3.996030	-1.932760
H	7.711961	-5.364899	10.670711	C	2.161641	-2.746975	-1.301075
C	7.761697	-7.138359	11.878672	H	3.054480	-2.260927	-0.915625
H	7.945728	-8.211060	11.745802	C	1.024457	-4.553822	-2.406203
H	8.535199	-6.775381	12.566356	H	1.042712	-5.520462	-2.897879
C	6.381580	-6.921009	12.491379	C	-0.166309	-3.860489	-2.239781
H	6.285996	-7.433262	13.450892	H	-1.106364	-4.264969	-2.595802
H	6.191378	-5.856576	12.660855	C	-0.142861	-2.628313	-1.603706
H	5.595922	-7.300454	11.830617	H	-1.048587	-2.051126	-1.448404

N	1.003086	-2.096162	-1.148333	C	8.178128	4.980847	2.808470
C	9.409987	-9.484891	-2.555070	C	8.218403	6.217814	3.489301
H	10.246752	-9.892649	-1.984885	C	6.995143	6.761837	3.954242
H	8.517328	-9.862972	-2.057516	H	6.974029	7.672493	4.538575
C	9.472837	-9.927152	-4.015598	C	5.803324	6.126924	3.691629
H	10.393195	-9.532185	-4.461579	H	4.876799	6.561411	4.051650
H	8.642432	-9.463535	-4.563494	C	5.761981	4.915999	2.966402
C	9.413845	-11.447482	-4.173308	C	6.960101	4.351429	2.549209
H	9.599649	-11.694547	-5.224279	H	6.985137	3.412403	2.004288
H	10.230625	-11.911325	-3.603457	C	4.514657	4.304860	2.651728
C	8.080503	-12.065628	-3.750302	C	3.450069	3.809620	2.354465
H	7.261157	-11.548323	-4.270964	C	2.196801	3.268319	1.960978
H	7.909345	-11.917686	-2.674669	C	2.144416	2.044199	1.280005
C	8.000797	-13.561543	-4.052247	H	3.048806	1.474309	1.080818
H	8.152166	-13.717043	-5.126955	C	0.991166	3.939673	2.209782
H	8.828617	-14.074056	-3.547168	H	1.005381	4.885615	2.740153
C	6.672337	-14.175928	-3.622391	C	-0.203243	3.387247	1.768989
H	6.634960	-15.242736	-3.851631	H	-1.150709	3.882840	1.944266
H	6.516104	-14.059885	-2.545224	C	-0.172621	2.180473	1.086834
H	5.834448	-13.694764	-4.136117	H	-1.079604	1.714557	0.715186
N	9.419372	6.870440	3.689760	N	0.982419	1.534066	0.857239
O	9.391522	3.251268	1.753247	C	9.411873	8.208599	4.296357
C	9.409470	4.323225	2.350640	H	10.244490	8.776939	3.878489
C	10.653143	5.029627	2.673968	H	8.515210	8.721724	3.948982
C	10.624748	6.271182	3.348421	C	9.481351	8.169625	5.822108
C	11.858522	6.881100	3.666202	H	10.436548	7.721895	6.120347
H	11.896951	7.803260	4.229770	H	8.697875	7.498392	6.196917
C	13.045648	6.292465	3.290863	C	9.318124	9.554550	6.451840
H	13.983774	6.773168	3.547499	H	9.545778	9.480783	7.520751
C	13.072618	5.067343	2.593508	H	10.060637	10.245374	6.029940
C	11.867117	4.441986	2.305732	C	7.917004	10.146291	6.286955
H	11.846814	3.484153	1.792928	H	7.175557	9.426210	6.663594
C	14.318226	4.487063	2.214035	H	7.686368	10.305169	5.223656
C	15.389423	4.013660	1.908596	C	7.742858	11.474299	7.022790
C	16.648263	3.439601	1.573029	H	7.954583	11.322608	8.087796
C	16.701939	2.149829	1.033715	H	8.491341	12.187869	6.657735
H	15.792619	1.580990	0.847771	C	6.343983	12.058338	6.850678
C	17.852955	4.120305	1.783854	H	6.239801	13.005726	7.383212
H	17.833565	5.123461	2.197074	H	6.123697	12.243425	5.794642
C	19.052336	3.500683	1.462785	H	5.583446	11.372689	7.236814
H	20.001921	4.001826	1.609760	Pd	9.326698	-0.308880	-0.093260
C	19.024969	2.215005	0.943597	Pd	26.107653	-0.374228	-0.011579
H	19.927192	1.670091	0.679908	N	17.976709	7.489510	-1.351022
N	17.866702	1.573242	0.740800	O	17.895239	3.387805	-1.628452

C	17.913230	4.613818	-1.556374	H	18.929237	9.188910	-0.613954
C	19.162974	5.386411	-1.616474	H	17.201851	9.216758	-0.483177
C	19.156362	6.797976	-1.547669	C	17.930369	9.735642	-2.462402
C	20.391861	7.475785	-1.691445	H	17.000487	9.477467	-2.984981
H	20.435209	8.556163	-1.708348	H	18.747876	9.427748	-3.126501
C	21.564946	6.773706	-1.845311	C	17.993537	11.241455	-2.215239
H	22.499602	7.312785	-1.957163	H	17.179167	11.530351	-1.538566
C	21.574919	5.362234	-1.863962	H	18.929428	11.488825	-1.694004
C	20.364204	4.690170	-1.760659	C	17.906873	12.052381	-3.508252
H	20.310595	3.606136	-1.797847	H	16.935184	11.863733	-3.984595
C	22.802782	4.644628	-1.979779	H	18.670646	11.688706	-4.206889
C	23.845345	4.032449	-2.053564	C	18.086100	13.557784	-3.300789
C	25.036578	3.251697	-2.067588	H	19.079541	13.747414	-2.876063
C	25.074046	2.078250	-1.304969	H	18.072564	14.048385	-4.279221
H	24.213119	1.758154	-0.728282	C	17.016886	14.183824	-2.407653
C	26.180311	3.599337	-2.797941	H	17.131439	15.268889	-2.362553
H	26.184569	4.504845	-3.394781	H	16.013704	13.970459	-2.791847
C	27.294893	2.770880	-2.750010	H	17.071807	13.807980	-1.381575
H	28.192903	3.008539	-3.307831	N	17.780208	-8.116278	2.082064
C	27.250824	1.620719	-1.974797	O	17.805879	-4.026100	1.684759
H	28.094972	0.941410	-1.913785	C	17.790716	-5.246930	1.815992
N	26.157133	1.295272	-1.264047	C	19.022673	-6.033212	1.964540
C	16.693270	5.420282	-1.427387	C	18.983175	-7.435666	2.128178
C	16.755405	6.829432	-1.354413	C	20.207331	-8.113900	2.343342
C	15.537863	7.544516	-1.293012	H	20.229299	-9.178609	2.531812
H	15.525476	8.625811	-1.298162	C	21.399856	-7.426293	2.349314
C	14.333993	6.876664	-1.259216	H	22.325920	-7.964600	2.520435
H	13.410191	7.443422	-1.213224	C	21.438967	-6.031063	2.141947
C	14.273928	5.468302	-1.292032	C	20.241040	-5.353141	1.962196
C	15.462524	4.760092	-1.390563	H	20.216356	-4.276256	1.825481
H	15.468149	3.675747	-1.443726	C	22.673803	-5.318187	2.135293
C	13.014761	4.801132	-1.225581	C	23.704261	-4.683126	2.125196
C	11.934135	4.257492	-1.169525	C	24.896915	-3.907699	2.115096
C	10.656818	3.628263	-1.097680	C	24.985424	-2.794378	1.269631
C	10.561163	2.273247	-0.765719	H	24.166865	-2.539974	0.602319
H	11.445994	1.675736	-0.555576	C	25.993796	-4.205547	2.933643
C	9.470887	4.334536	-1.333272	H	25.954024	-5.067366	3.590826
H	9.518173	5.387333	-1.590773	C	27.115566	-3.387310	2.897266
C	8.253532	3.677917	-1.230204	H	27.977992	-3.589198	3.521385
H	7.318706	4.197982	-1.402609	C	27.120607	-2.290593	2.049347
C	8.241275	2.331302	-0.896778	H	27.965905	-1.612231	1.998585
H	7.321398	1.761983	-0.792312	N	26.073614	-2.017036	1.250973
N	9.379592	1.663701	-0.675100	C	16.547879	-6.026229	1.854600
C	18.014907	8.946548	-1.159033	C	16.576104	-7.430667	2.010879

C	15.340443	-8.112004	2.094918	H	20.303223	-3.167017	-8.730164
H	15.302554	-9.177552	2.275970	C	21.417959	-2.968312	-6.943647
C	14.152988	-7.424560	1.975080	H	22.355269	-3.189788	-7.442734
H	13.214678	-7.965575	2.037729	C	21.417302	-2.714784	-5.554675
C	14.126096	-6.028291	1.778521	C	20.203763	-2.471397	-4.926077
C	15.333215	-5.344854	1.741061	H	20.142991	-2.297807	-3.855772
H	15.363615	-4.266043	1.621347	C	22.638190	-2.700559	-4.818767
C	12.880989	-5.355095	1.601692	C	23.679019	-2.661338	-4.201041
C	11.808821	-4.818790	1.428945	C	24.907125	-2.568171	-3.489416
C	10.545524	-4.198525	1.201823	C	24.976612	-1.782903	-2.331849
C	10.485194	-2.868456	0.772397	H	24.101635	-1.273095	-1.937234
H	11.389075	-2.279275	0.628875	C	26.074126	-3.214128	-3.920118
C	9.339756	-4.888063	1.383189	H	26.048671	-3.828229	-4.813647
H	9.360079	-5.920990	1.714902	C	27.248511	-3.059726	-3.195575
C	8.138170	-4.237820	1.140473	H	28.164689	-3.551751	-3.500094
H	7.186089	-4.737073	1.278648	C	27.240612	-2.257501	-2.063929
C	8.161354	-2.918505	0.710078	H	28.132521	-2.105358	-1.464595
H	7.248028	-2.363858	0.510207	N	26.122118	-1.633830	-1.657521
N	9.318803	-2.269715	0.532961	C	16.545719	-2.235958	-5.741827
C	17.776615	-9.585122	2.131696	C	16.617380	-2.438337	-7.138254
H	18.669741	-9.941056	1.615040	C	15.404462	-2.498436	-7.861976
H	16.939281	-9.938786	1.527491	H	15.398831	-2.707581	-8.923034
C	17.704304	-10.143048	3.550194	C	14.197252	-2.326199	-7.221336
H	16.805619	-9.754784	4.046238	H	13.277267	-2.379901	-7.793696
H	18.557954	-9.769793	4.130022	C	14.128116	-2.090489	-5.832709
C	17.690033	-11.670154	3.560877	C	15.312398	-2.060568	-5.110124
H	16.838991	-12.026887	2.966414	H	15.313051	-1.900457	-4.036372
H	18.594224	-12.050185	3.064839	C	12.868103	-1.890963	-5.194238
C	17.611862	-12.242147	4.976611	C	11.791302	-1.724387	-4.665340
H	16.673323	-11.912571	5.442939	C	10.528488	-1.519252	-4.036879
H	18.423883	-11.812864	5.576730	C	10.475802	-1.124884	-2.695465
C	17.695858	-13.768929	5.029699	H	11.382099	-0.968448	-2.115781
H	18.654984	-14.092875	4.607640	C	9.319756	-1.695999	-4.720815
H	17.702409	-14.080868	6.078878	H	9.332560	-2.001122	-5.761937
C	16.550960	-14.470836	4.301746	C	8.123656	-1.477427	-4.052476
H	16.596796	-15.551547	4.451531	H	7.170192	-1.601564	-4.552514
H	15.581165	-14.123226	4.673475	C	8.156009	-1.087402	-2.720862
H	16.582760	-14.290096	3.223153	H	7.253101	-0.893619	-2.149239
N	17.841691	-2.579149	-7.775256	N	9.315939	-0.921172	-2.072794
O	17.732266	-2.066220	-3.698298	C	17.887909	-2.668872	-9.242092
C	17.758367	-2.226336	-4.915622	H	18.818142	-2.207914	-9.578835
C	19.010869	-2.449382	-5.650199	H	17.095739	-2.032418	-9.640854
C	19.014664	-2.654240	-7.048179	C	17.761506	-4.096029	-9.767867
C	20.252145	-2.941227	-7.673802	H	16.831379	-4.539830	-9.390864

H	18.577278	-4.706556	-9.360526	C	14.107510	1.023781	5.757542
C	17.781365	-4.140927	-11.294246	C	15.302357	1.099236	5.056359
H	16.971602	-3.510073	-11.683137	H	15.311631	1.157865	3.972018
H	18.718777	-3.702347	-11.664104	C	12.853498	0.973665	5.080139
C	17.639206	-5.562681	-11.838466	C	11.779928	0.918575	4.523283
H	16.670367	-5.970998	-11.519953	C	10.520974	0.818321	3.862784
H	18.408622	-6.196187	-11.379687	C	10.478320	0.438451	2.517467
C	17.752159	-5.652828	-13.361697	H	11.396116	0.241204	1.971081
H	18.740014	-5.291856	-13.672757	C	9.308388	1.059675	4.519054
H	17.706880	-6.707260	-13.651973	H	9.314125	1.354142	5.563232
C	16.665028	-4.878080	-14.103974	C	8.117294	0.913982	3.821726
H	16.727321	-5.052002	-15.180251	H	7.158341	1.092777	4.294049
H	15.668525	-5.189643	-13.773073	C	8.158395	0.528998	2.489962
H	16.751682	-3.799286	-13.943444	H	7.251460	0.407177	1.904445
N	17.795434	0.988569	7.806169	N	9.323279	0.299541	1.870087
O	17.754951	1.278951	3.706173	C	17.818321	0.796560	9.263021
C	17.757662	1.206142	4.932141	H	18.717735	0.230640	9.513301
C	19.001779	1.234694	5.714060	H	16.986806	0.141853	9.529141
C	18.985119	1.157601	7.124317	C	17.760652	2.104021	10.048080
C	20.220560	1.263566	7.809431	H	16.844401	2.646886	9.783416
H	20.258611	1.271981	8.890107	H	18.594736	2.747450	9.740869
C	21.401298	1.389480	7.113861	C	17.812222	1.863553	11.555442
H	22.335819	1.472233	7.658471	H	16.982896	1.205624	11.845168
C	21.417973	1.417455	5.702822	H	18.736332	1.325086	11.809959
C	20.208898	1.351382	5.024566	C	17.748469	3.163540	12.357390
H	20.162985	1.394065	3.940502	H	16.785545	3.655510	12.164139
C	22.645698	1.514003	4.983512	H	18.524849	3.845710	11.989095
C	23.678381	1.580472	4.354974	C	17.923316	2.964609	13.864442
C	24.873351	1.626083	3.582818	H	18.910120	2.526477	14.057956
C	24.957305	0.859357	2.413401	H	17.924404	3.946686	14.347819
H	24.125706	0.236136	2.091924	C	16.840542	2.092282	14.496361
C	25.978833	2.408207	3.943037	H	16.952833	2.054972	15.582008
H	25.941591	3.007359	4.846349	H	15.843167	2.488704	14.278122
C	27.107204	2.409033	3.132918	H	16.881669	1.062317	14.129491
H	27.975766	3.007273	3.381290	B	13.548488	-0.214900	0.586156
C	27.113044	1.628955	1.986357	F	14.782926	-0.381263	-0.107991
H	27.967443	1.603383	1.317817	F	12.464937	-0.353903	-0.318771
N	26.056573	0.868913	1.649990	F	13.443139	-1.199019	1.564054
C	16.528335	1.103775	5.726780	F	13.507531	1.059353	1.141390
C	16.578941	1.023848	7.136561	B	5.040399	-0.421414	0.425341
C	15.355766	0.988459	7.842859	F	6.172772	-0.182733	-0.375122
H	15.335713	0.988921	8.924078	F	3.850202	-0.267040	-0.354687
C	14.156305	0.983402	7.165759	F	5.062644	-1.732685	0.896623
H	13.227479	0.953267	7.725393	F	4.998934	0.492945	1.469385

B	22.218181	-0.885525	0.240734
F	23.314670	-0.065906	-0.156467
F	21.006154	-0.232136	-0.059723
F	22.299829	-2.081880	-0.472510
F	22.315289	-1.110810	1.609338