

## SUPPORTING INFORMATION

### **Topology of Metallacalix[4]arenes with Uracil and Cytosine Ligands: Favorable and Unfavorable Assemblies**

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Supporting Information content:

- Figures
- Molecular coordinates

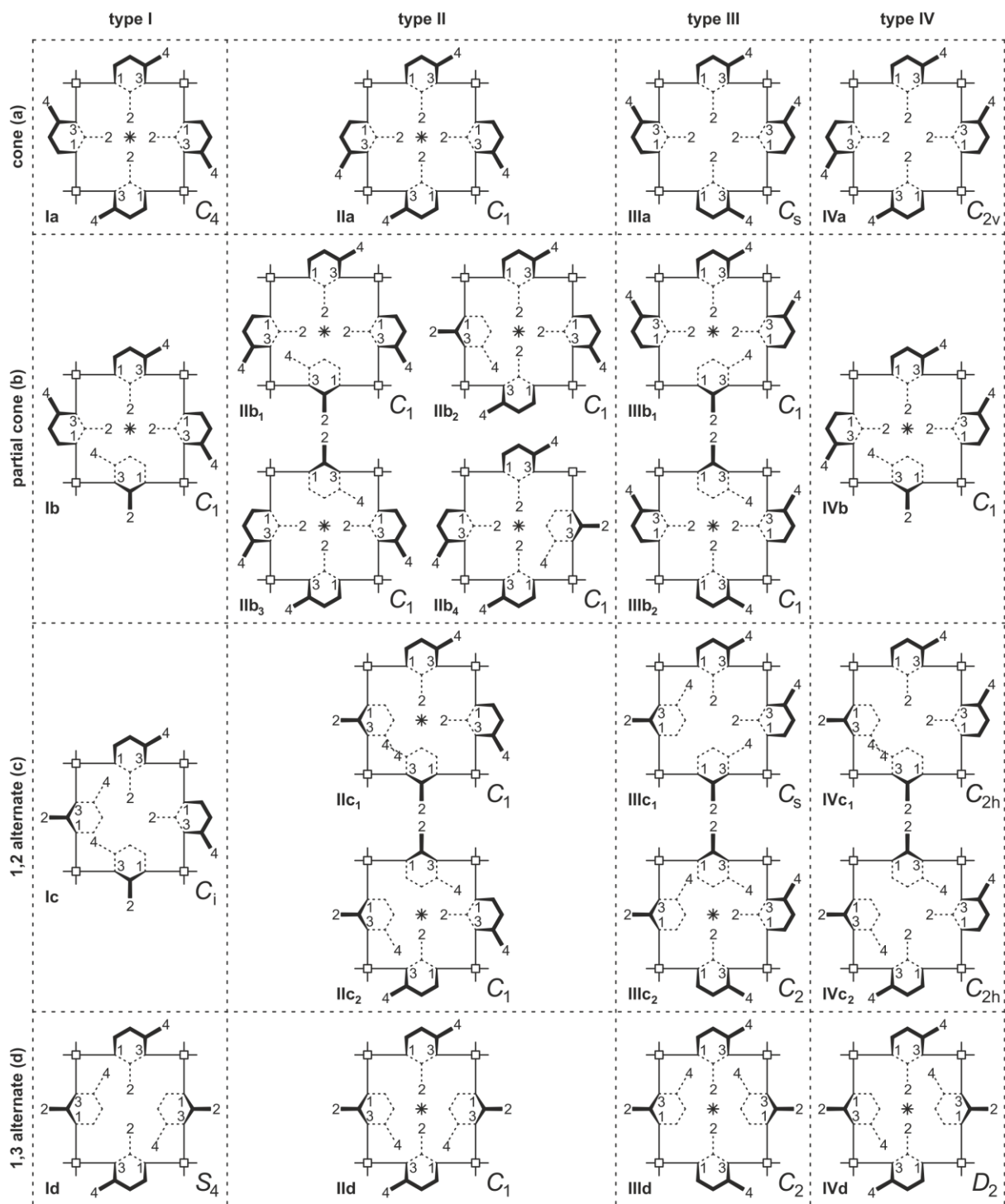


Figure S11. Resume of the possible metallacalix[4]arene isomers.<sup>S1</sup> Exocyclic (2 or 4) sites inside the molecular square point down; while outside placed sites point up (an inverse criterion is likewise valid: inside, up; outside, down). Asterisks in the center of the molecular square denote chirality. Bottom left: isomer numbering (**Ia** to **IVd**). Bottom right: highest symmetric point group.

#### Reference

S1 Adapted from: B. Lippert and P. J. Sanz Miguel, *Chem. Soc. Rev.*, 2011, **40**, 4475–4487.

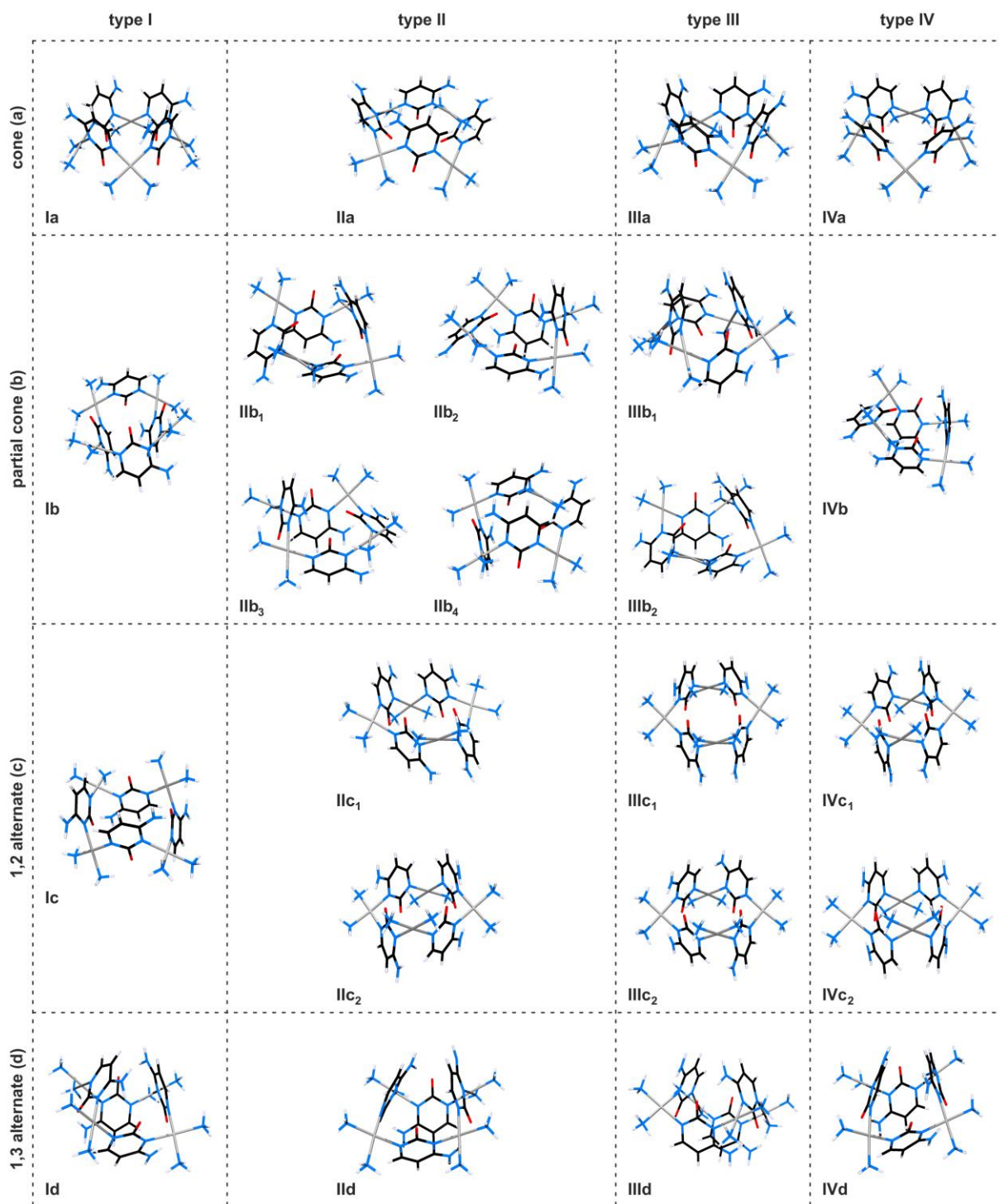


Figure SI2. View of the optimized *cis*-[Pt(NH<sub>3</sub>)<sub>2</sub>(cytosinate)]<sub>4</sub><sup>4+</sup> isomers.

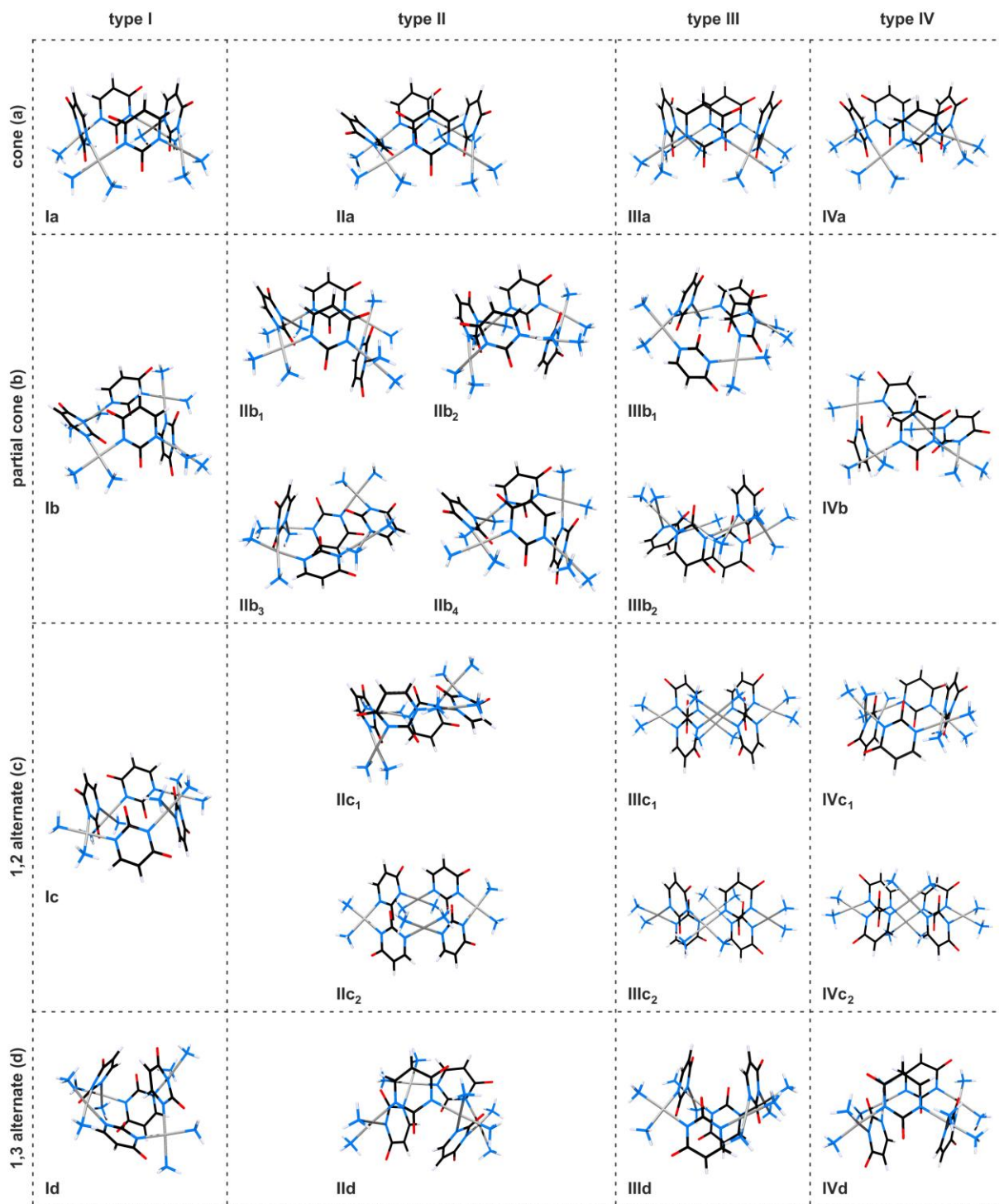


Figure SI3. View of the optimized *cis*-[Pt(NH<sub>3</sub>)<sub>2</sub>(uracilate)]<sub>4</sub> isomers.

## Abbreviations

C = cytosine; U = uracil; N1N1, N1N3, N3N3 = binding sites; hh = head-head conformation; ht = head-tail conformation.

## COORDINATES

<b>Pt–C–N1N1–hh (M11L, SMD water)</b>			
Pt	–0.001986	–1.119458	–0.256266
C	–2.663008	2.154020	–1.027428
C	–1.673822	1.214625	–1.106945
H	–2.795683	2.903158	–1.801381
H	–0.999464	1.188393	–1.960905
N	–1.486002	0.272183	–0.164068
N	–3.348169	1.145375	1.045381
C	2.735527	2.077662	–1.058510
H	2.917848	2.783333	–1.861994
N	3.311975	1.161892	1.090342
N	1.492638	0.257582	–0.158709
C	1.736117	1.149258	–1.137335
H	1.101228	1.085798	–2.019542
C	–3.498864	2.091120	0.105547
C	3.516721	2.060197	0.114552
C	–2.355081	0.237597	0.909341
O	–2.203236	–0.682061	1.778068
C	2.316576	0.257185	0.949878
O	2.122090	–0.630360	1.842447
H	1.177856	–3.492404	–0.185173
H	2.041783	–2.483893	–1.155315
H	2.112190	–2.305272	0.492014
H	–1.191067	–3.489991	–0.230980
H	–2.117891	–2.305748	0.469242
H	–2.048628	–2.459029	–1.182178
N	–1.510615	–2.528191	–0.321726
N	1.502034	–2.533954	–0.294421
N	–4.484549	2.971029	0.286810
N	4.505245	2.936532	0.298871
H	–4.649921	3.710661	–0.372036
H	–5.066955	2.907820	1.103236
H	4.710939	3.641720	–0.385823
H	5.048939	2.905402	1.143525

<b>Pt–C–N1N1–ht (M11L, SMD water)</b>			
Pt	0.000015	1.217698	–0.000032
C	–2.153199	–2.217488	–1.257419
C	–1.258115	–1.196339	–1.113950
H	–2.023354	–2.984345	–2.014380
H	–0.378230	–1.117089	–1.752903
N	–1.403393	–0.231382	–0.184674
N	–3.400101	–1.281007	0.577347
C	2.152146	–2.218661	1.256273
H	2.021459	–2.986187	2.012406
N	3.400686	–1.280751	–0.576598
N	1.403054	–0.231909	0.184124
C	1.257028	–1.197555	1.112572
H	0.376438	–1.119002	1.750657
C	–3.244615	–2.225256	–0.363580
C	3.244546	–2.225577	0.363674
C	–2.485476	–0.288100	0.667137

O	–2.611284	0.625785	1.546890
C	2.485991	–0.288041	–0.666741
O	2.612165	0.626011	–1.546281
H	1.202130	3.573264	–0.163008
H	1.848573	2.721248	1.086584
H	2.232446	2.306847	–0.476076
H	–1.201200	3.572885	0.164680
H	–1.848242	2.722531	–1.085805
H	–2.232568	2.306874	0.476251
N	–1.487492	2.644122	–0.137793
N	1.487675	2.643960	0.138510
N	–4.174316	–3.180207	–0.416671
N	4.174525	–3.180209	0.417266
H	–4.126266	–3.918382	–1.095679
H	–4.939895	–3.165445	0.233896
H	4.125653	–3.919117	1.095419
H	4.940509	–3.165150	–0.232816

<b>Pt–C–N1N3–hh (M11L, SMD water)</b>			
Pt	–0.483509	–1.007741	–0.091526
C	–2.481387	3.209998	0.615759
C	–2.627471	2.676990	–0.642779
H	–2.903448	4.190068	0.840092
C	1.485670	0.959038	–1.087215
H	0.638745	1.205059	–1.728276
C	2.664266	1.644016	–1.176547
H	2.795443	2.458213	–1.881173
H	–3.151221	3.195081	–1.439496
N	3.526956	0.233606	0.573411
N	1.302124	–0.057807	–0.223285
N	–1.842875	2.611973	1.630271
N	–1.400863	0.794174	0.140618
C	3.694389	1.235879	–0.303529
C	–2.047455	1.421802	–0.865410
C	2.336350	–0.406328	0.618819
O	2.149736	–1.357010	1.446953
C	–1.305793	1.386607	1.383172
O	–0.699089	0.752072	2.301860
N	–2.313309	–1.960877	0.030121
H	–2.324678	–2.636138	0.792616
H	–3.062807	–1.292372	0.200489
N	0.486471	–2.821279	–0.286920
H	–0.085605	–3.625044	–0.036359
H	0.831686	–2.965376	–1.232512
H	–2.532904	–2.461063	–0.829297
H	1.279813	–2.758131	0.356249
N	4.887825	1.831491	–0.313657
N	–2.101054	0.809192	–2.051299
H	5.605550	1.518310	0.316201
H	5.087197	2.592054	–0.938304
H	–1.633905	–0.074060	–2.190138
H	–2.563684	1.245385	–2.830031

<b>Pt-C-N1N3-ht (M11L, SMD water)</b>			
Pt	0.566528	-0.996825	-0.045818
C	2.244991	3.406197	0.215039
C	1.361998	3.027337	1.196050
H	2.627681	4.426664	0.195712
C	-1.483891	0.769021	-1.219986
H	-0.635816	1.011330	-1.861373
C	-2.692560	1.388200	-1.367991
H	-2.853822	2.143233	-2.130552
H	1.027572	3.706059	1.973368
N	-3.513542	0.066785	0.472030
N	-1.269095	-0.175093	-0.284056
N	2.701549	2.600335	-0.756029
N	1.328513	0.876906	0.176416
C	-3.714379	0.995100	-0.477679
C	0.904246	1.701984	1.160151
C	-2.294620	-0.507331	0.572700
O	-2.056697	-1.372383	1.479468
C	2.232405	1.325531	-0.763689
O	2.625852	0.497383	-1.648750
N	2.472559	-1.765872	0.141220
H	2.558413	-2.736216	-0.153054
H	3.050486	-1.183485	-0.468668
N	-0.284819	-2.868725	-0.232693
H	0.328933	-3.635083	0.035122
H	-1.091689	-2.852691	0.395315
H	2.822307	-1.696671	1.094026
H	-0.607601	-3.043611	-1.181575
N	-4.930859	1.537135	-0.539239
N	0.069796	1.216574	2.080818
H	-5.642543	1.237883	0.104206
H	-5.154289	2.243078	-1.217580
H	-0.268434	0.266332	2.031523
H	-0.271454	1.812972	2.814740

<b>Pt-C-N3N3-hh (M11L, SMD water)</b>			
Pt	-0.024214	-1.009557	0.034043
C	3.382376	1.577477	0.431345
C	3.247833	2.315448	-0.721314
H	4.174808	1.756941	1.150026
H	3.951212	3.120916	-0.934141
N	2.295526	2.123489	-1.641303
N	1.450440	0.366448	-0.254608
C	-2.331279	2.450930	1.195997
H	-2.301454	3.231556	1.948413
N	-1.423451	0.462161	0.250866
N	-3.367827	1.459212	-0.730693
C	-3.283661	2.411876	0.208414
H	-4.045271	3.190330	0.158049
C	-1.376365	1.422075	1.199799
C	2.432112	0.574202	0.648828
C	-2.430027	0.478320	-0.696744
O	-2.459876	-0.468950	-1.547492
C	1.399556	1.124708	-1.408652
O	0.492699	0.864015	-2.255526
H	-2.242001	-2.141092	-0.380885
H	-1.256743	-3.351940	0.193146
H	-1.949132	-2.293831	1.244805
H	2.282218	-2.175659	-0.437749

H	1.392385	-3.166112	0.529246
H	1.074248	-3.081568	-1.081861
N	-1.537218	-2.382046	0.318596
N	1.343023	-2.531683	-0.266461
N	2.446032	-0.184978	1.751401
N	-0.426949	1.359146	2.133887
H	-0.373930	2.068901	2.843519
H	0.244776	0.609659	2.154810
H	3.173930	-0.064369	2.435038
H	1.800775	-0.951279	1.868547

<b>Pt-C-N3N3-ht (M11L, SMD water)</b>			
Pt	0.002109	0.966766	-0.012906
C	-2.723494	-2.011120	1.395783
C	-3.580211	-2.064217	0.324431
H	-2.883360	-2.591483	2.298039
H	-4.467132	-2.696621	0.372619
N	-3.414276	-1.390955	-0.826374
N	-1.453193	-0.438956	0.148938
C	2.708214	-2.072564	-1.338711
H	2.863042	-2.686266	-2.219455
N	1.447999	-0.450860	-0.147052
N	3.410015	-1.371836	0.856209
C	3.568762	-2.088666	-0.269193
H	4.453364	-2.725581	-0.297299
C	1.601546	-1.213031	-1.253323
C	-1.612547	-1.160780	1.281263
C	2.319991	-0.568391	0.910444
O	2.059955	0.117197	1.956734
C	-2.321341	-0.593438	-0.907143
O	-2.054498	0.048473	-1.978799
H	1.884994	2.453650	-1.056450
H	1.214194	3.311627	0.174804
H	2.259508	2.085974	0.507527
H	-1.971267	2.357600	0.976889
H	-1.143320	3.354131	-0.033831
H	-2.163389	2.221097	-0.653211
N	1.506618	2.379688	-0.114156
N	-1.483253	2.401350	0.084309
N	-0.707992	-1.023680	2.250078
N	0.695297	-1.104125	-2.223675
H	0.792860	-1.660932	-3.055546
H	-0.133493	-0.524445	-2.124385
H	-0.813293	-1.548722	3.101607
H	0.125136	-0.454288	2.132673

<b>Pt-U-N1N1-hh (M11L, SMD water)</b>			
Pt	0.065681	-1.235520	-0.139804
C	-3.303515	1.188313	-1.073293
C	-2.321478	0.243320	-1.088178
H	-3.942330	1.348220	-1.936391
H	-2.132719	-0.379067	-1.964903
N	-1.519032	0.016396	-0.025984
N	-2.657964	1.730624	1.177297
C	1.817409	2.506946	-1.151435
H	1.590744	3.305618	-1.851308
N	3.173421	1.586137	0.603083
N	1.296491	0.374364	-0.231073
C	1.039033	1.390139	-1.085098

H	0.168823	1.260967	-1.730101
C	-3.469994	1.974332	0.109077
O	-4.360526	2.889444	0.188528
C	2.941019	2.605130	-0.276002
O	3.728596	3.612408	-0.294078
C	-1.714204	0.769354	1.113660
O	-0.974396	0.514519	2.128326
C	2.367864	0.508775	0.627495
O	2.585519	-0.445859	1.460874
H	1.537331	-3.432061	0.070158
H	2.114421	-2.525433	-1.175306
H	2.386060	-2.034612	0.396545
H	-0.815860	-3.691303	-0.513241
H	-1.461336	-3.093172	0.876098
H	-2.083796	-2.646137	-0.578197
N	-1.218391	-2.859405	-0.085206
N	1.717646	-2.480171	-0.240291

**Pt-U-N1N1-ht (M11L, SMD water)**

Pt	0.000045	1.174571	-0.000022
C	-2.156671	-2.267845	-1.229923
C	-1.253772	-1.257179	-1.090224
H	-2.013966	-3.048845	-1.971406
H	-0.357106	-1.195176	-1.709820
N	-1.407012	-0.268341	-0.180998
N	-3.429528	-1.289678	0.557134
C	2.156164	-2.268332	1.229519
H	2.013238	-3.049440	1.970844
N	3.429600	-1.289818	-0.556936
N	1.406997	-0.268454	0.180940
C	1.253422	-1.257520	1.089871
H	0.356668	-1.195519	1.709337
C	-3.299333	-2.280961	-0.373344
O	-4.195061	-3.190084	-0.452831
C	3.299007	-2.281386	0.373185
O	4.194858	-3.190363	0.452969
C	-2.506423	-0.315656	0.650630
O	-2.626854	0.616861	1.527709
C	2.506610	-0.315686	-0.650423
O	2.627343	0.617015	-1.527269
H	1.214879	3.529121	-0.172013
H	1.854127	2.683524	1.086336
H	2.230414	2.241791	-0.474263
H	-1.214769	3.529163	0.172103
H	-1.854141	2.683530	-1.086157
H	-2.230253	2.241812	0.474468
N	-1.493133	2.601262	-0.138921
N	1.493236	2.601236	0.139059

**Pt-U-N1N3-hh (M11L, SMD water)**

Pt	-0.506858	-1.000290	-0.036886
C	-2.172852	3.377062	0.374723
C	-2.668099	2.615220	-0.654169
H	-2.464843	4.425205	0.465270
C	1.446828	0.921286	-1.119791
H	0.561692	1.179324	-1.704279
C	2.618543	1.605752	-1.249537
H	2.709466	2.436521	-1.942950
H	-3.357465	3.014505	-1.392329

N	3.571314	0.163454	0.418585
N	1.305249	-0.120818	-0.271592
N	-1.335455	2.933200	1.326719
N	-1.355967	0.828950	0.196221
C	3.731653	1.204714	-0.450184
O	4.865991	1.790412	-0.529795
C	-2.240023	1.271203	-0.752288
O	-2.629709	0.459818	-1.669521
C	2.388295	-0.473677	0.505142
O	2.238166	-1.453451	1.324476
C	-0.948506	1.629411	1.235413
O	-0.197707	1.128529	2.138048
N	-2.396270	-1.828602	0.102955
H	-2.446397	-2.802298	-0.187974
H	-2.780761	-1.760333	1.042021
N	0.406072	-2.847014	-0.265660
H	-0.147085	-3.625455	0.084214
H	0.643480	-3.040058	-1.235558
H	-2.960469	-1.259052	-0.531825
H	1.263758	-2.758222	0.288389

**Pd-U-N1N3-ht (M11L, SMD water)**

Pt	0.485619	-1.001625	-0.030821
C	2.362520	3.303493	0.236064
C	1.504092	2.941395	1.240735
H	2.774991	4.313831	0.208941
C	-1.445106	0.943622	-1.112727
H	-0.556245	1.194138	-1.695047
C	-2.611639	1.636228	-1.246493
H	-2.695196	2.465952	-1.942107
H	1.219503	3.626710	2.033170
N	-3.578944	0.204512	0.422554
N	-1.313496	-0.097315	-0.261650
N	2.770185	2.492804	-0.758486
N	1.366466	0.813160	0.199218
C	-3.729818	1.244524	-0.449366
O	-4.860187	1.837158	-0.533868
C	0.984041	1.622396	1.239419
O	0.207718	1.165006	2.145988
C	-2.400568	-0.440585	0.513518
O	-2.258856	-1.419391	1.335549
C	2.257642	1.234737	-0.754844
O	2.613841	0.400050	-1.662992
N	2.362683	-1.858721	0.107918
H	2.399510	-2.830320	-0.191979
H	2.931870	-1.289556	-0.523479
N	-0.454141	-2.833324	-0.270203
H	0.089165	-3.623123	0.069743
H	-1.308493	-2.738192	0.287623
H	2.748119	-1.804187	1.047358
H	-0.697874	-3.013784	-1.240895

**Pt-U-N3N3-hh (M11L, SMD water)**

Pt	0.002090	-1.000047	0.001768
C	3.380362	1.547304	0.546366
C	3.199241	2.430340	-0.488267
H	4.188369	1.652590	1.263795
H	3.872319	3.282341	-0.603082
N	2.235968	2.333542	-1.419594

N	1.459846	0.399846	-0.251542
C	-2.325659	2.319012	1.352787
H	-2.288785	3.044804	2.159225
N	-1.453119	0.401871	0.257978
N	-3.386444	1.483751	-0.639117
C	-3.275432	2.371037	0.366525
H	-4.021593	3.167904	0.366726
C	-1.369734	1.272825	1.312821
O	-0.469603	1.105947	2.206245
C	2.466255	0.476063	0.674066
O	2.538264	-0.417095	1.595078
C	-2.460658	0.489229	-0.669135
O	-2.527639	-0.411658	-1.580375
C	1.378095	1.280966	-1.300565
O	0.479971	1.097683	-2.190014
H	-2.225338	-2.066333	-0.450998
H	-1.228597	-3.350845	-0.092999
H	-1.879786	-2.460003	1.128693
H	2.226102	-2.085132	0.455397
H	1.218235	-3.357100	0.091571
H	1.878205	-2.466341	-1.125474
N	-1.502445	-2.411465	0.185788
N	1.499776	-2.418669	-0.182917

**Pt-U-N3N3-ht (M11L, SMD water)**

Pt	-0.000036	-0.998733	0.000021
C	2.325666	2.320758	1.350612
C	3.277105	2.372087	0.365867
H	2.286878	3.047752	2.155918
H	4.022470	3.169725	0.366049
N	3.390356	1.483583	-0.638522
N	1.456534	0.401481	0.256973
C	-2.325478	2.320790	-1.350761
H	-2.286603	3.047728	-2.156120
N	-1.456415	0.401607	-0.256901
N	-3.390127	1.483896	0.638534
C	-3.276816	2.372325	-0.365905
H	-4.022101	3.170038	-0.366078
C	-1.369984	1.274224	-1.310164
O	-0.466789	1.108913	-2.200817
C	1.370043	1.274325	1.310037
O	0.466782	1.109246	2.200644
C	-2.465377	0.488365	0.668575
O	-2.534201	-0.413536	1.578755
C	2.465485	0.488165	-0.668515
O	2.534161	-0.413702	-1.578759
H	-1.878533	-2.461222	-1.131789
H	-1.228469	-3.350470	0.091720
H	-2.227042	-2.066566	0.446979
H	1.878342	-2.461429	1.131830
H	1.227860	-3.350771	-0.091395
H	2.226616	-2.067143	-0.447094
N	-1.502681	-2.411564	-0.188344
N	1.502320	-2.411870	0.188439

**Pt-C-Ia (M11L, SMD water)**

Pt	-2.879870	-2.903784	-0.414911
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Pt	2.903784	-2.879870	-0.414911
Pt	2.879870	2.903784	-0.414911
Pt	-2.903784	2.879870	-0.414911
C	0.048037	-4.224352	2.469841
C	-1.168015	-3.999942	1.800158
C	1.193696	-3.833006	1.842248
H	0.066039	-4.711326	3.437365
H	2.167932	-3.997184	2.298617
C	-3.833006	-1.193696	1.842248
C	-4.224352	-0.048037	2.469841
H	-3.997184	-2.167932	2.298617
C	-3.999942	1.168015	1.800158
H	-4.711326	-0.066039	3.437365
C	3.999942	-1.168015	1.800158
C	4.224352	0.048037	2.469841
C	3.833006	1.193696	1.842248
H	4.711326	0.066039	3.437365
H	3.997184	2.167932	2.298617
N	3.247515	1.193696	0.629553
N	1.193696	-3.247515	0.629553
N	-1.171269	-3.356129	0.612161
N	-3.247515	-1.193696	0.629553
N	-3.356129	1.171269	0.612161
C	1.168015	3.999942	1.800158
C	-0.048037	4.224352	2.469841
C	-1.193696	3.833006	1.842248
H	-0.066039	4.711326	3.437365
H	-2.167932	3.997184	2.298617
N	-1.193696	3.247515	0.629553
N	1.171269	3.356129	0.612161
H	-4.585230	1.627031	-1.932580
H	-5.438622	2.536550	-0.857864
H	-4.812143	3.233289	-2.208472
H	-1.475546	4.489926	-1.842265
H	-3.040090	4.761450	-2.266680
H	-2.449929	5.394736	-0.869848
H	3.233289	4.812143	-2.208472
H	1.627031	4.585230	-1.932580
H	2.536550	5.438622	-0.857864
H	5.394736	2.449929	-0.869848
H	4.489926	1.475546	-1.842265
H	4.761450	3.040090	-2.266680
H	-5.394736	-2.449929	-0.869848
H	-4.489926	-1.475546	-1.842265
H	-4.761450	-3.040090	-2.266680
H	-1.627031	-4.585230	-1.932580
H	-2.536550	-5.438622	-0.857864
H	-3.233289	-4.812143	-2.208472
H	2.449929	-5.394736	-0.869848
H	1.475546	-4.489926	-1.842265
H	3.040090	-4.761450	-2.266680
H	4.585230	-1.627031	-1.932580
H	5.438622	-2.536550	-0.857864
H	4.812143	-3.233289	-2.208472
N	4.634329	-2.540373	-1.482575
N	2.423754	-4.577253	-1.477030
N	-2.540373	-4.634329	-1.482575
N	-4.577253	-2.423754	-1.477030
N	-4.634329	2.540373	-1.482575
N	-2.423754	4.577253	-1.477030



N	2.540373	4.634329	-1.482575
N	4.577253	2.423754	-1.477030
N	3.356129	-1.171269	0.612161
C	-0.003296	3.001617	0.003851
O	0.014457	2.462141	-1.136046
C	-3.001617	-0.003296	0.003851
O	-2.462141	0.014457	-1.136046
C	0.003296	-3.001617	0.003851
O	-0.014457	-2.462141	-1.136046
C	3.001617	0.003296	0.003851
O	2.462141	-0.014457	-1.136046
H	-4.277017	3.183899	1.781756
H	-4.894375	2.360620	3.179236
H	3.183899	4.277017	1.781756
H	2.360620	4.894375	3.179236
H	4.894375	-2.360620	3.179236
H	4.277017	-3.183899	1.781756
H	-3.183899	-4.277017	1.781756
H	-2.360620	-4.894375	3.179236
N	-2.326155	-4.416938	2.294399
N	-4.416938	2.326155	2.294399
N	2.326155	4.416938	2.294399
N	4.416938	-2.326155	2.294399

**Pt-C-IIa (M11L, SMD water)**

Pt	3.920615	1.789756	-0.046325
Pt	1.613203	-3.511898	-0.726495
Pt	-3.849128	-1.675219	-0.152791
Pt	-1.554542	3.663737	-0.628028
C	-0.261252	2.886457	1.922140
C	-4.796485	2.126073	1.658775
C	0.731628	2.515210	2.779746
H	-1.247147	3.167379	2.289086
C	4.754823	-0.663558	1.396239
C	-0.724561	-2.593557	2.718491
H	5.468834	0.048096	1.811552
C	4.777158	-1.977768	1.758554
C	0.272046	-2.940725	1.856677
H	1.242274	-3.271107	2.223929
H	-0.584662	-2.625103	3.792517
H	5.497474	-2.362211	2.471581
H	0.575480	2.482459	3.851567
H	-5.543643	2.528756	2.332938
N	2.943693	-2.326899	0.271856
N	3.863399	-0.163515	0.519121
N	0.113170	-2.922919	0.518620
N	-2.113679	-2.168843	0.825945
N	-3.855112	0.270288	0.484313
N	-2.908162	2.427659	0.247835
N	-0.082595	2.953964	0.588650
N	2.152976	2.232256	0.886035
C	3.827932	-2.826235	1.163124
C	-1.966622	-2.230051	2.167097
C	-3.831357	2.910501	1.100553
C	1.989261	2.213428	2.226893
C	2.938931	-0.995041	-0.049386
O	2.098236	-0.551399	-0.875006
C	1.122367	2.589351	0.060033
O	1.304763	2.604687	-1.190876
C	-1.074649	-2.498545	-0.004122

O	-1.234250	-2.428102	-1.256075
C	-2.900658	1.095241	-0.058274
O	-2.039539	0.626769	-0.847095
N	3.982353	3.762285	-0.635075
H	4.783971	4.001297	-1.216571
H	3.134912	3.949817	-1.171700
N	5.687452	1.364473	-1.013632
H	6.238429	2.193734	-1.230367
H	6.276093	0.749555	-0.452576
N	0.290504	-4.724908	-1.739747
H	0.666191	-5.110842	-2.604222
H	-0.006721	-5.505604	-1.158138
N	3.153392	-4.064003	-1.981564
H	2.937674	-4.878839	-2.553905
H	3.366690	-3.291415	-2.610870
N	-5.549242	-1.252453	-1.233511
H	-5.745295	-0.252646	-1.255389
H	-5.436683	-1.557828	-2.199472
N	-3.871830	-3.618385	-0.831784
H	-3.838632	-4.275633	-0.054897
H	-4.690324	-3.848007	-1.393178
N	-0.208923	4.955457	-1.508028
H	-0.554955	5.363224	-2.374747
H	0.035983	5.720789	-0.883434
N	-3.049993	4.404176	-1.837973
H	-2.929117	5.394822	-2.043444
H	-3.064221	3.904349	-2.725807
H	-6.370438	-1.723091	-0.856304
H	-3.967862	4.292594	-1.409573
H	0.632775	4.415095	-1.716839
H	-3.039424	-3.760845	-1.404110
H	4.002613	-4.276723	-1.460556
H	3.991755	4.385167	0.170412
H	5.495459	0.885604	-1.892288
H	-0.525121	-4.150763	-1.962123
C	-4.807875	0.766078	1.305915
H	-3.771714	3.976229	1.316537
N	-3.010791	-1.953781	2.935897
N	-5.748934	-0.056692	1.758367
N	3.772090	-4.122412	1.447600
N	3.036195	1.922491	2.988278
H	-3.916426	-1.772221	2.537165
H	-2.926251	-1.985668	3.937718
H	-5.765244	-1.031722	1.497190
H	-6.468350	0.287196	2.371968
H	3.067814	-4.715441	1.033325
H	4.421718	-4.525753	2.101662
H	2.945425	1.907917	3.989995
H	3.949540	1.785524	2.584508

**Pt-C-IIIa (M11L, SMD water)**

Pt	2.820029	2.869621	-0.439801
Pt	-2.973946	2.826199	-0.420204
Pt	-2.989507	-2.958611	-0.293673
Pt	2.827274	-3.012981	-0.386712
C	-0.128441	2.571866	2.736928
C	1.101085	2.679130	2.061191
C	-1.266124	2.601862	1.988798
H	-0.158475	2.495494	3.817500
H	-2.248740	2.554812	2.455448

C	5.333249	-0.086010	1.413707
C	4.724795	-1.233157	1.000800
H	6.238502	-0.098778	2.009633
C	-4.586095	1.163345	1.485971
C	-5.060862	-0.041975	2.032142
C	-4.577342	-1.203317	1.503884
H	-5.785492	-0.037878	2.837591
H	-4.905536	-2.174450	1.871544
N	-3.672484	-1.224697	0.507218
N	-1.246414	2.708603	0.645897
N	1.123501	2.748946	0.711558
N	3.613530	1.125691	0.281857
N	3.595737	-1.240663	0.266305
C	-0.082530	-2.630627	2.797242
H	-0.090744	-2.540790	3.877154
N	1.126949	-2.854675	0.749905
N	-1.239692	-2.780060	0.727287
H	4.479937	-2.504140	-2.311969
H	5.358810	-3.014392	-1.019222
H	4.614336	-4.108304	-1.986359
H	1.148660	-4.656499	-1.388040
H	2.636917	-5.227404	-1.815750
H	2.066314	-5.505103	-0.301120
H	-2.874505	-5.076388	-1.862307
H	-1.360868	-4.528332	-1.487212
H	-2.212000	-5.449097	-0.405170
H	-5.564188	-3.033024	-0.626051
H	-4.880624	-2.401685	-1.981154
H	-4.908146	-4.029308	-1.754603
H	5.044143	3.821748	-1.441748
H	5.042766	2.186513	-1.644893
H	4.155524	3.136454	-2.644779
H	1.170967	4.461969	-1.575028
H	2.009441	5.346029	-0.454149
H	2.682677	5.040022	-1.921648
H	-2.209278	5.302627	-0.690737
H	-1.320989	4.312927	-1.679365
H	-2.823485	4.828784	-2.139003
H	-4.899983	2.023496	-1.949352
H	-5.534857	3.083463	-0.863053
H	-4.750955	3.639512	-2.192064
N	-4.740994	2.913072	-1.478532
N	-2.262315	4.525349	-1.345466
N	2.097210	4.645688	-1.187584
N	4.458972	3.021451	-1.678348
N	4.511995	-3.189187	-1.558507
N	2.099318	-4.819783	-1.052961
N	-2.290418	-4.718335	-1.109306
N	-4.789897	-3.135413	-1.280180
N	-3.676411	1.138261	0.487917
C	-0.053702	-2.842426	0.056931
O	-0.038880	-2.919466	-1.205601
C	3.019176	-0.053979	-0.098258
O	1.969831	-0.034117	-0.790966
C	-0.046711	2.732321	-0.002188
O	-0.007435	2.762389	-1.265764
C	-3.204154	-0.048338	-0.004774
O	-2.353708	-0.048487	-0.933975
H	-5.688300	2.401715	2.659068
H	-4.630174	3.200799	1.540445

H	3.128241	2.845887	2.260208
H	2.245189	2.683776	3.733435
N	2.245780	2.724238	2.728506
N	-5.005851	2.344871	1.922228
C	-1.233909	-2.648323	2.068023
C	4.744916	1.126847	1.020807
C	1.130430	-2.773764	2.099085
H	-2.209178	-2.572905	2.547230
N	5.275582	2.297034	1.371778
N	2.291484	-2.847735	2.735923
H	4.903940	3.173585	1.033923
H	6.130791	2.318742	1.902826
H	3.148601	-3.017097	2.235486
H	2.322748	-2.804494	3.740095
H	5.137498	-2.210008	1.253864

<b>Pt-C-IVa (M11L, SMD water)</b>			
Pt	4.126374	-1.231005	-0.077227
Pt	-1.098347	-3.707199	-0.743075
Pt	-4.126935	1.236902	-0.068755
Pt	1.091538	3.722243	-0.721873
C	3.358979	3.308428	1.105185
C	-1.004145	2.357056	2.727454
C	4.388092	2.681125	1.741053
H	3.131188	4.357367	1.291710
C	-4.373643	-2.666315	1.756842
C	1.030417	-2.435522	2.721484
C	-3.349668	-3.295307	1.112259
H	-3.113706	-4.340887	1.307427
H	-4.992329	-3.177873	2.484225
H	0.853020	-2.443356	3.790449
H	5.019203	3.196463	2.455011
H	-0.817708	2.334637	3.794795
N	0.309573	-2.917324	0.506705
N	2.452904	-1.962898	0.865183
N	-2.576043	-2.676339	0.200445
N	-3.829349	-0.696403	0.522928
N	-2.427669	1.905420	0.867636
N	-0.309384	2.916518	0.523068
N	2.568984	2.683001	0.211647
N	3.816171	0.698221	0.537985
C	0.100844	-2.895217	1.838097
C	-4.615483	-1.322438	1.425431
C	-0.095598	2.872456	1.852989
C	4.620502	1.332025	1.419518
C	1.482865	-2.422843	0.012613
O	1.696753	-2.401762	-1.233639
C	2.783282	1.365326	-0.075669
O	2.053186	0.763894	-0.905396
C	-2.805275	-1.365004	-0.102964
O	-2.095975	-0.770115	-0.954298
C	-1.473372	2.408950	0.022503
O	-1.696145	2.418658	-1.222417
N	5.737534	-0.503410	-1.140424
H	6.243590	-1.229269	-1.645560
H	5.392525	0.165258	-1.828409
N	4.455889	-3.157491	-0.722324
H	5.184183	-3.243458	-1.429277
H	4.711460	-3.761489	0.056256
N	-2.560180	-4.488425	-1.965346

H	-2.207483	-5.125392	-2.677438
H	-3.251404	-4.995926	-1.415045
N	0.359703	-4.832318	-1.666318
H	0.058295	-5.253487	-2.542652
H	1.144152	-4.206236	-1.854446
N	-4.440368	3.176880	-0.683479
H	-3.570595	3.518509	-1.094681
H	-5.175294	3.273063	-1.382327
N	-5.802037	0.599142	-1.083348
H	-6.662253	0.815345	-0.581708
H	-5.865980	1.038735	-2.000988
N	2.550743	4.513870	-1.940798
H	2.196643	5.160118	-2.643905
H	3.245488	5.013381	-1.387616
N	-0.368526	4.856771	-1.630376
H	-0.069725	5.290805	-2.501233
H	-1.150691	4.229923	-1.825446
H	-4.684228	3.773526	0.104447
H	-0.688498	5.599185	-1.012174
H	3.031225	3.760876	-2.431533
H	-5.773255	-0.408642	-1.232963
H	0.677076	-5.584127	-1.058255
H	6.414242	-0.018064	-0.553830
H	3.584498	-3.501110	-1.128804
H	-3.044431	-3.731037	-2.445557
C	-2.215834	1.874247	2.201771
H	0.848444	3.286449	2.203130
C	2.259503	-1.992441	2.202102
H	-0.853778	-3.288206	2.183463
N	-3.165765	1.397836	2.995140
N	-5.606952	-0.637335	1.991573
N	3.247336	-1.610514	2.999500
N	5.633819	0.663893	1.962475
H	-3.023920	1.373219	3.990930
H	-4.044328	1.065336	2.632239
H	-5.848318	0.295663	1.690331
H	-6.208343	-1.088010	2.661119
H	4.160673	-1.403394	2.632826
H	3.124192	-1.620032	3.997880
H	6.241176	1.120962	2.621770
H	5.823814	-0.298466	1.727271

**Pt-C-Ib (M11L, SMD water)**

Pt	1.973035	3.576817	0.254531
Pt	3.800803	-1.853449	-0.072376
Pt	-1.736164	-3.602402	-0.161831
Pt	-3.563549	2.010510	-0.611499
C	2.500173	0.960813	-3.073078
C	-0.908318	1.476818	2.675986
C	-2.008928	1.580675	1.876582
H	-2.982546	1.228896	2.214165
C	1.864538	-1.491192	2.136337
C	-5.229185	-1.556229	1.086828
H	2.759204	-1.080421	2.599339
C	0.687008	-1.582340	2.815593
C	-4.281715	-2.475479	0.753939
H	-4.398508	-3.525337	1.023483
H	-6.128498	-1.829905	1.626141
H	0.590020	-1.239799	3.839570
H	-0.962368	1.029586	3.662163

N	-0.273673	-2.598772	0.877878
N	1.995051	-1.910290	0.862785
N	-3.141189	-2.153050	0.107988
N	-3.873423	0.093430	0.017439
N	-1.961508	2.114958	0.639900
N	0.347820	2.540950	0.950546
N	3.219769	-0.203075	-1.117290
N	2.491542	2.037372	-0.956597
C	2.250879	2.043256	-2.280360
H	1.842099	2.965542	-2.690024
H	2.304601	0.976215	-4.138839
C	-4.976123	-0.219772	0.734260
C	0.313254	1.952818	2.167828
C	2.972850	-0.206456	-2.445416
C	-0.404730	-2.173803	2.154041
C	3.021656	0.925448	-0.371211
O	3.335655	0.938567	0.850150
C	0.914705	-2.429224	0.211688
O	1.009631	-2.780520	-0.997233
C	-2.938324	-0.861358	-0.298043
O	-1.922780	-0.551800	-0.972802
C	-0.770296	2.589543	0.165331
O	-0.695243	3.091814	-0.991602
N	1.434814	5.139650	1.484912
H	1.385884	6.022538	0.978714
H	0.519834	4.977256	1.903503
N	3.579205	4.655500	-0.450051
H	3.429022	5.662049	-0.406844
H	4.414839	4.442738	0.092106
N	4.382410	-3.501189	1.016404
H	4.633482	-4.280665	0.410615
H	5.190290	-3.288639	1.599947
N	5.655378	-1.813604	-0.975645
H	5.810876	-0.939097	-1.474329
H	6.400373	-1.908834	-0.287132
N	-0.384915	-5.140833	-0.389097
H	-0.047921	-5.467678	0.514590
H	-0.761302	-5.946298	-0.884813
N	-3.144729	-4.672402	-1.216192
H	-3.515298	-5.438191	-0.655496
H	-3.929810	-4.088413	-1.500922
N	-3.317028	3.966906	-1.206151
H	-3.794470	4.186573	-2.077634
H	-3.659955	4.608477	-0.494633
N	-5.171287	1.864587	-1.897127
H	-5.525909	0.911246	-1.957611
H	-5.943600	2.462687	-1.607037
H	0.407811	-4.771338	-0.914169
H	3.632539	-3.815666	1.630235
H	5.755827	-2.574322	-1.645915
H	3.774975	4.417431	-1.421751
H	2.105117	5.254599	2.243076
H	-2.312935	4.108042	-1.331181
H	-2.743899	-5.074597	-2.062837
H	-4.900044	2.145236	-2.838890
N	-5.802654	0.758359	1.085019
N	1.451722	1.872515	2.846588
N	-1.563700	-2.350773	2.775903
N	3.192173	-1.325372	-3.125934
H	-6.634808	0.551398	1.612018

H	-5.578323	1.724048	0.894606
H	-2.335632	-2.814527	2.327082
H	-1.668595	-2.065097	3.734692
H	3.420761	-2.185344	-2.651492
H	3.002973	-1.360319	-4.113346
H	1.464280	1.396374	3.734145
H	2.324577	1.958767	2.337469

**Pt-C-IIb1 (M11L, SMD water)**

Pt	-0.702306	3.693670	0.091652
Pt	-4.431562	-0.701759	-0.081678
Pt	0.623063	-3.620573	-0.465581
Pt	4.391855	0.901086	-0.253575
C	1.347775	0.953217	2.693601
C	-2.479345	-1.092401	2.177036
C	-1.302096	-1.588516	2.764856
C	-0.433778	-2.270492	1.963283
H	-1.096766	-1.426010	3.817079
H	0.492018	-2.680281	2.364387
N	-0.662432	-2.482038	0.651445
N	0.596111	2.355726	0.917800
N	2.774468	1.444421	0.853072
C	3.049196	-3.406437	1.236345
C	4.303824	-2.898829	1.614869
C	4.686024	-1.709651	1.069943
H	4.933787	-3.436451	2.313257
H	5.642181	-1.251968	1.320205
N	3.909910	-1.017975	0.212717
N	2.286597	-2.734729	0.342701
H	3.956518	3.333163	-0.826422
H	5.299678	3.313348	0.149868
H	5.454009	2.997887	-1.457034
H	6.849500	0.821427	-1.140935
H	6.217445	-0.694429	-1.224171
H	5.825162	0.421254	-2.364987
H	1.952271	-5.734354	-1.230664
H	1.617849	-4.816271	-2.555008
H	2.855991	-4.398189	-1.561845
H	-0.696726	-5.202923	-2.103349
H	-1.368098	-5.281961	-0.604929
H	-1.658776	-3.958159	-1.563942
H	-2.504472	5.571164	0.027436
H	-1.466872	5.804510	-1.227611
H	-2.651708	4.669341	-1.340879
H	0.939010	4.801827	1.786101
H	0.536706	5.920946	0.648489
H	-0.508260	5.578733	1.872935
H	-5.445749	-3.022546	0.492349
H	-5.189639	-2.229273	1.908370
H	-6.514119	-1.882421	1.002969
H	-6.613540	-0.904099	-1.497198
H	-6.804245	0.319975	-0.414451
H	-5.938165	0.565191	-1.790232
N	-6.144261	-0.112948	-1.058457
N	-5.523728	-2.116900	0.952407
N	0.168884	5.170434	1.230327
N	-1.979439	5.095847	-0.705225
N	4.849807	2.869508	-0.647971
N	6.010070	0.292157	-1.371517
N	1.910573	-4.777971	-1.579276

N	-0.959115	-4.649504	-1.289512
N	-2.714801	-1.306415	0.863762
C	2.696331	-1.528023	-0.163953
O	1.963910	-0.908195	-0.979738
C	1.799647	2.214609	0.290471
O	2.008809	2.814772	-0.805240
C	-1.805536	-1.976094	0.088802
O	-2.038575	-2.136193	-1.140300
C	-2.003970	1.070128	-3.061143
H	-1.750579	0.860915	-4.094090
N	-3.320624	0.636453	-1.128786
N	-1.611451	2.259012	-1.033065
C	-2.659703	1.611885	-0.445452
O	-3.011213	1.921020	0.728861
H	3.126082	-5.074686	2.391623
H	-3.237973	-0.245062	3.857458
N	-3.391805	-0.430283	2.880119
N	2.585126	-4.550141	1.724628
H	1.668592	-4.887041	1.467151
H	-4.144605	0.053872	2.413321
C	2.541949	0.854819	2.043842
H	1.170679	0.456237	3.640997
C	-3.010906	0.410411	-2.419996
C	-1.236308	1.971090	-2.299954
C	0.331198	1.704260	2.074720
H	-3.597926	-0.355811	-2.922772
H	3.364924	0.279986	2.465236
N	-0.883939	1.816570	2.593199
H	-1.099792	1.312960	3.438833
H	-1.659024	2.140820	2.017778
N	-0.142021	2.557359	-2.768945
H	0.521086	2.977567	-2.122754
H	0.166916	2.350548	-3.704623

**Pt-C-IIb2 (M11L, SMD water)**

Pt	4.333339	-1.017377	-0.098405
Pt	1.093123	3.740439	0.229193
Pt	-4.068162	1.180683	-0.432578
Pt	-0.791857	-3.781800	-0.335372
C	2.390998	-1.222945	2.131246
C	1.275912	-1.618453	2.808146
H	3.192360	-0.675795	2.625536
C	-0.128677	1.790896	2.149535
C	-1.208495	1.075694	2.701006
C	-2.370335	1.040414	1.986207
H	-1.105435	0.554822	3.646690
H	-3.237583	0.492124	2.349884
N	-2.517578	1.660828	0.798148
N	2.580007	-1.496783	0.826268
N	0.486009	-2.614594	0.784012
C	-4.778207	-1.409500	0.830760
C	-4.625217	-2.767755	1.158243
C	-3.469643	-3.372986	0.769563
H	-5.394806	-3.299833	1.705331
H	-3.283787	-4.424302	0.993335
N	-2.484436	-2.726145	0.111172
N	-3.819998	-0.772653	0.120378
H	1.230778	-5.365308	0.092870
H	0.600846	-5.759178	-1.372506
H	1.528578	-4.393248	-1.212768

H	-1.553042	-5.161352	-2.405730
H	-2.112572	-5.910639	-1.050293
H	-2.898087	-4.595413	-1.653135
H	-5.380828	0.927480	-2.658262
H	-5.751633	-0.364358	-1.717921
H	-6.477832	1.086177	-1.442895
H	-4.857554	3.262871	-1.842855
H	-4.894619	3.644487	-0.242933
H	-3.435503	3.561748	-1.038753
H	5.972041	0.159300	-1.751206
H	6.772460	-0.140413	-0.347448
H	6.550472	-1.348489	-1.443020
H	4.625619	-3.103540	1.446431
H	5.772379	-3.167074	0.270955
H	5.974613	-2.171375	1.564936
H	0.043591	6.039840	0.862645
H	-0.493616	4.910719	1.931656
H	1.011304	5.555288	2.101375
H	2.023623	5.856409	-0.975616
H	3.082867	5.422839	0.207452
H	3.070544	4.612278	-1.222906
N	2.477111	5.061720	-0.527421
N	0.325675	5.234588	1.419584
N	5.286236	-2.541756	0.911523
N	6.112504	-0.533388	-1.016720
N	0.827541	-4.978964	-0.758739
N	-1.977901	-5.002436	-1.492734
N	-5.598631	0.642613	-1.704077
N	-4.367276	3.148747	-0.958249
N	-0.307340	2.472586	0.993756
C	-2.652604	-1.411037	-0.227713
O	-1.763742	-0.794935	-0.870278
C	1.605305	-2.155001	0.131750
O	1.739323	-2.369318	-1.105046
C	-1.481157	2.399461	0.305260
O	-1.601972	3.030679	-0.785469
C	2.195200	1.165607	-3.038241
C	3.083167	0.345695	-2.406987
H	1.955647	1.048608	-4.088586
N	1.877700	2.278990	-0.953316
N	3.371133	0.460122	-1.095864
C	2.818999	1.476314	-0.374880
O	3.174992	1.683778	0.820252
H	-6.594063	-1.186469	1.707052
H	1.224336	1.306349	3.561958
N	1.065832	1.843484	2.724550
N	-5.855793	-0.727791	1.199241
H	-5.942238	0.259520	1.010124
H	1.877696	2.106253	2.168990
H	1.139963	-1.399064	3.861178
C	1.519878	2.113789	-2.247282
C	0.316712	-2.367745	2.102574
N	-0.749705	-2.866369	2.715157
N	0.529147	2.862221	-2.717330
H	3.585855	-0.462598	-2.936368
H	-0.889161	-2.706641	3.698577
H	-1.399164	-3.459985	2.228000
H	-0.116790	3.296826	-2.064849
H	0.238690	2.747922	-3.674468

<b>Pt-C-Iib3 (M11L, SMD water)</b>			
Pt	-2.380598	3.380236	0.160595
Pt	-3.699057	-2.286689	0.089519
Pt	1.982214	-3.345481	-0.524964
Pt	3.312514	2.417947	-0.391107
C	-0.569185	2.547867	2.353915
C	0.609785	2.275780	2.981850
H	-1.512028	2.572470	2.897518
C	-1.708791	-2.206033	2.269702
C	-0.513311	-2.373544	2.900724
H	-0.411336	-2.251964	3.972901
N	0.459979	-2.867706	0.776307
N	-0.638518	2.823852	1.038055
N	1.700188	2.508085	0.869609
C	4.369143	-2.099352	0.737654
C	5.251566	-1.061318	1.077657
C	4.884702	0.203725	0.730721
H	6.185655	-1.269179	1.586012
H	5.526633	1.056834	0.951695
N	3.726949	0.483134	0.100414
N	3.206979	-1.826192	0.103435
H	3.048120	4.990958	-0.072868
H	3.570231	4.741617	-1.611580
H	1.991316	4.429671	-1.215908
H	4.588985	2.490883	-2.650679
H	5.560949	3.144638	-1.495891
H	5.433229	1.512332	-1.638394
H	3.841882	-4.748226	-1.726769
H	3.017669	-3.864683	-2.841594
H	4.182223	-3.150627	-1.934494
H	1.248405	-5.398003	-1.996706
H	0.741803	-5.637245	-0.451934
H	-0.069100	-4.569471	-1.428973
H	-4.877405	4.107828	0.015370
H	-4.049269	4.868061	-1.186376
H	-4.506476	3.298465	-1.364581
H	-1.558983	5.144773	1.904451
H	-2.181067	5.936684	0.606668
H	-3.187071	5.298836	1.741377
H	-4.484015	-4.750185	0.458015
H	-3.478289	-4.351245	1.692660
H	-5.036165	-3.832630	1.706207
H	-5.791971	-3.096534	-1.241120
H	-6.297621	-2.104035	-0.029788
H	-5.673634	-1.466978	-1.410768
N	-5.582714	-2.232210	-0.744285
N	-4.232787	-4.003176	1.103405
N	-2.321138	5.141960	1.228177
N	-4.157251	3.982505	-0.694684
N	2.955091	4.383157	-0.883742
N	4.909668	2.385161	-1.689139
N	3.427479	-3.834840	-1.908543
N	0.850743	-4.935814	-1.181266
N	-1.853511	-2.369451	0.940853
C	2.868689	-0.533406	-0.221863
O	1.790224	-0.299104	-0.824606
C	0.495221	2.787534	0.281360
O	0.439549	3.033190	-0.955270
C	-0.758988	-2.651809	0.177827
O	-0.862141	-2.751363	-1.076090

C	-2.582527	0.444693	-2.968118
H	-2.432241	0.404995	-4.040548
N	-3.196339	-0.608186	-0.927369
N	-2.499025	1.646747	-0.907877
C	-2.942927	0.540490	-0.234677
O	-3.130773	0.593730	1.011655
H	5.515563	-3.585427	1.505318
N	4.651413	-3.365520	1.038059
H	4.062947	-4.130392	0.740508
H	0.658370	2.076425	4.045930
C	-3.029479	-0.633831	-2.262658
C	1.780294	2.295393	2.201853
N	2.978237	2.124776	2.745372
H	3.068206	1.965176	3.734449
H	3.815964	2.222439	2.194979
C	0.590479	-2.756290	2.116455
C	-2.280209	1.609130	-2.241427
H	-2.610840	-1.946301	2.821699
H	-3.259706	-1.577649	-2.754260
N	-1.798323	2.704060	-2.819449
N	1.761984	-3.027801	2.676397
H	-1.355053	3.403197	-2.238781
H	-1.602380	2.702697	-3.806785
H	1.870015	-2.967316	3.674722
H	2.545450	-3.353510	2.135427

**Pt-C-IIb4 (M11L, SMD water)**

Pt	-3.188003	2.683214	-0.194082
Pt	-2.806260	-3.014929	0.391561
Pt	2.917554	-2.919533	-0.634778
Pt	2.599801	2.937398	-0.187257
C	-0.330053	1.984407	2.875725
C	-0.756872	-1.720970	2.181220
C	0.560995	-1.522832	2.633282
C	1.575818	-1.949698	1.826581
H	0.755036	-1.043584	3.586691
H	2.615572	-1.838403	2.128867
N	1.362453	-2.523166	0.625885
N	-1.448262	2.366381	0.814851
N	0.920406	2.455054	0.895977
C	4.897397	-1.144664	0.598565
C	5.442164	-0.014162	1.128244
H	6.374927	-0.031084	1.679291
N	3.580818	1.194110	0.241112
N	3.738522	-1.143471	-0.088658
H	2.276473	5.371642	-1.151405
H	0.863471	4.505170	-1.210380
H	1.363683	5.199330	0.202974
H	4.694189	4.299007	-0.965257
H	4.897087	2.737847	-1.445531
H	3.898082	3.730267	-2.286370
H	4.946420	-4.177497	-1.701293
H	4.183390	-3.307457	-2.870955
H	5.212840	-2.560567	-1.831963
H	1.135014	-4.615093	-1.259683
H	2.531916	-5.156458	-1.981177
H	2.279808	-5.439097	-0.380742
H	-5.723390	3.215701	-0.498814
H	-4.908258	3.825840	-1.791284
H	-5.257898	2.220105	-1.719761

H	-2.572700	4.702118	1.347075
H	-3.559025	5.247268	0.150586
H	-4.193868	4.443353	1.437613
H	-1.707549	-4.643929	2.106891
H	-3.313161	-4.535764	2.449360
H	-2.794903	-5.494730	1.216895
H	-4.584867	-4.722080	-0.476076
H	-5.340490	-3.608640	0.471643
H	-4.942106	-3.234793	-1.078933
N	-4.627744	-3.730545	-0.246061
N	-2.637026	-4.607057	1.691064
N	-3.401328	4.477010	0.798191
N	-4.974986	3.025979	-1.163767
N	1.680382	4.723832	-0.639668
N	4.212169	3.486437	-1.347521
N	4.499106	-3.284535	-1.902271
N	2.137710	-4.763462	-1.128432
N	-0.968848	-2.357070	1.007258
C	3.069874	0.033779	-0.289248
O	2.006437	0.065054	-0.958857
C	-0.250340	2.496959	0.176473
O	-0.208189	2.687794	-1.069184
C	0.077220	-2.710668	0.200748
O	-0.156691	-3.228533	-0.927307
C	-2.660275	-0.508770	-3.048892
H	-2.485777	-0.624634	-4.112073
N	-2.946340	-1.453918	-0.890169
N	-3.010760	0.892886	-1.150255
C	-3.143415	-0.213959	-0.357681
O	-3.453699	-0.086479	0.857844
H	-1.691188	-0.833012	3.739064
N	-1.820294	-1.334916	2.875646
H	-2.707260	-1.242476	2.393645
H	-0.359251	1.768009	3.937597
C	-2.729570	-1.583143	-2.211765
C	-2.771115	0.770016	-2.474432
C	-1.468461	2.100098	2.135037
H	-2.607973	-2.599448	-2.581672
N	-2.658942	1.872702	-3.206052
H	-2.622621	2.783433	-2.775035
H	-2.466104	1.804187	-4.191117
C	0.897963	2.199542	2.222371
C	4.736359	1.185913	0.943179
N	2.040585	2.176718	2.896594
N	5.178622	2.330197	1.458163
H	4.698144	3.204689	1.306612
H	6.041454	2.345316	1.976620
H	2.037879	2.002781	3.887431
H	2.921656	2.368955	2.451443
H	-2.453296	1.991885	2.586866
H	5.380852	-2.113859	0.718094

**Pt-C-IIIb1 (M11L, SMD water)**

Pt	3.694535	-1.626251	-0.349056
Pt	1.225316	3.756986	-0.578771
Pt	-4.086152	1.506512	0.202369
Pt	-1.667265	-3.767943	0.062636
C	-0.129068	-2.598251	2.304501
C	-2.436573	-0.802887	-2.963667
H	-1.060116	-2.829611	2.819382

C	0.944999	-2.087438	2.970176
C	-2.045766	1.885061	2.324250
C	4.839839	2.271030	1.066192
H	-2.834015	1.412971	2.908746
C	-0.898143	2.332694	2.908908
C	3.776934	3.017573	0.659960
H	3.755826	4.096544	0.815575
H	5.696287	2.712720	1.561523
H	-0.727386	2.244852	3.975383
H	0.918013	-1.895218	4.036336
N	-0.156102	3.019799	0.745156
N	-2.287410	2.018147	1.005804
N	2.701628	2.489242	0.042503
N	3.721395	0.354965	0.176487
N	2.126503	-2.064191	0.895271
N	-0.099040	-2.864731	0.984651
N	-3.235305	0.023431	-0.883943
N	-2.162164	-2.077544	-0.965675
C	-3.061443	0.148398	-2.212109
H	-2.290237	-0.683756	-4.030822
H	-3.443779	1.063613	-2.660542
C	4.794157	0.892757	0.799626
C	2.117307	-1.849387	2.228456
C	-1.955546	-1.941850	-2.293677
C	0.044187	2.969700	2.080472
C	2.657587	1.143521	-0.201568
O	1.671181	0.628599	-0.787169
C	1.022090	-2.578551	0.265499
O	1.057146	-2.804388	-0.975394
C	-1.322470	2.547052	0.198043
O	-1.507869	2.630640	-1.047090
C	-2.796735	-1.100252	-0.246998
O	-2.977270	-1.248599	0.993179
N	-0.204275	5.103901	-1.196509
H	-0.478988	5.719174	-0.433779
H	0.084095	5.689002	-1.978227
N	2.565924	4.502324	-1.953267
H	2.456375	4.016179	-2.842218
H	2.429674	5.497134	-2.127213
N	5.221147	-1.243931	-1.681804
H	5.462110	-0.254677	-1.728487
H	6.069425	-1.757634	-1.445232
N	3.741420	-3.611197	-0.888351
H	2.793741	-3.860383	-1.175326
H	4.379299	-3.803616	-1.658635
N	-3.281402	-4.674824	-0.843350
H	-3.435735	-5.634058	-0.537585
H	-4.128873	-4.147540	-0.638796
N	-1.183639	-5.475389	1.112076
H	-1.754348	-6.282296	0.864696
H	-0.210686	-5.723611	0.940121
N	-5.896952	0.963676	-0.615993
H	-6.047951	-0.036507	-0.495845
H	-6.694824	1.444473	-0.204172
N	-4.962900	3.034280	1.279666
H	-4.904574	3.911027	0.764027
H	-5.946871	2.860118	1.479834
H	3.532099	4.376414	-1.655324
H	-1.014869	4.549194	-1.477788
H	4.014808	-4.200459	-0.105004

H	4.941347	-1.529625	-2.619842
H	-3.165499	-4.693625	-1.855704
H	-1.289979	-5.322159	2.114207
H	-4.494206	3.174265	2.173797
H	-5.904680	1.158954	-1.616050
N	3.230455	-1.432794	2.816969
N	-1.314001	-2.915708	-2.929450
N	5.801836	0.099302	1.153553
N	1.128895	3.548921	2.579054
H	5.809965	-0.886750	0.938956
H	6.608228	0.492922	1.609787
H	1.305429	3.531652	3.569267
H	1.740434	4.092538	1.990978
H	-1.125434	-2.833078	-3.914463
H	-0.807404	-3.609411	-2.398766
H	4.089672	-1.331805	2.302495
H	3.246082	-1.262456	3.808222

**Pt-C-IIIb2 (M11L, SMD water)**

Pt	-0.531490	3.724141	-0.418905
Pt	-4.321987	-0.789925	-0.300875
Pt	0.705389	-3.689252	0.036513
Pt	4.457086	0.692107	-0.023007
C	2.043905	-1.012135	-3.055290
C	1.286118	1.567006	2.779243
C	-4.175617	3.055121	1.628176
C	-1.369296	-1.047527	2.716305
H	-4.782945	3.623794	2.322487
H	-1.208527	-0.598961	3.690730
H	1.060150	1.386449	3.824367
N	-2.771168	-1.456366	0.836003
N	-0.592805	-2.368526	0.890998
N	-3.816854	1.090083	0.319026
N	-2.208927	2.825269	0.305981
N	0.697355	2.506082	0.671958
N	2.736280	1.312617	0.900746
N	1.635386	-2.239816	-1.054166
N	3.345839	-0.617850	-1.105023
H	1.798033	-0.781227	-4.085528
C	-2.983409	3.522039	1.162004
C	0.438006	2.269307	1.973325
C	3.046688	-0.366175	-2.393810
C	-2.557387	-0.927590	2.058775
C	-2.611861	1.588051	-0.113557
O	-1.899251	0.914972	-0.904121
C	1.846792	2.004552	0.121787
O	2.106135	2.195340	-1.098254
C	-1.788933	-2.204094	0.256276
O	-1.983097	-2.763231	-0.863540
C	2.678790	-1.605058	-0.445423
O	3.020449	-1.937038	0.725757
N	-4.808039	-2.696409	-0.906172
H	-5.347965	-3.187720	-0.197361
H	-5.338226	-2.720549	-1.775386
N	-5.862764	-0.055392	-1.458071
H	-5.732049	-0.318917	-2.433711
H	-6.764027	-0.423550	-1.156366
N	-1.750247	4.997358	-1.484237
H	-2.735398	4.846451	-1.272014
H	-1.540171	5.973928	-1.281821

N	1.099072	4.763919	-1.131330
H	1.804119	4.074051	-1.396151
H	0.876224	5.338077	-1.942399
N	6.165465	0.069508	-0.988505
H	6.980704	0.641731	-0.773087
H	6.388344	-0.891428	-0.734278
N	5.556315	2.072854	1.043012
H	6.239307	1.621368	1.649408
H	6.064005	2.693091	0.413672
N	1.999636	-5.047710	-0.811089
H	2.959956	-4.721057	-0.718165
H	1.948168	-5.974423	-0.391502
N	-0.219108	-5.170477	1.127962
H	-0.893618	-5.671659	0.552599
H	0.441261	-5.852366	1.498605
H	-5.918138	0.961221	-1.424097
H	-3.919672	-3.181533	-1.047525
H	1.484302	5.375968	-0.415541
H	-1.628553	4.855002	-2.485910
H	6.028189	0.096315	-1.997945
H	4.962456	2.656754	1.630487
H	-0.724081	-4.773052	1.918469
H	1.803907	-5.149467	-1.805570
H	3.638426	0.409006	-2.877004
C	1.268986	-1.925662	-2.317177
C	-0.339726	-1.759460	2.073130
H	-3.391723	-0.386054	2.500914
H	-0.494248	2.680126	2.359218
C	2.476388	1.082410	2.207441
C	-4.589481	1.788678	1.180147
H	-2.599921	4.495726	1.464737
N	-5.730798	1.247405	1.589491
N	0.875523	-1.877834	2.589273
N	3.375577	0.413507	2.919700
N	0.175393	-2.497740	-2.805022
H	-5.993447	0.310970	1.321091
H	-6.328041	1.749365	2.224831
H	-0.495148	-2.924172	-2.170902
H	-0.126623	-2.270111	-3.738123
H	1.653563	-2.179760	2.005201
H	1.086608	-1.403708	3.452826
H	4.155015	-0.040181	2.467073
H	3.206367	0.218464	3.892427

**Pt-C-IVb (M11L, SMD water)**

Pt	-4.096949	-1.404856	-0.416702
Pt	1.195791	-3.708885	0.302576
Pt	4.285044	1.134768	-0.172281
Pt	-0.958707	3.626184	-0.366986
C	2.421995	1.363149	2.122400
C	2.140481	-1.147492	-3.025984
H	3.267972	0.882338	2.611405
C	1.313845	1.736519	2.822760
C	-4.784683	2.442554	1.189895
C	-1.187020	-1.005051	2.649371
C	-4.888190	1.171331	0.711406
C	-2.355398	-1.048972	1.945937
H	-3.235422	-0.506715	2.287246
H	-5.782113	0.573322	0.883677
H	-5.582116	2.912481	1.753469

H	-1.091682	-0.428749	3.563194
H	1.228085	1.563584	3.889593
N	-2.495596	-1.745899	0.799404
N	-0.257737	-2.472838	1.019095
N	-3.904076	0.573300	0.012398
N	-2.606173	2.543563	0.206265
N	0.395393	2.584968	0.787118
N	2.545809	1.575824	0.798491
N	1.917783	-2.250800	-0.923648
N	3.345732	-0.385473	-1.124346
C	3.017556	-0.292090	-2.427280
H	3.477871	0.527367	-2.976968
H	1.868094	-1.048225	-4.070045
C	-3.594017	3.133865	0.917521
C	0.290571	2.401260	2.122334
C	1.520837	-2.110795	-2.209280
C	-0.090450	-1.719144	2.130272
C	-2.745931	1.256140	-0.252903
O	-1.822948	0.724708	-0.921647
C	1.504826	2.131572	0.111177
O	1.567123	2.263680	-1.142304
C	2.845638	-1.409701	-0.378412
O	3.236111	-1.589607	0.810705
C	-1.443870	-2.486997	0.345350
O	-1.560057	-3.206743	-0.689954
H	-4.867047	-3.605621	-1.640428
H	-3.404437	-3.799637	-0.874982
H	-4.827370	-3.876280	-0.017790
H	-5.574582	-1.418541	-2.561777
H	-6.565270	-1.376256	-1.248610
H	-5.829808	-0.000663	-1.773183
H	0.325063	5.494385	-1.692883
H	0.919106	5.418408	-0.163347
H	1.352610	4.266726	-1.277131
H	-2.299408	5.659737	-1.325057
H	-1.851928	4.671354	-2.561131
H	-3.152552	4.286765	-1.639442
H	4.840255	2.829496	1.732441
H	6.213749	2.583973	0.866073
H	5.042895	3.582074	0.285694
H	5.906694	-0.024376	-1.854001
H	6.458795	1.501048	-1.584662
H	6.735212	0.316877	-0.476469
H	3.352486	-4.467483	-0.935684
H	3.129621	-5.465191	0.352520
H	2.252128	-5.687309	-1.022669
H	0.127935	-5.977223	0.997426
H	1.222070	-5.553641	2.152096
H	-0.265041	-4.854759	2.132687
N	-4.346840	-3.413779	-0.786693
N	-5.701556	-1.002560	-1.640161
N	2.650213	-4.981594	-0.405594
N	0.490511	-5.195707	1.540495
N	6.049361	0.683812	-1.134835
N	5.205901	2.711514	0.788463
N	0.589266	4.856023	-0.944785
N	-2.214741	4.684421	-1.608444
N	0.547197	-2.897750	-2.649863
N	-3.402664	4.374157	1.365389
N	-0.771648	2.876906	2.759686



N	1.106860	-1.708552	2.702403
H	1.925789	-1.982147	2.162849
H	1.252285	-1.124819	3.510358
H	-1.482049	3.409034	2.285809
H	-0.858726	2.750569	3.753852
H	-2.586972	4.914387	1.112574
H	-4.133486	4.834787	1.882898
H	0.227412	-2.798782	-3.599413
H	-0.059939	-3.364714	-1.983162

**Pt-C-Ic (M11L, SMD water)**

Pt	-0.664394	-3.709687	0.598149
Pt	4.438714	-0.784747	0.039319
Pt	0.670720	3.710307	-0.590698
Pt	-4.439156	0.784240	-0.048546
C	3.444961	2.536211	2.481923
C	1.589034	-2.331380	-2.748941
C	0.682408	-2.906948	-1.911174
H	-0.155079	-3.474090	-2.308774
C	-0.682809	2.899700	1.911077
C	-3.452242	-2.552244	-2.468771
H	0.157212	3.460650	2.311836
C	-1.596238	2.331041	2.745370
C	-3.852202	-1.344711	-1.980642
H	-4.474416	-0.682419	-2.581032
H	-3.764343	-2.906232	-3.444337
H	-1.503769	2.397089	3.823128
H	1.492201	-2.396420	-3.826348
N	-2.775309	1.597677	0.809653
N	-0.763024	2.819883	0.567434
N	-3.527405	-0.904286	-0.746852
N	-2.160850	-2.823047	-0.485953
N	0.764735	-2.823050	-0.568152
N	2.770372	-1.592698	-0.817596
N	2.163129	2.818645	0.494534
N	3.527646	0.898115	0.751292
C	3.845744	1.330601	1.989487
H	4.463349	0.664029	2.589854
H	3.752317	2.884549	3.460994
C	-2.618231	-3.330972	-1.649654
C	2.658519	-1.637397	-2.162480
C	2.616237	3.320323	1.662649
C	-2.671373	1.647663	2.155870
C	-2.669024	-1.649129	0.018884
O	-2.346425	-1.286544	1.177153
C	1.818044	-2.147404	-0.011286
O	1.925492	-2.047764	1.245086
C	2.673278	1.647669	-0.014555
O	2.356642	1.291645	-1.176568
C	-1.818517	2.150697	0.006982
O	-1.923493	2.055437	-1.249976
N	-2.131676	-4.584239	1.746864
H	-1.775948	-5.239893	2.440221
H	-2.647310	-3.856857	2.240689
N	0.835457	-4.608837	1.685043
H	0.527338	-4.955278	2.591850
H	1.242582	-5.390394	1.176219
N	-6.220691	0.064426	-0.804458
H	-7.002393	0.334156	-0.208220
H	-6.404565	0.439847	-1.734385

N	-5.429551	2.479375	0.577358
H	-4.769718	3.214411	0.828881
H	-6.033979	2.848797	-0.154969
N	-0.824281	4.615164	-1.679536
H	-1.232818	5.394789	-1.168846
H	-0.511894	4.965565	-2.583406
N	2.143200	4.590218	-1.728696
H	2.661226	3.865412	-2.223763
H	1.790532	5.249303	-2.420356
N	6.214835	-0.066345	0.806661
H	6.390260	-0.440289	1.738883
N	7.004840	-0.332048	0.219529
H	5.408430	-2.483577	-0.613936
H	6.400084	-2.493420	-0.379573
H	4.985525	-3.308480	-0.190795
H	5.334554	-2.584150	-1.625676
H	6.224944	0.950581	0.874011
H	-1.542006	3.903720	-1.836412
H	2.801402	5.090227	-1.133672
H	-6.234225	-0.952401	-0.872178
H	-6.011603	2.291001	1.392250
H	-2.792714	-5.087237	1.157508
H	1.553062	-3.895924	1.835944
N	3.595586	-1.050189	-2.898802
N	-2.239323	-4.556159	-1.996110
N	-3.616943	1.075761	2.890398
N	2.237159	4.544272	2.013257
H	4.261702	-0.422053	-2.474363
H	3.525402	-1.066802	-3.902497
H	-1.667724	-5.112763	-1.376740
H	-2.550370	-4.959128	-2.864061
H	-3.555362	1.098797	3.894385
H	-4.314314	0.485143	2.463374
H	2.544188	4.942670	2.884728
H	1.669119	5.104497	1.393812

**Pt-C-IIc1 (M11L, SMD water)**

Pt	-2.315767	3.252148	0.471950
Pt	-3.400654	-2.566770	0.167073
Pt	2.422013	-3.186810	-0.772168
Pt	3.519691	2.500538	0.099856
C	0.006718	-2.838587	2.710331
C	1.005383	-3.039566	1.807750
H	0.183532	-2.881869	3.778512
H	2.012026	-3.280795	2.139629
N	0.817997	-2.966147	0.474767
C	4.433058	-0.999793	2.333467
C	4.143360	0.269273	1.928085
H	4.901418	-1.201265	3.289834
H	4.341148	1.118874	2.579469
N	3.618144	0.555004	0.718232
N	3.427308	-1.772373	0.317791
H	2.580639	4.890984	-0.329120
H	4.192387	5.048360	-0.046712
H	3.662492	4.524451	-1.511570
H	5.953948	3.423923	0.275896
H	5.428533	3.065941	1.789275
H	5.972748	1.870526	0.797745
H	3.903590	-3.900784	-2.834793
H	4.401541	-2.445221	-2.253352

H	4.836138	-3.833505	-1.482426
H	1.316271	-5.474142	-1.351488
H	0.419046	-4.216679	-1.960973
H	1.755447	-4.768220	-2.771201
H	-0.441875	4.491605	1.666713
H	-1.229777	5.607166	0.724605
H	-1.853030	5.191388	2.186699
H	-3.651736	3.499149	2.681006
H	-4.401261	4.416076	1.538873
H	-4.632347	2.785406	1.572157
H	-5.875904	-1.840569	-0.369623
H	-5.500209	-3.157927	-1.285490
H	-5.881280	-3.333503	0.301956
H	-3.977677	-5.109025	0.261100
H	-2.577537	-4.866580	1.084205
H	-4.020145	-4.510136	1.793137
N	-3.506507	-4.483048	0.913198
N	-5.390640	-2.736644	-0.363353
N	-3.940388	3.522213	1.703481
N	-1.358321	4.832998	1.371910
N	3.491726	4.470405	-0.508188
N	5.437360	2.737265	0.824183
N	4.076917	-3.372256	-1.981717
N	1.364912	-4.587319	-1.848389
N	-1.481549	-2.581012	0.866028
C	3.282145	-0.477176	-0.116984
O	2.841858	-0.259816	-1.273115
C	0.467529	2.603784	-2.787170
C	-0.440602	-2.724666	-0.007165
O	-0.649501	-2.656743	-1.251572
C	-4.148635	-0.488802	-1.755351
C	-4.564857	0.736197	-2.183009
H	-4.408416	-1.387135	-2.313008
H	-5.190110	0.852806	-3.059782
N	-3.428875	-0.675174	-0.627499
N	-3.285782	1.681084	-0.414641
C	-2.948635	0.425341	0.034712
O	-2.213613	0.315539	1.046985
C	0.533055	2.710982	-0.037731
O	0.563313	2.752976	1.225085
N	-0.645258	2.965096	-0.701195
N	1.664018	2.433628	-0.744885
H	0.439224	2.566837	-3.869880
C	4.086804	-2.047441	1.462865
C	-1.276616	-2.584155	2.202274
C	-4.176239	1.844595	-1.414733
C	1.606192	2.349156	-2.087997
N	4.361914	-3.315127	1.749013
N	-2.313639	-2.385221	3.006758
N	-4.638636	3.067574	-1.663795
H	-3.214020	-2.118410	2.638188
H	-2.183703	-2.394029	4.004596
H	-5.305693	3.211394	-2.403952
H	-4.444772	3.839331	-1.042381
H	4.119088	-4.057545	1.110576
H	4.837314	-3.549750	2.604037
C	-0.671770	2.980233	-2.053910
H	2.535006	2.088601	-2.589699
N	-1.776205	3.366468	-2.675071
H	-1.814061	3.360777	-3.680257

H	-2.579310	3.709433	-2.174071
<b>Pt-C-Hc2 (M11L, SMD water)</b>			
Pt	0.289000	3.658901	0.628936
Pt	-4.508493	0.267702	-0.125983
Pt	-0.299400	-3.783276	-0.420780
Pt	4.528947	-0.418483	-0.163675
C	-2.652282	-2.242177	2.809800
C	-1.727356	2.115416	-2.798922
C	-0.928183	2.788439	-1.926211
H	-0.142653	3.442810	-2.293968
C	3.126785	2.820454	-2.489763
C	2.287147	-2.567299	2.755439
C	3.625235	1.634072	-2.043088
H	4.275070	1.033867	-2.678445
H	3.388291	3.222644	-3.461277
H	2.375093	-2.765968	3.816892
H	-1.586938	2.187017	-3.870999
N	3.058475	-1.472924	0.782955
N	1.223679	-2.960795	0.663237
N	3.372477	1.141289	-0.811460
N	1.854631	2.931349	-0.479963
N	-1.058407	2.702442	-0.586586
N	-2.915995	1.268540	-0.917023
N	-1.716604	-2.820423	0.698749
N	-3.317411	-1.079447	0.839030
H	-2.731713	-2.404661	3.878232
C	2.264614	3.516520	-1.625860
C	-2.736996	1.304980	-2.256527
C	-1.849868	-3.014633	2.024293
C	1.374726	-3.213475	1.977275
C	-2.074945	1.941451	-0.071990
O	-2.254803	1.868564	1.175383
C	2.459553	1.784655	-0.017703
O	2.169772	1.355772	1.127137
C	2.099332	-2.107647	0.045372
O	2.035589	-1.924571	-1.202979
C	-2.510659	-1.888932	0.084434
O	-2.514901	-1.786695	-1.171776
N	1.681538	4.605127	1.812080
H	1.293640	4.989198	2.672554
H	2.415929	3.948405	2.071907
N	-1.264660	4.414111	1.748151
H	-0.983206	4.711669	2.680427
H	-1.699716	5.210009	1.286666
N	-5.770439	1.613698	-1.049705
H	-6.315777	1.163231	-1.783502
H	-6.425674	2.007458	-0.375388
N	-6.173627	-0.721099	0.583381
H	-6.728210	-0.126756	1.198654
H	-6.769431	-1.000914	-0.194806
N	-1.834558	-4.577965	-1.538235
H	-2.459565	-3.799278	-1.753386
H	-1.526070	-4.993602	-2.414893
N	1.143811	-4.713608	-1.556164
H	1.618330	-5.443598	-1.028685
H	0.784010	-5.135055	-2.410657
N	6.161861	0.541304	-0.990346
H	6.067204	1.555654	-0.961710

H	7.012208	0.307981	-0.478426
N	5.784472	-1.957043	0.387769
H	5.255967	-2.787843	0.651360
H	6.398535	-2.220740	-0.381759
H	-5.266437	2.391002	-1.474822
H	2.118347	5.372544	1.303601
H	-1.950217	3.660908	1.838458
H	6.309699	0.269106	-1.961630
H	6.371524	-1.696386	1.179005
H	-2.352858	-5.286669	-1.023774
H	1.826909	-3.999859	-1.814224
H	-5.937187	-1.565214	1.102932
C	3.118884	-1.628283	2.124973
H	0.733535	-3.982140	2.399367
C	-3.356717	-1.200393	2.185019
H	-1.287941	-3.839760	2.452435
N	-3.547791	0.591705	-3.028168
N	1.812208	4.731113	-1.916960
N	4.004452	-0.911329	2.807400
N	-4.091660	-0.341254	2.882253
H	1.216819	5.230013	-1.272401
H	2.084181	5.182600	-2.774058
H	-4.167361	-0.096525	-2.628208
H	-3.431220	0.607874	-4.027608
H	-4.137041	-0.419616	3.884369
H	-4.492457	0.476512	2.448370
H	4.532643	-0.177695	2.358175
H	4.083453	-1.023047	3.804198

**Pt-C-IIIc1 (M11L, SMD water)**

Pt	-0.451246	-3.843208	-0.765653
Pt	-4.472826	0.327281	0.055451
Pt	0.320096	3.729279	0.488355
Pt	4.419207	-0.586030	0.104143
C	-2.097819	2.256355	-2.829500
H	-2.134744	2.357311	-3.907923
N	-1.073379	2.811397	-0.735924
C	3.493821	2.762347	-2.259522
H	3.932990	3.186658	-3.154776
N	3.362794	0.999945	-0.658413
N	1.954107	2.897708	-0.449165
H	6.169345	-1.861500	1.571963
H	5.086934	-2.957221	0.990254
H	6.281892	-2.394322	0.018641
H	6.895574	0.204142	0.213253
H	6.453620	0.171268	-1.368269
H	6.016672	1.439056	-0.410268
H	1.213110	5.018736	2.602008
H	2.300518	3.877410	2.139244
H	2.217793	5.310787	1.336414
H	-1.825711	5.169231	0.794434
H	-1.878889	3.829949	1.766406
H	-1.034258	5.176519	2.234545
H	1.675681	-3.903282	-2.150464
H	1.452814	-5.435538	-1.558846
H	0.636032	-4.954419	-2.902437
H	-1.696562	-4.771311	-2.898547
H	-2.543137	-5.190553	-1.551340
H	-2.593350	-3.628282	-2.104379
H	-6.519474	-0.194205	1.599394

H	-6.826193	-0.784752	0.095889
H	-5.864404	-1.625931	1.124183
H	-6.535430	1.940312	-0.112461
H	-5.266020	2.627278	-0.894254
H	-6.127074	1.426536	-1.620211
N	-5.747935	1.745138	-0.729104
N	-6.104762	-0.686944	0.809645
N	-1.996451	-4.447656	-1.980964
N	0.987837	-4.643865	-1.998568
N	5.625653	-2.125831	0.750987
N	6.139030	0.427368	-0.432996
N	1.660202	4.590643	1.792928
N	-1.286436	4.593832	1.438229
N	-2.948776	1.360014	-0.805181
C	1.979971	-2.989574	2.627336
C	-2.658946	-2.544388	2.654177
H	-2.726440	-2.813590	3.701565
N	-3.275494	-1.128322	0.838277
N	-1.844931	-2.975968	0.458826
N	1.069466	-3.199801	0.439501
N	2.866448	-1.710028	0.818800
H	2.003076	-3.284144	3.670116
C	3.824792	1.517590	-1.817197
C	-1.968404	-3.305218	1.758970
C	1.144828	-3.580550	1.728690
C	-2.969516	1.467532	-2.148509
H	0.505184	-4.406776	2.025412
H	-1.490700	-4.229558	2.070773
H	-3.741689	0.896619	-2.662420
H	4.513861	0.893574	-2.383574
C	-2.577813	-1.926034	-0.028520
O	-2.628015	-1.708524	-1.269748
C	-1.977916	1.997065	-0.090820
O	-1.912458	1.860740	1.163115
C	2.376152	1.670310	0.015999
O	1.853730	1.195682	1.055826
C	1.975890	-2.291125	-0.039703
O	2.002553	-2.007572	-1.269308
C	2.599341	3.502048	-1.469725
C	-1.157992	2.984205	-2.075691
N	2.350749	4.785570	-1.728342
N	-0.352367	3.848314	-2.671248
H	2.829750	5.238173	-2.490302
H	1.860156	5.372598	-1.069711
H	-0.401869	3.972488	-3.668516
H	0.310411	4.407694	-2.160481
C	2.817242	-1.969113	2.146847
C	-3.265490	-1.374325	2.168323
N	3.606547	-1.275871	2.958663
N	-3.869102	-0.511382	2.976822
H	-4.229565	0.363998	2.627087
H	-3.883685	-0.675506	3.969451
H	4.155129	-0.501122	2.616502
H	3.602899	-1.464551	3.947227

**Pt-C-IIIc2 (M11L, SMD water)**

Pt	0.016757	-3.740766	-0.446566
Pt	4.525452	0.024335	-0.171945
Pt	-0.022127	3.648735	0.752499
Pt	-4.626773	-0.032213	-0.174370

C	-3.601762	-1.769054	1.898985
C	-2.944675	3.166668	-2.348734
H	-4.385380	-1.212799	2.412263
C	-2.971880	-2.811789	2.508254
C	1.130956	2.863625	-1.868704
C	2.161826	-1.964632	2.798628
H	0.366469	3.560508	-2.200447
C	1.884693	2.186105	-2.777981
H	2.111752	-2.006882	3.880165
H	1.729272	2.301863	-3.844217
H	-3.238793	-3.139601	3.505946
N	3.059439	1.212576	-0.950615
N	1.283415	2.728139	-0.535881
N	3.147275	-1.119769	0.801861
N	1.339977	-2.644631	0.667616
N	-1.598268	-2.989445	0.567696
N	-3.330478	-1.381035	0.636449
N	-1.628255	3.038055	-0.367727
N	-3.296181	1.406484	-0.775230
H	-3.193034	3.652181	-3.284814
C	1.314244	-2.687711	2.014935
C	-1.983029	-3.479812	1.766731
C	-3.536524	2.002170	-1.963195
C	2.856551	1.301913	-2.283374
C	-2.294430	-1.966985	-0.032765
O	-1.978737	-1.598586	-1.195209
C	2.274112	-1.857334	0.049128
O	2.348238	-1.819430	-1.209886
C	2.281008	1.913754	-0.067886
O	2.499891	1.812752	1.169349
C	-2.302368	1.904370	0.025050
O	-2.003978	1.353018	1.115093
N	-1.326917	-4.843753	-1.550679
H	-2.119915	-4.260096	-1.814027
H	-0.930021	-5.226062	-2.407903
N	1.624374	-4.526622	-1.462749
H	2.188098	-5.114308	-0.851609
H	1.368053	-5.082774	-2.276295
N	-6.105100	-1.380670	0.332574
H	-6.583220	-1.099972	1.188003
H	-6.807966	-1.446292	-0.403174
N	-6.113063	1.240818	-0.835102
H	-6.344054	1.069956	-1.813392
H	-6.968255	1.108935	-0.296287
N	1.561989	4.338163	1.869772
H	2.001505	5.137896	1.419121
H	1.303476	4.618030	2.813941
N	-1.373934	4.549689	2.015369
H	-2.070556	3.868409	2.313094
H	-0.952616	4.945385	2.854194
N	6.030942	-1.166435	0.583991
H	6.599708	-0.663254	1.263230
H	5.662105	-1.995877	1.045863
N	5.957562	1.187784	-1.096483
H	6.404770	0.695789	-1.869350
H	5.559622	2.048877	-1.469362
H	6.648011	-1.482816	-0.162438
H	-1.861872	5.303230	1.532986
H	-5.851568	2.221433	-0.743204
H	-5.735784	-2.319562	0.477262

H	-1.684103	-5.624001	-1.002148
H	2.191505	-3.732784	-1.766519
H	6.689009	1.454061	-0.438827
H	2.235979	3.572114	1.925862
C	3.096037	-1.139715	2.152037
H	0.573305	-3.345164	2.462486
H	-4.257681	1.507097	-2.610861
C	-2.012114	3.729174	-1.463350
N	-1.404328	-4.588985	2.214472
N	3.954026	-0.392351	2.835742
N	-1.465210	4.919251	-1.684114
N	3.603983	0.564543	-3.095622
H	4.503914	0.315534	2.373809
H	3.935460	-0.400762	3.841439
H	-0.730203	-5.084676	1.649591
H	-1.656940	-4.966043	3.112401
H	-1.715061	5.451403	-2.501124
H	-0.817960	5.319845	-1.019826
H	3.464647	0.617786	-4.090705
H	4.202199	-0.162840	-2.736042

**Pt-C-IVc1 (M11L, SMD water)**

Pt	3.987555	-1.382922	0.631715
Pt	1.335468	3.864972	0.120043
Pt	-3.982953	1.404093	-0.631365
Pt	-1.327924	-3.867704	-0.103598
C	3.225189	2.619202	-1.742372
C	-1.434377	2.183651	2.767753
H	2.875686	3.458996	-2.341195
C	4.321217	1.903701	-2.120914
C	1.458233	-2.251213	-2.758600
C	-4.425508	-1.944425	2.011875
C	0.311714	-2.604226	-2.118314
C	-3.310654	-2.649687	1.671069
H	-2.991906	-3.500353	2.271148
H	-0.605053	-2.810714	-2.667385
H	1.511832	-2.169852	-3.837925
H	-5.041764	-2.223829	2.858876
H	4.894648	2.161363	-3.004183
N	-2.558020	-2.372332	0.583725
N	-3.899755	-0.446325	0.242089
N	0.245311	-2.760391	-0.780968
N	2.505332	-2.076942	-0.614899
N	3.888087	0.447030	-0.290212
N	2.530995	2.365916	-0.610502
N	-2.486534	2.042972	0.625163
N	-0.236661	2.757909	0.798422
C	-0.297815	2.577225	2.132812
H	0.615039	2.793923	2.684393
H	-1.482049	2.076882	3.845151
C	2.601778	-2.049039	-1.964252
C	4.697463	0.826235	-1.301337
C	-2.576209	1.971954	1.973182
C	-4.757340	-0.845556	1.203755
C	2.843568	1.245483	0.114083
O	2.199210	0.931285	1.146520
C	-1.320328	2.462152	0.028439
O	-1.267310	2.585412	-1.227746
C	-2.831501	-1.231550	-0.126406
O	-2.130751	-0.885022	-1.109778

C	1.331230	-2.466093	-0.013260
O	1.271953	-2.566527	1.244812
H	4.872848	-0.198858	2.740112
H	5.983028	-1.350961	2.348477
H	5.960883	0.079200	1.542464
H	4.413041	-3.939118	0.910768
H	4.564064	-3.258392	2.400810
H	3.056582	-3.465317	1.741850
H	2.912499	5.926275	0.309809
H	3.773132	4.723185	-0.393260
H	2.702609	5.597569	-1.286390
H	-0.763376	5.277386	0.754490
H	0.439350	5.604326	1.826611
H	0.434070	6.326604	0.348400
H	-4.564277	3.317044	-2.352299
H	-4.400010	3.969902	-0.851190
H	-3.051138	3.508702	-1.702249
H	-5.138744	0.890871	-2.900674
H	-5.594562	-0.260386	-1.820846
H	-6.316098	1.219421	-1.800289
H	0.795007	-5.270653	-0.688854
H	-0.398172	-6.322610	-0.278713
H	-0.392823	-5.624542	-1.768573
N	5.369106	-0.634888	1.963797
N	4.029838	-3.232073	1.533954
N	2.857902	5.171220	-0.373098
N	0.236709	5.455384	0.838681
N	-4.023014	3.273927	-1.490581
N	-5.428259	0.738292	-1.935376
N	-0.202746	-5.457664	-0.780911
N	-2.839408	-5.194768	0.372511
H	-2.699290	-5.608384	1.294211
H	-3.764963	-4.767782	0.362121
H	-2.860210	-5.958702	-0.302332
N	5.822586	0.151606	-1.512214
N	3.785071	-1.841139	-2.519405
N	-5.881746	-0.157726	1.380979
N	-3.750307	1.717343	2.531203
H	-6.528216	-0.428049	2.103278
H	-6.151025	0.585333	0.753958
H	-3.825224	1.648353	3.532226
H	-4.592671	1.625788	1.987292
H	6.133749	-0.569359	-0.879015
H	6.427041	0.406204	-2.275319
H	4.622214	-1.754541	-1.967208
H	3.870735	-1.792737	-3.520695

**Pt-C-IVc2 (M11L, SMD water)**

Pt	-3.749768	0.466755	-0.003601
Pt	0.002935	-0.005786	4.521788
Pt	3.749768	-0.466755	0.003601
Pt	-0.002935	0.005786	-4.521788
C	2.373443	2.821295	2.372254
C	-2.452029	-2.794687	2.421530
C	-2.373443	-2.821295	-2.372254
C	2.452029	2.794687	-2.421530
H	-2.556846	-3.888000	-2.422315
H	2.663846	3.854877	-2.494448
H	-2.663846	-3.854877	2.494448
N	1.234471	0.874628	-3.145841

N	2.903401	0.656795	-1.480209
N	-1.219516	-0.881452	-3.140552
N	-2.873424	-0.681614	-1.455597
N	-2.903401	-0.656795	1.480209
N	-1.234471	-0.874628	3.145841
N	2.873424	0.681614	1.455597
N	1.219516	0.881452	3.140552
H	2.556846	3.888000	2.422315
C	-3.103624	-2.004297	-1.562741
C	-3.176092	-1.968750	1.615725
C	3.103624	2.004297	1.562741
C	3.176092	1.968750	-1.615725
C	-1.971891	-0.083454	2.304716
O	-1.808274	1.166777	2.304024
C	1.960365	0.098652	2.295006
O	1.813872	-1.154098	2.304745
C	1.971891	0.083454	-2.304716
O	1.808274	-1.166777	-2.304024
C	-1.960365	-0.098652	-2.295006
O	-1.813872	1.154098	-2.304745
H	-3.803363	1.834259	2.132908
H	-4.935272	2.527865	1.143208
H	-5.309980	1.156552	1.973385
H	-5.269569	1.079969	-2.033820
H	-4.995175	2.465941	-1.194385
H	-3.794685	1.830884	-2.144348
H	-1.441476	-0.098407	6.682390
H	-2.043419	-1.210803	5.638223
H	-0.692755	-1.554647	6.511092
H	2.055730	1.202477	5.619050
H	0.719150	1.514752	6.524810
H	1.487932	0.064866	6.655072
H	4.995175	-2.465941	1.194385
H	5.269569	-1.079969	2.033820
H	3.794685	-1.830884	2.144348
H	4.935272	-2.527865	-1.143208
H	3.803363	-1.834259	-2.132908
H	5.309980	-1.156552	-1.973385
H	-2.055730	-1.202477	-5.619050
H	-1.487932	-0.064866	-6.655072
H	-0.719150	-1.514752	-6.524810
N	-4.563688	1.640621	1.478172
N	-4.565659	1.600519	-1.514835
N	-1.179553	-0.814750	6.006417
N	1.204361	0.789983	5.997524
N	4.565659	-1.600519	1.514835
N	4.563688	-1.640621	-1.478172
N	-1.204361	-0.789983	-5.997524
N	1.179553	0.814750	-6.006417
H	0.692755	1.554647	-6.511092
H	2.043419	1.210803	-5.638223
H	1.441476	0.098407	-6.682390
C	-1.354595	-2.227965	-3.134091
C	-1.397795	-2.218583	3.148874
H	-4.023476	-2.345035	1.049358
H	-3.920838	-2.404351	-0.970222
H	4.023476	2.345035	-1.049358
H	1.397795	2.218583	-3.148874
C	3.920838	2.404351	0.970222
C	1.354595	2.227965	3.134091

N	-0.537389	-2.953321	-3.887629
N	-0.574140	-2.957607	3.881603
N	0.537389	2.953321	3.887629
N	0.574140	2.957607	-3.881603
H	0.258737	-2.534483	-4.344288
H	-0.630731	-3.955000	-3.909302
H	0.689733	3.956738	-3.912635
H	-0.240532	2.553637	-4.318778
H	0.240532	-2.553637	4.318778
H	-0.689733	-3.956738	3.912635
H	-0.258737	2.534483	4.344288
H	0.630731	3.955000	3.909302

**Pt-C-Id (M11L, SMD water)**

Pt	-1.797384	3.645362	-0.356066
Pt	3.645362	1.797384	0.356066
Pt	-3.645362	-1.797384	0.356066
Pt	1.797384	-3.645362	-0.356066
C	-0.153539	-1.681699	2.879837
C	0.736174	-2.353100	2.093333
H	0.130808	-1.275478	3.843669
H	1.768621	-2.502329	2.401748
N	0.398601	-2.868473	0.896509
N	-1.797384	-2.044740	1.187986
C	0.153539	1.681699	2.879837
C	-0.736174	2.353100	2.093333
H	-0.130808	1.275478	3.843669
H	-1.768621	2.502329	2.401748
N	-0.398601	2.868473	0.896509
N	1.797384	2.044740	1.187986
C	-1.681699	0.153539	-2.879837
C	1.681699	-0.153539	-2.879837
N	2.868473	0.398601	-0.896509
N	2.044740	-1.797384	-1.187986
C	2.353100	0.736174	-2.093333
H	1.275478	0.130808	-3.843669
H	2.502329	1.768621	-2.401748
H	-1.275478	-0.130808	-3.843669
C	-2.353100	-0.736174	-2.093333
N	-2.868473	-0.398601	-0.896509
N	-2.044740	1.797384	-1.187986
H	-2.502329	-1.768621	-2.401748
C	1.451284	1.491403	2.371341
C	1.491403	-1.451284	-2.371341
C	-1.451284	-1.491403	2.371341
C	-1.491403	1.451284	-2.371341
C	0.890641	2.763585	0.455039
O	1.249893	3.323248	-0.615820
C	2.763585	-0.890641	-0.455039
O	3.323248	-1.249893	0.615820
C	-0.890641	-2.763585	0.455039
O	-1.249893	-3.323248	-0.615820
C	-2.763585	0.890641	-0.455039
O	-3.323248	1.249893	0.615820
N	-5.490446	-1.518853	-0.515492
H	-5.437013	-1.701882	-1.516191
H	-6.218098	-2.119213	-0.131762
N	-4.398498	-3.225305	1.637237
H	-4.876948	-2.792106	2.425634
H	-5.063780	-3.843635	1.175774

N	-3.225305	4.398498	-1.637237
H	-3.843635	5.063780	-1.175774
H	-2.792106	4.876948	-2.425634
N	-1.518853	5.490446	0.515492
H	-2.119213	6.218098	0.131762
H	-1.701882	5.437013	1.516191
N	4.398498	3.225305	1.637237
H	4.876948	2.792106	2.425634
H	5.063780	3.843635	1.175774
N	5.490446	1.518853	-0.515492
H	5.437013	1.701882	-1.516191
H	6.218098	2.119213	-0.131762
N	1.518853	-5.490446	0.515492
H	0.553057	-5.789145	0.393591
H	2.119213	-6.218098	0.131762
N	3.225305	-4.398498	-1.637237
H	3.805285	-3.649078	-2.010532
H	3.843635	-5.063780	-1.175774
H	3.649078	3.805285	2.010532
H	5.789145	0.553057	-0.393591
H	1.701882	-5.437013	1.516191
H	2.792106	-4.876948	-2.425634
H	-3.649078	-3.805285	2.010532
H	-5.789145	-0.553057	-0.393591
H	-3.805285	3.649078	-2.010532
H	-0.553057	5.789145	0.393591
N	-2.367614	-0.788186	3.026015
N	-0.788186	2.367614	-3.026015
N	2.367614	0.788186	3.026015
N	0.788186	-2.367614	-3.026015
H	3.251385	0.571527	2.588859
H	2.127787	0.322393	3.884894
H	-0.322393	2.127787	-3.884894
H	-0.571527	3.251385	-2.588859
H	-2.127787	-0.322393	3.884894
H	-3.251385	-0.571527	2.588859
H	0.571527	-3.251385	-2.588859
H	0.322393	-2.127787	-3.884894

**Pt-C-IId (M11L, SMD water)**

Pt	4.555185	0.036854	0.060639
Pt	0.043530	3.690143	0.093946
Pt	-4.428532	0.022654	-0.140103
Pt	0.066385	-3.628655	-0.020379
C	-1.422093	-0.912941	-2.997390
C	-2.569241	-0.489709	-2.391660
H	-1.131150	-0.553508	-3.977938
H	-3.234412	0.225144	-2.872790
N	-2.940822	-0.907428	-1.165597
N	-0.995892	-2.240520	-1.065901
C	1.689681	1.090959	-2.911787
C	2.801262	0.639675	-2.260000
H	1.472182	0.801140	-3.933884
H	3.513160	-0.024884	-2.747279
N	3.077712	0.965615	-0.983548
N	1.110232	2.276988	-0.925466
C	1.541699	-0.865104	2.916721
C	-1.633368	1.059893	2.989620
N	-1.094326	2.306120	1.042274
N	-2.971680	0.866892	1.020916

C	-0.835841	1.932148	2.309682
H	-1.423043	0.772281	4.013896
H	0.044934	2.376456	2.771018
H	1.251382	-0.503582	3.896571
N	1.113396	-2.201943	0.989330
N	3.075130	-0.892770	1.098105
C	2.706022	-0.471312	2.323051
H	3.387042	0.221281	2.812930
C	0.794675	1.897505	-2.184847
C	-2.726195	0.501970	2.298829
C	-0.583021	-1.772650	-2.266364
C	0.698247	-1.720315	2.184364
C	2.293761	-1.794143	0.436640
O	2.659971	-2.263687	-0.679347
C	2.244965	1.818955	-0.313212
O	2.523442	2.196576	0.857054
C	-2.187827	1.802980	0.400410
O	-2.487354	2.204631	-0.758679
C	-2.175698	-1.830311	-0.514736
O	-2.554998	-2.312971	0.589603
N	5.993423	-0.965507	1.143816
H	6.926577	-0.901048	0.740239
H	6.042770	-0.596770	2.092077
N	5.989873	1.036547	-1.029254
H	6.923319	0.976065	-0.625628
H	6.039981	0.660606	-1.974742
N	-1.009783	-5.069956	-1.024433
H	-0.783778	-6.024875	-0.750792
H	-2.004431	-4.928130	-0.854332
N	1.149829	-5.031845	1.028884
H	1.113082	-5.964112	0.619918
H	2.129673	-4.754386	1.067990
N	-5.840621	-0.851320	-1.358166
H	-6.757935	-0.413099	-1.290861
H	-5.549934	-0.801866	-2.333958
N	-5.910268	1.025521	0.886871
H	-6.526936	1.524316	0.247240
H	-6.484344	0.382402	1.430064
N	-1.018631	5.121822	1.126391
H	-0.875606	5.006602	2.128848
H	-0.765533	6.079553	0.888324
N	1.218044	5.099529	-0.845990
H	0.964422	5.173643	-1.829887
H	1.142883	6.030254	-0.438412
H	5.755181	2.024562	-1.102944
H	5.758893	-1.954192	1.209305
H	-0.853638	-4.993535	-2.028210
H	0.810473	-5.101662	1.986800
H	-5.952529	-1.835247	-1.121303
H	-5.520702	1.711437	1.531653
H	-2.014298	5.012712	0.940679
H	2.198907	4.826594	-0.800459
N	-0.356735	2.325671	-2.690589
N	-0.495974	-2.096722	2.626293
N	-3.540524	-0.373571	2.874196
N	0.605080	-2.164678	-2.712055
H	-1.088492	2.643306	-2.060084
H	-0.632382	2.011845	-3.607248
H	0.952709	-1.776367	-3.574598
H	1.287438	-2.543842	-2.059654

H	-0.837097	-1.720687	3.497025
H	-1.177502	-2.489542	1.981061
H	-4.231289	-0.867498	2.330351
H	-3.375225	-0.670157	3.821432

**Pt-C-IIIId (M11L, SMD water)**

Pt	0.000000	3.672487	0.113006
Pt	0.000000	0.000000	-4.347394
Pt	0.000000	-3.672487	0.113006
Pt	0.000000	0.000000	4.590346
C	2.908688	-0.872490	1.611480
H	3.895358	-0.513917	1.341861
N	0.986346	-2.204594	1.137329
N	1.057218	-0.892843	3.103103
C	3.001842	1.078555	-1.437900
C	2.283098	1.948443	-0.672429
H	4.011629	0.784693	-1.173128
H	2.694139	2.381419	0.238401
N	1.036043	2.333242	-1.001933
N	1.101850	0.887792	-2.872426
C	-2.908688	0.872490	1.611480
C	-3.001842	-1.078555	-1.437900
N	-1.101850	-0.887792	-2.872426
N	-1.036043	-2.333242	-1.001933
H	-4.011629	-0.784693	-1.173128
H	-3.895358	0.513917	1.341861
C	-2.290182	0.474531	2.761306
N	-1.057218	0.892843	3.103103
N	-0.986346	2.204594	1.137329
H	-2.767537	-0.217956	3.452039
C	2.290182	-0.474531	2.761306
C	-2.283098	-1.948443	-0.672429
H	2.767537	0.217956	3.452039
H	-2.694139	-2.381419	0.238401
C	2.366071	0.521850	-2.564247
C	-2.366071	-0.521850	-2.564247
C	2.196724	-1.735168	0.756953
C	-2.196724	1.735168	0.756953
C	0.452258	1.836527	-2.129946
O	-0.680331	2.254072	-2.497663
C	-0.402774	1.785304	2.301186
O	0.727680	2.234209	2.635356
C	0.402774	-1.785304	2.301186
O	-0.727680	-2.234209	2.635356
C	-0.452258	-1.836527	-2.129946
O	0.680331	-2.254072	-2.497663
N	1.004686	5.162253	-0.896472
H	0.910873	6.082163	-0.468438
H	1.999532	4.945380	-0.938849
N	-1.058936	5.014583	1.263681
H	-0.862736	5.991512	1.052889
H	-2.058449	4.868124	1.130333
N	1.103861	0.930343	-5.818558
H	1.632463	0.257257	-6.371664
H	0.493956	1.441932	-6.454504
N	-1.103861	-0.930343	-5.818558
H	-1.632463	-0.257257	-6.371664
H	-0.493956	-1.441932	-6.454504
N	1.108972	-0.975706	6.028904
H	2.094275	-0.985582	5.767354

H	1.042138	-0.548597	6.951242
N	-1.108972	0.975706	6.028904
H	-2.094275	0.985582	5.767354
H	-1.042138	0.548597	6.951242
N	1.058936	-5.014583	1.263681
H	0.862736	-5.991512	1.052889
H	2.058449	-4.868124	1.130333
N	-1.004686	-5.162253	-0.896472
H	-0.910873	-6.082163	-0.468438
H	-1.999532	-4.945380	-0.938849
H	-0.803776	1.943406	6.115329
H	0.803776	-1.943406	6.115329
H	0.662271	5.228921	-1.853431
H	-0.854178	4.866108	2.250738
H	-1.767287	-1.597791	-5.427777
H	1.767287	1.597791	-5.427777
H	-0.662271	-5.228921	-1.853431
H	0.854178	-4.866108	2.250738
N	-2.676108	2.131572	-0.416664
N	-2.986575	0.352733	-3.347326
N	2.986575	-0.352733	-3.347326
N	2.676108	-2.131572	-0.416664
H	3.557641	-1.761391	-0.735675
H	2.043790	-2.515275	-1.114536
H	-2.043790	2.515275	-1.114536
H	-3.557641	1.761391	-0.735675
H	3.919772	-0.653137	-3.119153
H	2.480662	-0.868817	-4.050019
H	-2.480662	0.868817	-4.050019
H	-3.919772	0.653137	-3.119153

**Pt-C-IVd (M11L, SMD water)**

Pt	0.000000	3.668006	0.000000
Pt	-4.509069	0.000000	0.000000
Pt	0.000000	-3.668006	0.000000
Pt	4.509069	0.000000	0.000000
C	-1.589966	0.981082	2.941425
C	-2.713272	0.545683	2.299695
H	-1.340811	0.646692	3.942089
H	-3.401267	-0.152217	2.773679
N	-3.032777	0.928571	1.047987
N	-1.082951	2.259702	0.995700
C	1.589966	-0.981082	2.941425
C	2.713272	-0.545683	2.299695
H	1.340811	-0.646692	3.942089
H	3.401267	0.152217	2.773679
N	3.032777	-0.928571	1.047987
N	1.082951	-2.259702	0.995700
C	2.239823	-1.835513	0.405254
O	2.571826	-2.292297	-0.725825
C	1.589966	0.981082	-2.941425
C	-2.239823	1.835513	0.405254
O	-2.571826	2.292297	-0.725825
C	-1.589966	-0.981082	-2.941425
C	-2.239823	-1.835513	-0.405254
O	-2.571826	-2.292297	0.725825
H	1.744681	-4.728708	1.623129
H	0.458697	-5.748355	1.502831
H	1.589346	-5.702673	0.307075
H	-0.458697	-5.748355	-1.502831

H	-1.589346	-5.702673	-0.307075
H	-1.744681	-4.728708	-1.623129
H	-5.594017	-1.390500	-1.919282
H	-6.364583	-1.746327	-0.511274
H	-6.736291	-0.367360	-1.327382
H	-6.736291	0.367360	1.327382
H	-5.594017	1.390500	1.919282
H	-6.364583	1.746327	0.511274
N	1.071383	-5.131041	0.972315
N	-1.071383	-5.131041	-0.972315
N	-5.971432	-0.986041	-1.063290
N	-5.971432	0.986041	1.063290
N	-1.082951	-2.259702	-0.995700
N	-3.032777	-0.928571	-1.047987
C	-2.713272	-0.545683	-2.299695
H	-3.401267	0.152217	-2.773679
H	-1.340811	-0.646692	-3.942089
H	1.340811	0.646692	-3.942089
C	2.713272	0.545683	-2.299695
N	1.082951	2.259702	-0.995700
N	3.032777	0.928571	-1.047987
C	2.239823	1.835513	-0.405254
O	2.571826	2.292297	0.725825
H	3.401267	-0.152217	-2.773679
H	-1.589346	5.702673	0.307075
H	-1.744681	4.728708	1.623129
H	-0.458697	5.748355	1.502831
H	0.458697	5.748355	-1.502831
H	1.589346	5.702673	-0.307075
H	1.744681	4.728708	-1.623129
H	5.594017	1.390500	-1.919282
H	6.364583	1.746327	-0.511274
H	6.736291	0.367360	-1.327382
H	6.364583	-1.746327	0.511274
H	6.736291	-0.367360	1.327382
H	5.594017	-1.390500	1.919282
N	5.971432	0.986041	-1.063290
N	5.971432	-0.986041	1.063290
N	1.071383	5.131041	-0.972315
N	-1.071383	5.131041	0.972315
C	0.720430	-1.821353	2.223845
C	-0.720430	-1.821353	-2.223845
C	0.720430	1.821353	-2.223845
C	-0.720430	1.821353	2.223845
N	0.449042	2.226674	2.705662
N	-0.449042	2.226674	-2.705662
N	-0.449042	-2.226674	2.705662
N	0.449042	-2.226674	-2.705662
H	-1.156644	-2.585521	2.069029
H	-0.760263	-1.868099	3.594459
H	0.760263	-1.868099	-3.594459
H	1.156644	-2.585521	-2.069029
H	0.760263	1.868099	3.594459
H	1.156644	2.585521	2.069029
H	-1.156644	2.585521	-2.069029
H	-0.760263	1.868099	-3.594459

**Pt-U-Ia (M11L, SMD water)**



Pt	-2.920478	2.900943	-0.395214
Pt	2.900943	2.920478	-0.395214
Pt	2.920478	-2.900943	-0.395214
Pt	-2.900943	-2.920478	-0.395214
C	-3.773774	-1.172211	1.853505
C	0.019890	-4.118908	2.491973
C	-4.118908	-0.019890	2.491973
H	-3.922712	-2.148430	2.313337
C	1.172211	-3.773774	1.853505
H	2.148430	-3.922712	2.313337
C	-1.172211	3.773774	1.853505
C	4.118908	0.019890	2.491973
H	-2.148430	3.922712	2.313337
C	-0.019890	4.118908	2.491973
C	3.773774	1.172211	1.853505
H	3.922712	2.148430	2.313337
H	4.558843	0.032243	3.482739
H	-0.032243	4.558843	3.482739
H	-4.558843	-0.032243	3.482739
H	0.032243	-4.558843	3.482739
N	1.172211	3.316087	0.596681
N	-1.187233	3.233171	0.615592
N	3.233171	1.187233	0.615592
N	3.316087	-1.172211	0.596681
N	1.187233	-3.233171	0.615592
N	-1.172211	-3.316087	0.596681
N	-3.233171	-1.187233	0.615592
N	-3.316087	1.172211	0.596681
C	1.220486	3.906667	1.832826
O	2.346382	4.237880	2.322401
C	3.906667	-1.220486	1.832826
O	4.237880	-2.346382	2.322401
C	-1.220486	-3.906667	1.832826
O	-2.346382	-4.237880	2.322401
C	-3.906667	1.220486	1.832826
O	-4.237880	2.346382	2.322401
C	0.000151	2.999969	-0.020838
O	0.003072	2.499064	-1.188249
C	-2.999969	0.000151	-0.020838
O	-2.499064	0.003072	-1.188249
C	2.999969	-0.000151	-0.020838
O	2.499064	-0.003072	-1.188249
C	-0.000151	-2.999969	-0.020838
O	-0.003072	-2.499064	-1.188249
N	-4.686316	2.583010	-1.419431
H	-4.814873	3.203991	-2.216300
H	-4.715618	1.624874	-1.764774
N	-2.491775	4.643134	-1.423406
H	-2.987369	4.726389	-2.309270
H	-2.722767	5.459721	-0.860187
N	4.643134	2.491775	-1.423406
H	4.726389	2.987369	-2.309270
H	5.459721	2.722767	-0.860187
N	2.583010	4.686316	-1.419431
H	3.203991	4.814873	-2.216300
H	1.624874	4.715618	-1.764774
N	2.491775	-4.643134	-1.423406
H	1.493613	-4.676624	-1.627034
H	2.987369	-4.726389	-2.309270
N	4.686316	-2.583010	-1.419431

H	5.480483	-2.712559	-0.795895
H	4.814873	-3.203991	-2.216300
N	-4.643134	-2.491775	-1.423406
H	-4.726389	-2.987369	-2.309270
H	-5.459721	-2.722767	-0.860187
N	-2.583010	-4.686316	-1.419431
H	-3.203991	-4.814873	-2.216300
H	-1.624874	-4.715618	-1.764774
H	2.722767	-5.459721	-0.860187
H	-2.712559	-5.480483	-0.795895
H	-4.676624	-1.493613	-1.627034
H	4.715618	-1.624874	-1.764774
H	2.712559	5.480483	-0.795895
H	-5.480483	2.712559	-0.795895
H	-1.493613	4.676624	-1.627034
H	4.676624	1.493613	-1.627034

**Pt-U-IIa (M11L, SMD water)**

Pt	3.839308	1.977666	-0.036667
Pt	1.802891	-3.528215	-0.650021
Pt	-3.812374	-1.872282	-0.120943
Pt	-1.742078	3.637815	-0.595100
C	-0.418831	2.710825	1.890148
C	-4.897152	1.866674	1.619123
C	0.582822	2.316922	2.723123
H	-1.426936	2.896488	2.259711
C	4.788553	-0.452172	1.339834
C	-0.566878	-2.274869	2.645033
H	5.443239	0.301909	1.777194
C	4.902001	-1.768048	1.671483
C	0.437570	-2.660220	1.811732
H	1.437279	-2.880406	2.185967
H	-0.405339	-2.166919	3.711886
H	5.649103	-2.112811	2.377702
H	0.411555	2.175070	3.784446
H	-5.648619	2.221548	2.315844
N	3.087931	-2.197120	0.191488
N	3.878148	0.007439	0.455524
N	0.264586	-2.816577	0.479424
N	-1.992174	-2.166707	0.742582
N	-3.886709	0.098131	0.382080
N	-3.038701	2.290611	0.192727
N	-0.232650	2.913322	0.565448
N	2.026973	2.277987	0.833913
C	4.022661	-2.698060	1.061286
O	4.060332	-3.954266	1.269521
C	-1.859055	-2.037792	2.103142
O	-2.872741	-1.743002	2.809081
C	-3.977394	2.706664	1.071295
C	1.885041	2.116359	2.189731
O	2.898000	1.822468	2.896309
C	3.006558	-0.873035	-0.123531
O	2.146232	-0.462939	-0.959565
C	1.000428	2.667376	0.032631
O	1.197012	2.831178	-1.216337
C	-0.959933	-2.541736	-0.059279
O	-1.143972	-2.668916	-1.314874
C	-2.985232	0.967972	-0.155267
O	-2.116598	0.571058	-0.988729
N	3.791818	3.977527	-0.542089

H	4.556782	4.280807	-1.140872
H	2.912673	4.123798	-1.040226
N	5.679841	1.680499	-0.937244
H	6.064631	2.517608	-1.372048
H	6.365746	1.347512	-0.261217
N	0.527753	-4.918287	-1.496559
H	0.887218	-5.322063	-2.359187
H	0.329671	-5.682788	-0.855048
N	3.421414	-4.281660	-1.680740
H	3.222165	-5.129081	-2.208910
H	3.797844	-3.592494	-2.328128
N	-5.678007	-1.599789	-0.964725
H	-5.644000	-0.918265	-1.719313
H	-6.100807	-2.448823	-1.333944
N	-3.734367	-3.869348	-0.646944
H	-3.721138	-4.462993	0.179944
H	-4.503281	-4.177485	-1.238303
N	-0.473403	5.074055	-1.364590
H	-0.819298	5.491954	-2.226028
H	-0.315013	5.824311	-0.695944
N	-3.277936	4.398247	-1.742050
H	-3.076027	4.289740	-2.734540
H	-4.153340	3.913196	-1.552531
H	-6.272894	-1.231929	-0.221710
H	-3.427882	5.389491	-1.561678
H	0.410657	4.599640	-1.556371
H	-2.859513	-4.003532	-1.155152
H	4.139476	-4.497621	-0.988706
H	3.795126	4.565592	0.288843
H	5.593632	0.970537	-1.662818
H	-0.338468	-4.415954	-1.699970
C	-4.868398	0.495761	1.252990
O	-5.705777	-0.362893	1.681113
H	-3.956579	3.769729	1.313351

**Pt-U-IIIa (M11L, SMD water)**

Pt	3.189215	-2.800307	-0.240761
Pt	-2.634085	-3.156770	-0.417625
Pt	-3.073732	2.742012	-0.349580
Pt	2.796408	3.036230	-0.404367
C	-0.051483	2.373620	2.671994
C	5.114754	0.316484	1.926466
C	1.358497	-2.596733	2.080178
C	-5.236571	-0.419467	1.517891
H	2.316999	-2.448883	2.578747
C	0.189703	-2.666589	2.773420
C	-4.541880	-1.516444	1.107872
H	-4.818790	-2.520341	1.429639
H	-6.094747	-0.502858	2.175233
H	0.165290	-2.578945	3.854018
H	5.867730	0.379168	2.704092
H	-0.009242	2.230121	3.746051
N	-0.937164	-2.938748	0.690225
N	1.413578	-2.725516	0.736215
N	-3.480954	-1.443810	0.277212
N	-3.714359	0.903062	0.249277
N	-1.303660	2.615738	0.660155
N	1.056464	2.694793	0.589124
N	3.617011	1.360507	0.397762
N	3.734236	-0.991289	0.493360

C	-1.022352	-2.884845	2.061330
O	-2.147010	-3.045452	2.625662
C	-4.824791	0.856027	1.054097
O	-5.436591	1.938223	1.336628
C	1.080482	2.496201	1.926967
C	4.664929	-0.883653	1.465276
C	0.252873	-2.871234	0.035756
O	0.295500	-2.973419	-1.234735
C	3.187500	0.144070	-0.038490
O	2.302041	0.059178	-0.941627
C	-3.057088	-0.219273	-0.159992
O	-2.073698	-0.139180	-0.957627
C	-0.148311	2.718584	-0.050454
O	-0.187175	2.872535	-1.316467
N	5.018669	-2.875622	-1.195179
H	5.182761	-3.749649	-1.691294
H	5.090763	-2.119740	-1.874032
N	2.626688	-4.645595	-0.977479
H	3.240070	-5.008818	-1.704104
H	2.578629	-5.341547	-0.236637
N	-4.352724	-3.385666	-1.545138
H	-4.380875	-4.256723	-2.072383
H	-5.178776	-3.365230	-0.948401
N	-1.812215	-4.904960	-1.141443
H	-2.315878	-5.306834	-1.929353
H	-0.868690	-4.661043	-1.448257
N	-2.460553	4.614200	-0.972168
H	-1.510000	4.503328	-1.327105
H	-3.038389	5.008105	-1.711761
N	-4.880690	2.909151	-1.332357
H	-5.593245	2.759844	-0.616042
H	-5.036819	3.814373	-1.770731
N	4.613345	3.399664	-1.308813
H	4.690729	4.331268	-1.712454
H	5.335190	3.303719	-0.594853
N	1.962621	4.740501	-1.226574
H	2.477802	5.097959	-2.028404
H	1.022444	4.479643	-1.530345
H	-2.449380	5.278124	-0.201314
H	1.894215	5.489994	-0.541963
H	4.801421	2.725422	-2.047672
H	-4.985895	2.195147	-2.049723
H	-1.748867	-5.617357	-0.417821
H	5.775731	-2.758480	-0.523608
H	1.692719	-4.521323	-1.372321
H	-4.435971	-2.619542	-2.211186
C	-1.314402	2.476266	2.027573
O	-2.420677	2.467288	2.649400
H	2.071188	2.458763	2.380165
H	5.045707	-1.826443	1.859504
C	4.588847	1.504638	1.354813
O	4.967725	2.676722	1.677375

**Pt-U-IVa (M11L, SMD water)**

Pt	-2.913934	3.214711	-0.071038
Pt	2.913934	2.636017	-0.657453
Pt	2.913934	-3.214711	-0.071038
Pt	-2.913934	-2.636017	-0.657453
C	-4.603771	-1.033422	1.161148
C	-0.274096	-2.417448	2.666262

C	-5.161337	0.066981	1.736193
H	-4.939864	-2.041160	1.407223
C	5.161337	-0.066981	1.736193
C	0.274096	2.417448	2.666262
C	4.603771	1.033422	1.161148
H	4.939864	2.041160	1.407223
H	5.962721	0.015048	2.462104
H	0.389050	2.263805	3.733577
H	-5.962721	-0.015048	2.462104
H	-0.389050	-2.263805	3.733577
N	1.237002	2.599089	0.494901
N	-1.098689	2.832272	0.768114
N	3.613792	0.956664	0.245616
N	3.660298	-1.392774	0.444796
N	1.098689	-2.832272	0.768114
N	-1.237002	-2.599089	0.494901
N	-3.613792	-0.956664	0.245616
N	-3.660298	1.392774	0.444796
C	1.345921	2.402523	1.829004
C	4.687150	-1.349496	1.352026
O	5.174212	-2.440482	1.792402
C	-1.345921	-2.402523	1.829004
C	-4.687150	1.349496	1.352026
O	-5.174212	2.440482	1.792402
C	-0.005593	2.794602	-0.038864
O	-0.137296	2.967193	-1.295083
C	-3.126196	0.269870	-0.112960
O	-2.200998	0.348354	-0.976385
C	3.126196	-0.269870	-0.112960
O	2.200998	-0.348354	-0.976385
C	0.005593	-2.794602	-0.038864
O	0.137296	-2.967193	-1.295083
N	-4.777963	3.652169	-0.846885
H	-4.888431	4.625604	-1.122513
H	-5.004444	3.072591	-1.651778
N	-2.140657	5.044287	-0.640194
H	-2.762792	5.587087	-1.235832
H	-1.904142	5.618052	0.166687
N	4.648577	2.642601	-1.772406
H	4.673657	3.365046	-2.489318
H	5.457670	2.780970	-1.169118
N	2.258480	4.375433	-1.558331
H	2.725225	4.578676	-2.439436
H	1.260408	4.239033	-1.734648
N	2.140657	-5.044287	-0.640194
H	1.284850	-4.848580	-1.160749
H	2.762792	-5.587087	-1.235832
N	4.777963	-3.652169	-0.846885
H	5.442113	-3.448208	-0.098418
H	4.888431	-4.625604	-1.122513
N	-4.648577	-2.642601	-1.772406
H	-4.673657	-3.365046	-2.489318
H	-5.457670	-2.780970	-1.169118
N	-2.258480	-4.375433	-1.558331
H	-2.725225	-4.578676	-2.439436
H	-1.260408	-4.239033	-1.734648
H	1.904142	-5.618052	0.166687
H	-2.386015	-5.177437	-0.945942
H	-4.760677	-1.743744	-2.238672
H	5.004444	-3.072591	-1.651778

H	2.386015	5.177437	-0.945942
H	-5.442113	3.448208	-0.098418
H	-1.284850	4.848580	-1.160749
H	4.760677	1.743744	-2.238672
C	1.017490	-2.665081	2.128781
O	2.067696	-2.754197	2.836326
H	-2.356158	-2.238922	2.202257
C	-1.017490	2.665081	2.128781
O	-2.067696	2.754197	2.836326
H	2.356158	2.238922	2.202257

<b>Pt-U-Ib (M11L, SMD water)</b>			
Pt	-1.925659	-3.607797	0.348108
Pt	-3.816223	1.827132	-0.164280
Pt	1.697427	3.602914	-0.080587
Pt	3.615331	-1.955709	-0.655020
C	-2.557506	-1.072949	-3.036186
C	0.919633	-1.333037	2.593108
C	1.991800	-1.361271	1.754489
H	2.936804	-0.895049	2.031862
C	-1.951115	1.566592	2.150963
C	5.162051	1.530220	1.203660
H	-2.856394	1.166542	2.604930
C	-0.803053	1.728788	2.864156
C	4.162555	2.426765	0.977825
H	4.186443	3.426053	1.412700
H	6.020337	1.778034	1.818542
H	-0.743658	1.454612	3.911867
H	0.970911	-0.839991	3.557939
N	0.206120	2.608335	0.894613
N	-2.050259	1.901252	0.845331
N	3.090597	2.154641	0.204186
N	3.930741	-0.022955	-0.115508
N	1.966083	-1.975518	0.548379
N	-0.284666	-2.572743	0.961325
N	-3.259309	0.117984	-1.101302
N	-2.489794	-2.100736	-0.889749
C	-2.266698	-2.126287	-2.220247
H	-1.842706	-3.051461	-2.610362
H	-2.386183	-1.120740	-4.105696
C	5.052149	0.238658	0.631205
O	5.924944	-0.678426	0.783603
C	-0.276867	-1.995476	2.205548
O	-1.300256	-2.100697	2.950834
C	-3.075130	0.116326	-2.458149
O	-3.381681	1.157662	-3.125532
C	0.331860	2.303510	2.227158
O	1.413656	2.570499	2.837514
C	-3.030131	-0.977569	-0.327348
O	-3.326886	-0.967160	0.903239
C	-0.950914	2.392633	0.205151
O	-1.018996	2.688531	-1.031245
C	2.974619	0.918187	-0.367333
O	1.996315	0.656081	-1.128204
C	0.797628	-2.552563	0.136597
O	0.726389	-3.093170	-1.013217
N	-1.309622	-5.098775	1.635758
H	-1.953884	-5.884237	1.701240
H	-0.403330	-5.459983	1.344628
N	-3.568305	-4.695038	-0.283949

H	-3.419939	-5.701060	-0.228810
H	-4.388045	-4.471531	0.277728
N	-4.388681	3.564287	0.801839
H	-4.618194	4.306283	0.143352
H	-5.207795	3.405155	1.385148
N	-5.580823	1.763434	-1.227024
H	-6.197815	1.029650	-0.886911
H	-6.099107	2.639603	-1.215734
N	0.324926	5.115781	-0.379092
H	-0.008319	5.497605	0.503693
H	0.677296	5.889488	-0.938631
N	3.160045	4.685307	-1.065050
H	3.494340	5.453601	-0.486021
H	3.961020	4.100052	-1.297541
N	3.350550	-3.947326	-1.145179
H	3.821262	-4.214692	-2.006989
H	3.688709	-4.557630	-0.404960
N	5.334566	-1.878539	-1.787265
H	6.041908	-1.479515	-1.167638
H	5.660889	-2.785592	-2.114692
H	-0.464181	4.689194	-0.867390
H	-3.641704	3.905786	1.404109
H	-5.321183	1.552626	-2.192107
H	-3.789096	-4.469428	-1.253045
H	-1.203818	-4.702688	2.568993
H	2.342850	-4.076824	-1.259060
H	2.807978	5.082500	-1.934878
H	5.227858	-1.273992	-2.598171

**Pt-U-IIb1 (M11L, SMD water)**

Pt	-1.495937	-3.784524	-0.254787
Pt	3.934222	-1.552198	0.001575
Pt	1.591547	3.808035	0.034548
Pt	-3.843723	1.573597	-0.510566
C	2.344293	0.968240	-3.060124
C	-1.247807	2.215633	2.788368
C	-2.278463	1.884589	1.962288
H	-3.195895	1.437522	2.344987
C	-4.720471	-1.910927	1.797381
C	0.872952	-2.217241	2.909410
C	-3.764226	-2.772400	1.351845
C	-0.134602	-2.707473	2.135794
H	-1.101097	-2.980538	2.560257
H	-3.694849	-3.793673	1.727349
H	-5.447877	-2.206126	2.544795
H	0.751313	-2.079912	3.978069
H	-1.299645	2.039771	3.856917
N	-0.004478	-2.902179	0.805644
N	2.194644	-2.055150	0.934253
N	-2.843626	-2.429046	0.425501
N	-3.811893	-0.282903	0.315424
N	-2.249228	2.105933	0.629437
N	-0.076350	2.994222	0.868432
N	3.078981	-0.012929	-1.019115
N	2.070333	2.121396	-0.995635
C	1.918881	2.040054	-2.333860
H	1.439824	2.896404	-2.807863
H	2.223031	0.928305	-4.136908
C	-4.760678	-0.599700	1.252947
O	-5.619974	0.279371	1.583539

C	-0.091145	2.817665	2.229323
O	0.908556	3.206321	2.914999
C	2.980772	-0.104872	-2.383049
O	3.473478	-1.121155	-2.972653
C	2.113076	-1.899329	2.295262
O	3.138498	-1.502681	2.937250
C	-2.850112	-1.160985	-0.085905
O	-1.981390	-0.818774	-0.943273
C	1.167774	-2.552172	0.193632
O	1.295266	-2.721282	-1.060098
C	-1.131050	2.664081	0.075148
O	-1.088628	2.886319	-1.175392
C	2.652804	1.080351	-0.326674
O	2.809109	1.150134	0.930131
N	-3.862236	3.454121	-1.373373
H	-4.391184	3.497919	-2.242180
H	-4.240054	4.157345	-0.742824
N	-5.500418	1.010183	-1.604727
H	-6.088582	1.801398	-1.860924
H	-5.228695	0.534748	-2.462965
N	-0.127753	-5.173491	-0.931896
H	0.157991	-5.802206	-0.184829
H	-0.458426	-5.742188	-1.708626
N	-3.033322	-4.699665	-1.284466
H	-3.275877	-4.154350	-2.110032
H	-2.803151	-5.642499	-1.593185
N	4.821741	-3.069730	1.086340
H	5.837376	-3.082096	1.020840
H	4.561070	-2.904030	2.059466
N	5.684007	-1.080009	-0.989393
H	6.429422	-1.761621	-0.863031
H	5.444308	-1.042567	-1.981013
N	1.153799	5.512118	1.109286
H	1.854789	6.246322	1.033018
H	0.258452	5.908092	0.832836
N	3.297756	4.634996	-0.789803
H	3.473990	5.592034	-0.489549
H	4.107640	4.074240	-0.529345
H	4.480594	-3.986886	0.807664
H	6.041233	-0.170669	-0.705635
H	1.092920	5.219036	2.085390
H	3.238426	4.638103	-1.806761
H	-2.883047	3.671570	-1.571720
H	-6.071462	0.365812	-1.059984
H	-3.867991	-4.762994	-0.703149
H	0.684017	-4.633504	-1.239340

**Pt-U-IIb2 (M11L, SMD water)**

C	-2.579935	1.319053	-3.030907
C	-0.996922	-1.579075	2.753643
C	-0.166480	-2.209384	1.876075
C	4.454938	-2.910770	1.279750
C	1.215185	1.264182	2.680386
C	4.720365	-1.633681	0.890234
H	5.146530	-3.472312	1.897725
H	1.020173	0.862768	3.669061
H	-0.700889	-1.401703	3.781780
N	2.660794	1.571570	0.818073
N	0.477940	2.472402	0.766548
N	3.886945	-0.915393	0.110031

N	2.400298	-2.747022	0.082070
N	-0.508142	-2.461973	0.592199
N	-2.577101	-1.379587	0.986793
N	-1.881520	2.402059	-1.028730
N	-3.433783	0.632788	-0.920156
C	-1.818061	2.233535	-2.366715
C	0.255184	1.938605	1.989054
C	2.709091	-1.474892	-0.304549
O	1.928423	-0.827805	-1.065352
C	1.687062	2.263913	0.167705
O	1.904105	2.736008	-0.994714
C	-1.718857	-2.007817	0.137261
O	-2.046482	-2.195724	-1.076741
C	-2.721950	1.609784	-0.298091
O	-2.850649	1.807435	0.947059
Pt	4.309196	1.038930	-0.243212
Pt	-0.796800	3.821400	-0.070614
Pt	-4.368387	-0.730962	0.258478
Pt	0.691093	-3.662567	-0.551277
N	-0.971931	-4.714950	-1.187058
H	-0.802786	-5.255910	-2.032220
H	-1.298726	-5.355566	-0.467491
N	1.932466	-4.920467	-1.607760
H	1.451281	-5.672436	-2.097276
H	2.480642	-4.404281	-2.292328
N	4.722409	3.033037	-0.572192
H	5.015585	3.505230	0.279499
H	5.435021	3.194756	-1.281054
N	5.957228	0.480278	-1.362349
H	5.771742	0.615705	-2.354651
H	6.782732	1.027333	-1.123380
N	0.317138	5.264904	0.900620
H	-0.050795	6.207921	0.789067
H	0.348819	5.062784	1.898631
N	-2.050572	5.246862	-0.881451
H	-2.680990	5.623127	-0.175496
H	-1.528242	6.026280	-1.277932
N	-5.275340	-2.083110	1.529110
H	-6.287641	-1.989151	1.578203
H	-5.062841	-3.045238	1.274099
N	-6.155150	-0.104261	-0.562260
H	-6.945053	-0.712016	-0.355993
H	-6.400586	0.838494	-0.268742
H	1.274898	5.263454	0.554084
H	-2.624470	4.851974	-1.624661
H	-4.886917	-1.901068	2.455473
H	-5.994911	-0.102050	-1.570952
H	-1.696989	-4.017694	-1.373046
H	2.570039	-5.332707	-0.925413
H	6.188567	-0.502417	-1.226319
H	3.839804	3.438547	-0.890079
C	2.502890	1.105777	2.099935
O	3.486520	0.578818	2.705417
C	3.239758	-3.506876	0.859428
O	2.901513	-4.701023	1.152045
C	-2.280264	-1.167213	2.309280
O	-3.156786	-0.637729	3.066113
C	-3.444999	0.477959	-2.280682
O	-4.218409	-0.392116	-2.798062
H	-0.742059	2.094233	2.398731

H	5.633948	-1.123432	1.195750
H	0.819095	-2.562648	2.179821
H	-2.529564	1.216483	-4.109234
H	-1.123051	2.889556	-2.890284

**Pt-U-IIB3 (M11L, SMD water)**

Pt	-1.180564	-3.804780	-0.409872
Pt	4.092161	-1.347611	0.188043
Pt	1.503035	3.927574	0.086516
Pt	-3.802135	1.525841	-0.477476
C	2.607321	1.144422	-2.927889
C	-1.161552	2.113674	2.854980
C	-4.795555	-2.270869	1.181681
C	0.948218	-2.188843	2.940276
C	-3.702432	-3.016018	0.861429
H	-5.616690	-2.682234	1.757557
H	0.788475	-2.070251	4.006299
H	-1.173833	1.931496	3.923899
N	0.211535	-2.944724	0.806135
N	2.312454	-1.883724	1.012971
N	-2.672615	-2.532136	0.134949
N	-3.772492	-0.446310	0.039913
N	-2.222063	2.006926	0.721969
N	-0.056546	2.928976	0.914343
N	3.262937	0.189294	-0.848261
N	2.179854	2.279792	-0.879212
C	2.101125	2.195100	-2.224266
C	-0.086778	2.677576	2.241699
C	2.078219	-1.731127	2.335235
C	-2.702811	-1.230466	-0.282754
O	-1.748888	-0.768719	-0.980536
C	1.355960	-2.471737	0.236516
O	1.546592	-2.602641	-1.013895
C	-1.123912	2.570323	0.144712
O	-1.097068	2.788368	-1.108832
C	2.769968	1.266470	-0.176981
O	2.877906	1.348091	1.084986
N	-3.852459	3.522547	-1.011160
H	-4.461503	3.728657	-1.800315
H	-4.144868	4.107610	-0.231778
N	-5.435594	1.058194	-1.650867
H	-5.907823	1.866377	-2.050213
H	-5.182576	0.436793	-2.415509
N	0.284723	-5.142684	-0.977190
H	0.532294	-5.763694	-0.210440
H	0.031955	-5.718490	-1.777836
N	-2.589741	-4.676392	-1.645479
H	-3.087697	-3.949629	-2.157097
H	-2.194062	-5.319603	-2.328765
N	4.966632	-2.908554	1.228517
H	5.958908	-2.753740	1.399337
H	4.518433	-3.041960	2.134019
N	5.880322	-0.831302	-0.700800
H	6.641507	-1.484408	-0.527580
H	5.688605	-0.813924	-1.703684
N	0.803371	5.619754	1.045621
H	1.339205	6.459006	0.830006
H	-0.164855	5.795491	0.782331
N	3.099659	4.948445	-0.734383
H	3.373846	5.764315	-0.189507

H	3.909860	4.334501	-0.797848
H	4.874728	-3.780497	0.710270
H	6.190957	0.093997	-0.412995
H	0.828648	5.490891	2.056038
H	2.876693	5.265775	-1.676328
H	-2.892776	3.765023	-1.265374
H	-6.085553	0.571849	-1.031855
H	-3.275816	-5.194176	-1.098529
H	1.100139	-4.577385	-1.222742
C	-2.307687	1.791636	2.076388
O	-3.384403	1.345686	2.577945
C	-0.023016	-2.871326	2.156998
O	-1.060236	-3.416145	2.645419
C	-4.850479	-0.924235	0.740103
O	-5.844884	-0.155694	0.956655
C	3.239559	0.092570	-2.215774
O	3.793819	-0.909145	-2.773442
H	2.545818	1.102511	-4.009529
H	1.612668	3.032758	-2.722418
H	0.805933	2.966806	2.796193
H	-3.609344	-4.055721	1.175274
H	2.864575	-1.226063	2.896574

**Pt-U-IIb4 (M1 1L, SMD water)**

Pt	3.649133	1.846264	-0.110158
Pt	-1.909718	3.660345	-0.202083
Pt	-3.848304	-1.822627	0.374005
Pt	1.632688	-3.670907	-0.737793
C	-2.680179	0.528648	-2.997633
C	-0.362347	-2.362732	2.786971
C	4.894093	-1.958730	1.366898
C	0.627544	2.226743	2.902743
H	5.693237	-2.336834	1.994264
H	0.550988	2.094540	3.976350
H	-0.086829	-2.230446	3.826961
N	1.892339	2.123772	0.886502
N	-0.352213	2.859599	0.828911
N	3.770395	-0.143432	0.307513
N	2.966293	-2.343072	0.023232
N	0.220537	-2.999972	0.566049
N	-1.972277	-2.259323	1.037561
N	-2.410031	1.884201	-1.058628
N	-3.174556	-0.336625	-0.837286
C	-3.083513	-0.479547	-2.174243
C	-0.422632	2.680177	2.165614
C	2.854227	-1.001550	-0.224771
O	1.921094	-0.573856	-0.968003
C	0.812660	2.563547	0.180691
O	0.893179	2.727826	-1.078288
C	-1.051900	-2.720498	0.147800
O	-1.374316	-2.909632	-1.065425
C	-2.851826	0.864607	-0.270620
O	-2.986461	1.026006	0.979943
N	0.321996	-5.085096	-1.476021
H	0.592675	-5.449219	-2.387028
H	0.230254	-5.872564	-0.838907
N	3.091339	-4.346631	-2.032126
H	3.014648	-5.344543	-2.221841
H	3.025302	-3.856656	-2.922917
N	3.539147	3.858030	-0.571742

H	3.541897	4.426143	0.272855
H	4.290152	4.189470	-1.173042
N	5.457175	1.600459	-1.081484
H	5.371607	0.943334	-1.853481
H	5.857619	2.461103	-1.450061
N	-1.424359	5.483266	0.644377
H	-2.250042	6.026373	0.892156
H	-0.873464	5.357961	1.491974
N	-3.468317	4.495841	-1.265422
H	-3.503378	5.511972	-1.219183
H	-3.321714	4.216940	-2.236588
N	-4.537194	-3.283495	1.658909
H	-5.545422	-3.274773	1.798094
H	-4.272834	-4.218844	1.357962
N	-5.744910	-1.373219	-0.317312
H	-6.482908	-1.937164	0.099680
H	-5.957706	-0.394903	-0.129109
H	-0.869982	6.041951	-0.002131
H	-4.369313	4.138838	-0.954895
H	-4.085193	-3.084881	2.553582
H	-5.787514	-1.509644	-1.325931
H	-0.579863	-4.611042	-1.559525
H	4.024141	-4.177728	-1.658800
H	6.100699	1.208888	-0.392203
H	2.649767	3.998305	-1.052456
C	0.536292	-2.809434	1.866095
C	1.857907	1.947985	2.247919
O	2.906639	1.577969	2.862584
C	3.966607	-2.787813	0.815547
C	-2.329796	1.778081	-2.423641
O	-1.970824	2.794560	-3.103802
H	-2.625428	0.395609	-4.072299
H	-3.361883	-1.457763	-2.563729
H	-1.378656	2.930253	2.624220
C	-1.687720	-2.080316	2.367848
O	-2.614629	-1.695753	3.152503
C	4.811073	-0.567894	1.093461
O	5.654165	0.283560	1.524432
H	1.561222	-3.052855	2.145692
H	3.990360	-3.864857	0.983776

**Pt-U-IIIb1 (M1 1L, SMD water)**

Pt	2.739464	-2.900820	-0.403865
Pt	2.737887	3.043965	-0.480039
Pt	-3.076431	2.968656	0.128154
Pt	-3.079431	-2.907865	0.143931
C	-1.122431	-2.377192	2.306203
C	-2.821767	0.023917	-2.932217
H	-2.055032	-2.270393	2.859762
C	0.089221	-2.311472	2.921954
C	-1.086554	2.507556	2.268074
C	5.340809	0.110666	1.125921
H	-2.011856	2.368009	2.826204
C	0.129500	2.470957	2.876778
C	4.697007	1.254497	0.766768
H	5.096660	2.236601	1.020411
H	6.278182	0.131497	1.670227
H	0.224803	2.301256	3.943627
H	0.174495	-2.148971	3.990857
N	1.119288	2.853585	0.744421

N	-1.230567	2.733311	0.942263
N	3.534270	1.258045	0.081161
N	3.565581	-1.101333	0.095176
N	1.102655	-2.663322	0.794270
N	-1.252728	-2.591763	0.978437
N	-2.973103	1.203299	-0.868194
N	-3.037021	-1.149793	-0.872073
C	-2.833394	1.179023	-2.210746
H	-2.724108	0.029344	-4.011996
H	-2.739671	2.153136	-2.691253
C	4.765415	-1.132090	0.758152
O	5.314720	-2.257042	1.000673
C	1.266696	-2.506183	2.147843
O	2.429769	-2.561861	2.654992
C	-2.949484	-1.207862	-2.239472
O	-3.000731	-2.344356	-2.812394
C	1.297421	2.695673	2.096615
O	2.462419	2.775282	2.593922
C	2.945272	0.066234	-0.244197
O	1.845294	0.054591	-0.875063
C	-0.128741	-2.700840	0.211363
O	-0.235349	-2.868344	-1.044975
C	-0.115664	2.878198	0.169868
O	-0.234085	3.065561	-1.082437
C	-3.072462	0.024334	-0.184266
O	-3.210859	0.032383	1.076655
N	1.970737	4.870053	-1.062079
H	2.036147	5.557937	-0.315214
H	2.417870	5.265026	-1.887005
N	4.374397	3.239859	-1.733265
H	4.315008	2.562109	-2.491136
H	4.453333	4.164150	-2.154115
N	4.415346	-3.186233	-1.578132
H	5.213446	-3.029612	-0.960616
H	4.491377	-4.119799	-1.976428
N	1.930806	-4.723080	-0.953093
H	0.961811	-4.531175	-1.214356
H	2.400368	-5.159772	-1.743996
N	-4.910136	-3.253306	-0.739677
H	-5.252874	-4.205951	-0.635903
H	-5.625976	-2.623884	-0.384569
N	-3.129773	-4.704997	1.170765
H	-3.835673	-5.347308	0.814717
H	-2.228228	-5.174754	1.107804
N	-4.964960	3.225222	-0.665889
H	-5.613823	2.554860	-0.256947
H	-5.344543	4.157038	-0.506039
N	-3.218120	4.784161	1.101857
H	-3.132439	5.555104	0.441919
H	-4.110218	4.886237	1.583349
H	5.242075	3.062376	-1.229399
H	0.985960	4.700396	-1.275646
H	1.940557	-5.385721	-0.181241
H	4.456097	-2.517488	-2.343471
H	-4.773318	-3.068617	-1.734404
H	-3.327995	-4.546844	2.157470
H	-2.481171	4.891775	1.797352
H	-4.958603	3.068321	-1.672577

Pt-U-IIIb2 (M1 1L, SMD water)

Pt	-2.902393	2.981840	-0.449225
Pt	-2.878882	-2.866453	-0.338690
Pt	2.992624	-2.885855	0.004285
Pt	2.970099	2.968635	0.038500
C	2.576336	0.063875	-3.058006
C	-0.227868	2.633634	2.840647
C	-5.048248	0.098150	1.839487
C	-0.136687	-2.436095	2.880288
H	-5.814378	0.118442	2.606085
H	-0.213057	-2.307520	3.954218
H	-0.328468	2.504525	3.912463
N	-1.177669	-2.666722	0.752127
N	1.177522	-2.695910	0.911006
N	-3.591758	-1.110582	0.394618
N	-3.585169	1.247919	0.354248
N	-1.223017	2.876211	0.690590
N	1.126985	2.876616	0.898591
N	2.821721	-1.129755	-1.011905
N	2.737181	1.227587	-0.986723
H	2.470564	0.077522	-4.137071
C	-4.539690	1.244613	1.309816
C	-1.317446	2.701944	2.026744
C	2.593162	1.214398	-2.328110
C	-1.244390	-2.495989	2.090083
C	-3.092447	0.056302	-0.101140
O	-2.186914	0.044675	-0.989118
C	0.016121	2.967295	0.119521
O	0.119826	3.154995	-1.133044
C	0.048568	-2.750584	0.152505
O	0.121486	-2.904728	-1.106674
C	2.844356	0.041043	-0.315276
O	2.981426	0.039816	0.945647
N	-2.133603	-4.640021	-1.096768
H	-2.127033	-5.374557	-0.393073
H	-2.644550	-4.989213	-1.904830
N	-4.639943	-3.095541	-1.391894
H	-4.610259	-2.578783	-2.268798
H	-4.839326	-4.070132	-1.612677
N	-4.637325	3.077749	-1.561413
H	-5.449242	2.899605	-0.972221
H	-4.776771	3.980772	-2.012146
N	-2.215928	4.744563	-1.272847
H	-1.228249	4.581879	-1.482138
H	-2.695387	5.005343	-2.131716
N	4.844410	3.059446	-0.827679
H	5.445534	3.778902	-0.430806
H	5.317800	2.164381	-0.714460
N	3.261050	4.701550	1.118575
H	4.216903	5.050251	1.092776
H	2.647022	5.451633	0.810682
N	4.799742	-3.118602	-0.967842
H	5.480989	-2.427939	-0.661702
H	5.217161	-4.040231	-0.854730
N	3.216017	-4.635035	1.083111
H	2.558780	-5.352428	0.786395
H	4.152381	-5.030650	1.029196
H	-5.421584	-2.738142	-0.845653
H	-1.170953	-4.440394	-1.376989
H	-2.296403	5.521956	-0.622007
H	-4.626952	2.367463	-2.291196

H	4.764638	3.242318	-1.826636
H	3.028912	4.460449	2.084154
H	3.020620	-4.392619	2.055550
H	4.605080	-2.970944	-1.958932
H	2.498241	2.192124	-2.800941
C	2.720159	-1.174199	-2.378249
O	2.776956	-2.303336	-2.966429
C	1.141117	-2.557554	2.275467
O	2.235112	-2.564102	2.927746
H	-2.249955	-2.425234	2.506144
H	-2.329316	2.631180	2.424912
C	1.063052	2.733470	2.261968
O	2.145563	2.713406	2.932132
C	-4.563902	-1.148145	1.360611
O	-4.984110	-2.276135	1.772876
H	-4.885117	2.227104	1.632484

**Pt-U-IVb (M11L, SMD water)**

Pt	-0.488030	-3.680923	-0.559830
Pt	4.453225	-0.599315	0.313485
Pt	0.667999	3.785358	-0.121990
Pt	-4.354440	0.812752	-0.252093
C	-0.309085	1.868174	1.944295
C	2.622380	1.341580	-3.016954
H	0.682548	2.063363	2.350397
C	-1.241539	1.158635	2.637912
C	-4.224182	-3.127047	1.337371
C	1.089861	-1.556457	2.778679
C	-3.001516	-3.553348	0.920712
C	0.291230	-2.218378	1.895578
H	-0.684319	-2.604274	2.191497
H	-2.596257	-4.518151	1.227942
H	-4.844775	-3.729190	1.992076
H	0.777110	-1.386173	3.803024
H	-1.028586	0.762078	3.624760
N	0.653666	-2.458117	0.615097
N	2.680829	-1.306532	1.028301
N	-2.214057	-2.829877	0.093339
N	-3.845166	-1.127598	0.097307
N	-2.705204	1.411819	0.778781
N	-0.557236	2.395023	0.723358
N	3.472856	0.712036	-0.886840
N	1.839875	2.405157	-1.035396
C	1.809031	2.225354	-2.373418
H	1.093850	2.844852	-2.914033
H	2.595592	1.227874	-4.094937
C	-4.683667	-1.858807	0.897884
O	-5.823088	-1.380871	1.207034
C	-2.523182	0.949494	2.059414
O	-3.481663	0.380540	2.666751
C	3.509698	0.544254	-2.245189
O	4.324347	-0.298471	-2.743759
C	2.361873	-1.098987	2.345950
O	3.209416	-0.534174	3.109769
C	-2.635840	-1.595505	-0.323171
O	-1.912508	-0.917327	-1.113866
C	-1.763145	2.147356	0.131073
O	-2.005221	2.628483	-1.023567
C	2.705529	1.659514	-0.284330
O	2.805463	1.873374	0.960470

C	1.853012	-1.963134	0.170841
O	2.197751	-2.142538	-1.038932
H	1.050894	-5.210741	-2.057272
H	1.910566	-3.965962	-1.364722
H	1.536848	-5.331734	-0.490651
H	-1.409516	-5.936928	-1.510479
H	-2.628570	-4.834316	-1.514860
H	-1.484236	-4.795558	-2.693421
H	-5.520527	2.929126	-1.325125
H	-5.141424	3.265308	0.240614
H	-3.938818	3.215549	-0.905245
H	-6.712228	0.874241	-1.456960
H	-5.797288	-0.318963	-2.126564
H	-6.457876	-0.536942	-0.621554
H	-0.449681	5.103409	1.812310
H	-0.307286	6.152250	0.554091
H	-1.512095	5.034753	0.559738
H	2.447057	4.876550	-1.695016
H	1.321062	6.016617	-1.330794
H	2.496723	5.641216	-0.242428
H	6.442181	1.031963	-0.208031
H	7.032462	-0.502303	-0.274891
H	6.077002	0.067820	-1.505173
H	5.228557	-2.878683	1.347793
H	6.405243	-1.773249	1.664190
H	4.991579	-1.739844	2.523213
N	1.200604	-4.684076	-1.199540
N	-1.634732	-4.961375	-1.699548
N	6.226857	0.079879	-0.494978
N	5.398374	-1.908045	1.602100
N	1.869763	5.250836	-0.943694
N	-0.534622	5.190280	0.800888
N	-4.818723	2.793627	-0.600519
N	-6.032693	0.144635	-1.252543

**Pt-U-Ic (M11L, SMD water)**

Pt	0.762003	3.601911	-0.007060
Pt	0.223509	-0.064063	4.653211
Pt	-0.762003	-3.601911	0.007060
Pt	-0.223509	0.064063	-4.653211
C	2.492410	-3.084470	2.732880
C	-2.510774	2.187021	2.330684
C	-1.700285	2.795257	1.422633
H	-2.095568	3.489447	0.682421
C	1.700285	-2.795257	-1.422633
C	-2.492410	3.084470	-2.732880
H	2.095568	-3.489447	-0.682421
C	2.510774	-2.187021	-2.330684
C	-2.050258	2.022337	-3.459803
H	-2.690659	1.539414	-4.197610
H	-3.481354	3.503487	-2.884779
H	3.582160	-2.355136	-2.333488
H	-3.582160	2.355136	2.333488
N	0.567334	-1.168449	-3.245666
N	0.360944	-2.605151	-1.383054
N	-0.804928	1.507424	-3.337193
N	-0.432408	3.009053	-1.551715
N	-0.360944	2.605151	1.383054
N	-0.567334	1.168449	3.245666
N	0.432408	-3.009053	1.551715



N	0.804928	-1.507424	3.337193
C	2.050258	-2.022337	3.459803
H	2.690659	-1.539414	4.197610
H	3.481354	-3.503487	2.884779
C	-1.623894	3.650843	-1.764709
O	-1.904106	4.692619	-1.088945
C	-1.931429	1.322906	3.292198
O	-2.595499	0.711151	4.187533
C	1.623894	-3.650843	1.764709
O	1.904106	-4.692619	1.088945
C	1.931429	-1.322906	-3.292198
O	2.595499	-0.711151	-4.187533
C	0.026248	2.019949	-2.376801
O	1.215366	1.603978	-2.257697
C	0.210313	1.769030	2.306882
O	1.468043	1.573727	2.293626
C	-0.026248	-2.019949	2.376801
O	-1.215366	-1.603978	2.257697
C	-0.210313	-1.769030	-2.306882
O	-1.468043	-1.573727	-2.293626
N	1.862489	4.605434	-1.430495
H	2.748174	4.970991	-1.084830
H	2.064359	3.962806	-2.195569
N	1.996933	4.227302	1.527364
H	2.889182	4.595498	1.203269
H	1.551112	4.945020	2.093772
N	-0.953639	1.273364	-6.170497
H	-0.427883	1.150411	-7.034514
H	-1.929345	1.061332	-6.374993
N	0.302745	-1.359431	-6.051489
H	-0.490737	-1.635416	-6.627300
H	1.030929	-1.005446	-6.668824
N	-1.996933	-4.227302	-1.527364
H	-1.551112	-4.945020	-2.093772
H	-2.889182	-4.595498	-1.203269
N	-1.862489	-4.605434	1.430495
H	-2.064359	-3.962806	2.195569
H	-2.748174	-4.970991	1.084830
N	0.953639	-1.273364	6.170497
H	1.929345	-1.061332	6.374993
H	0.427883	-1.150411	7.034514
N	-0.302745	1.359431	6.051489
H	-1.030929	1.005446	6.668824
H	0.490737	1.635416	6.627300
H	-0.665466	2.195745	5.597326
H	0.897608	-2.259531	5.919875
H	-2.167866	-3.401599	-2.105348
H	-1.329456	-5.386257	1.807862
H	-0.897608	2.259531	-5.919875
H	0.665466	-2.195745	-5.597326
H	1.329456	5.386257	-1.807862
H	2.167866	3.401599	2.105348
<b>Pt-U-IIc1 (M11L, SMD water)</b>			
Pt	-0.211285	-3.811540	-0.846575
Pt	-4.491483	0.141535	0.165672
Pt	0.087573	3.848944	0.373851
Pt	4.493414	-0.244061	0.286657
C	-2.194584	2.087839	-2.812128
C	-2.132790	-2.360010	2.673827

C	-1.386854	-3.043421	1.762955
H	-0.670096	-3.800916	2.073282
C	2.587823	-3.397634	2.323315
C	3.453723	3.043198	-2.096285
C	3.250106	-2.269017	1.955340
C	3.859127	1.834889	-1.625652
H	4.655376	1.277716	-2.120189
H	3.956980	-1.790025	2.632274
H	2.766239	-3.873745	3.281292
H	3.921588	3.502239	-2.960174
H	-2.026639	-2.538094	3.738067
N	3.337031	1.252717	-0.516672
N	1.774788	3.020114	-0.417035
N	3.097409	-1.673582	0.746909
N	1.388250	-3.234700	0.280587
N	-1.496932	-2.856581	0.428112
N	-3.168195	-1.241084	0.851063
N	-1.207985	2.704990	-0.728075
N	-3.049099	1.223500	-0.767236
C	-3.062566	1.307620	-2.115772
H	-3.827791	0.713727	-2.615723
H	-2.232513	2.155923	-3.893725
C	1.664334	-3.962542	1.408272
O	1.070432	-5.072392	1.597429
C	-3.060125	-1.395936	2.209869
O	-3.797888	-0.692553	2.974752
C	-1.246077	2.865325	-2.093373
O	-0.466539	3.693713	-2.654008
C	2.432185	3.730451	-1.389143
O	2.109755	4.938088	-1.614841
C	-2.429832	-1.965384	-0.033792
O	-2.612612	-1.832979	-1.284133
C	2.125875	-2.145951	-0.094861
O	1.916352	-1.595522	-1.215872
C	2.230026	1.822592	0.056628
O	1.642749	1.256175	1.026720
C	-2.096861	1.907419	-0.067496
O	-2.059382	1.826770	1.200933
N	1.131442	-4.755729	-2.092872
H	0.710912	-5.148324	-2.933195
H	1.846592	-4.092018	-2.385490
N	-1.824967	-4.425583	-1.981041
H	-1.578022	-4.713926	-2.925417
H	-2.315379	-5.198545	-1.536992
N	-5.974110	-0.934359	1.117153
H	-6.884468	-0.479467	1.112388
H	-6.084875	-1.860530	0.710675
N	-5.875959	1.518185	-0.517393
H	-6.621374	1.061215	-1.040470
H	-6.307297	2.021010	0.256609
N	-1.595452	4.703516	1.215227
H	-2.194940	3.933842	1.515667
H	-1.390544	5.286675	2.024332
N	1.376649	5.058094	1.438216
H	2.042600	5.452112	0.774052
H	0.919394	5.828398	1.922211
N	5.889321	-1.624988	0.935049
H	5.558325	-2.582815	0.831247
H	6.750568	-1.544451	0.395397
N	6.067535	1.074646	0.037693

H	5.758893	2.046032	0.040431
H	6.743190	0.972332	0.794477
H	-5.658911	-1.035147	2.083603
H	1.596083	-5.513517	-1.595412
H	-2.444999	-3.613769	-2.029574
H	6.130175	-1.484205	1.915498
H	6.562425	0.907866	-0.837805
H	-2.103109	5.272765	0.542101
H	1.895320	4.517266	2.127047
H	-5.446917	2.208801	-1.131554

**Pt-U-IIc2 (M1 1L, SMD water)**

Pt	0.183253	3.560462	0.630259
Pt	-4.640497	0.141687	-0.080939
Pt	-0.164991	-3.668119	-0.460369
Pt	4.680345	-0.244221	-0.143590
C	-2.661222	-2.335684	2.768264
C	-2.049661	2.210328	-2.746739
C	-1.167596	2.800022	-1.893948
H	-0.373922	3.449473	-2.257379
C	2.926167	2.763996	-2.547838
C	2.505734	-2.545768	2.680333
C	3.565316	1.664342	-2.065436
H	4.262234	1.102495	-2.687093
H	3.111368	3.134618	-3.549875
H	2.610465	-2.776615	3.734278
H	-1.978632	2.351655	-3.819603
N	3.270602	-1.445529	0.712146
N	1.369902	-2.844307	0.606528
N	3.404301	1.206919	-0.801424
N	1.728453	2.844323	-0.497490
N	-1.224746	2.649863	-0.550811
N	-3.133846	1.284623	-0.843261
N	-1.611784	-2.768868	0.673594
N	-3.382413	-1.202973	0.801876
H	-2.754976	-2.537477	3.829333
C	2.009892	3.438663	-1.700271
O	1.434614	4.531109	-2.009936
C	-3.083096	1.406526	-2.209046
O	-3.965707	0.821450	-2.920175
C	-1.756396	-2.996654	1.996084
C	1.535301	-3.117838	1.918098
C	-2.230209	1.883515	-0.019593
O	-2.327972	1.751755	1.241678
C	2.472399	1.809826	-0.000343
O	2.302181	1.433587	1.196830
C	2.272355	-2.017682	-0.012681
O	2.181047	-1.819077	-1.264741
C	-2.472242	-1.892369	0.060591
O	-2.419737	-1.751345	-1.200280
N	1.628435	4.457808	1.791210
H	1.276098	4.836747	2.668684
H	2.337885	3.759005	2.010215
N	-1.352093	4.312300	1.790726
H	-1.053691	4.603257	2.719453
H	-1.799973	5.108322	1.342566
N	-5.937481	1.484545	-0.962972
H	-6.912970	1.194141	-0.946036
H	-5.877727	2.400558	-0.524376
N	-6.201804	-0.982574	0.670653

H	-7.116497	-0.551492	0.553556
H	-6.237215	-1.906707	0.246949
N	-1.706714	-4.499791	-1.544979
H	-2.314669	-3.717050	-1.795275
H	-1.409508	-4.971615	-2.396148
N	1.286851	-4.537044	-1.639058
H	1.775337	-5.284083	-1.149860
H	0.929215	-4.917593	-2.513558
N	6.210671	0.910119	-0.928136
H	5.973802	1.901492	-0.915154
H	7.074391	0.800469	-0.398601
N	6.038650	-1.664905	0.484476
H	5.902252	-2.549312	0.000320
H	7.012455	-1.393779	0.364286
H	-5.636845	1.562037	-1.935603
H	2.078818	5.216493	1.282789
H	-2.028048	3.550224	1.884379
H	6.412705	0.653051	-1.893637
H	5.865583	-1.804836	1.481195
H	-2.238727	-5.166842	-0.990704
H	1.950462	-3.790258	-1.856020
H	-6.011402	-1.082349	1.668894
C	3.403526	-1.640728	2.064420
O	4.338973	-1.041657	2.688949
H	0.856129	-3.853680	2.341663
C	-3.495275	-1.365821	2.159989
O	-4.350397	-0.673151	2.803242
H	-1.119777	-3.766406	2.424773

**Pt-U-IIIc1 (M1 1L, SMD water)**

Pt	-0.308718	3.743725	-0.447685
Pt	-4.480747	-0.553907	-0.107229
Pt	0.450011	-3.802837	0.723392
Pt	4.530502	0.343243	-0.049434
C	2.919708	1.399604	2.147673
C	2.741525	-2.510653	-2.660275
H	3.685796	0.833318	2.677849
C	1.996621	2.145781	2.807734
C	-1.202170	-3.550873	-1.732066
C	-3.544917	2.859842	2.164638
H	-0.526535	-4.342825	-2.044240
C	-2.119669	-3.032848	-2.591736
C	-3.888599	1.608386	1.761603
H	-4.607511	1.015528	2.326822
H	-3.996515	3.320677	3.036284
H	-2.183393	-3.360687	-3.623078
N	1.988193	2.215536	3.889799
H	-2.962448	-1.750265	-0.768653
N	-1.086794	-3.147427	-0.449292
N	-3.396549	1.023427	0.640297
N	-1.939994	2.871679	0.416513
N	1.062126	2.720620	0.685256
N	2.963511	1.319284	0.799385
N	1.858646	-2.940429	-0.487819
N	3.392443	-1.168648	-0.806109
C	1.972311	-3.233671	-1.800996
H	2.816627	-2.770247	-3.710202
H	1.426561	-4.108809	-2.144581
C	-2.605501	3.583299	1.381753
O	-2.359810	4.819128	1.537654

C	1.052010	2.891338	2.050958
O	0.232136	3.698873	2.581190
C	3.451874	-1.391473	-2.159402
O	4.159891	-0.620885	-2.886110
C	-3.015963	-2.048315	-2.109421
O	-3.885427	-1.472109	-2.842181
C	2.012818	1.963110	0.061954
O	2.029496	1.871224	-1.207192
C	-2.368170	1.649164	-0.017603
O	-1.827469	1.111156	-1.029138
C	-2.007588	-2.262566	0.051434
O	-1.969147	-1.948830	1.281500
C	2.644088	-1.941053	0.028546
O	2.684817	-1.762852	1.284407
N	1.312543	4.641004	-1.361140
H	1.915623	3.877883	-1.673464
H	1.063744	5.215861	-2.163683
N	-1.690026	4.811566	-1.543336
H	-2.291928	5.298313	-0.880089
H	-1.289657	5.499923	-2.177497
N	5.715405	1.858020	0.711908
H	6.051605	1.620006	1.643643
H	6.528811	2.054412	0.130838
N	6.167611	-0.615701	-0.861166
H	7.022315	-0.062764	-0.843115
H	6.357378	-1.494094	-0.384514
N	-0.994254	-4.597275	1.959733
H	-1.510574	-5.343464	1.498600
H	-0.634169	-4.964556	2.838728
N	1.998433	-4.453697	1.916128
H	2.604729	-3.638850	2.029912
H	1.704203	-4.775961	2.835667
N	-6.178316	0.544508	0.356988
H	-6.559566	0.292771	1.267671
H	-6.000704	1.547935	0.361452
N	-5.685065	-2.088595	-0.776081
H	-6.675054	-1.964256	-0.575596
H	-5.555253	-2.145725	-1.786710
H	-6.906200	0.375274	-0.337147
H	2.526094	-5.203258	1.474938
H	5.927410	-0.811117	-1.834441
H	5.178924	2.720871	0.788300
H	1.832592	5.223762	-0.709268
H	-2.271328	4.180610	-2.091975
H	-5.393441	-2.972009	-0.362890
H	-1.637567	-3.828124	2.158449

**Pt-U-IIIc2 (M11L, SMD water)**

Pt	0.000000	3.675190	0.025967
Pt	0.000000	0.000000	-4.613568
Pt	0.000000	-3.675190	0.025967
Pt	0.000000	0.000000	4.708829
C	-2.229898	1.491451	3.579262
C	2.919992	-2.441641	2.893396
H	-2.711547	0.892581	4.352598
C	-2.919992	2.441641	2.893396
C	2.348875	-2.453336	-1.316992
C	-3.066795	1.685270	-2.182650
H	2.833459	-3.050056	-0.546103
C	3.066795	-1.685270	-2.182650

H	-4.148387	1.631163	-2.125817
H	4.148387	-1.631163	-2.125817
H	-3.962233	2.651892	3.107037
N	1.010862	-1.075172	-3.209102
N	1.000863	-2.550861	-1.361506
N	-1.010862	1.075172	-3.209102
N	-1.000863	2.550861	-1.361506
N	-0.957453	2.791560	1.598294
N	-0.914551	1.240950	3.377180
N	0.957453	-2.791560	1.598294
N	0.914551	-1.240950	3.377180
H	3.962233	-2.651892	3.107037
C	-2.348875	2.453336	-1.316992
C	-2.234263	3.188070	1.900846
O	-2.746534	4.176512	1.284262
C	2.229898	-1.491451	3.579262
C	2.376652	-0.951904	-3.178260
O	2.953684	-0.215568	-4.044779
C	-0.271019	1.885333	2.356955
O	0.956337	1.668937	2.128149
C	-0.324685	1.858118	-2.332347
O	0.938586	1.966154	-2.423033
C	0.324685	-1.858118	-2.332347
O	-0.938586	-1.966154	-2.423033
C	0.271019	-1.885333	2.356955
O	-0.956337	-1.668937	2.128149
N	0.992728	4.774435	1.457525
H	1.465467	4.125044	2.085195
H	1.688144	5.418184	1.085151
N	0.980443	4.610360	-1.533304
H	0.349354	5.217692	-2.050967
H	1.781168	5.168748	-1.244999
N	-0.783597	1.211279	6.190512
H	-1.648574	0.827584	6.570321
N	-0.125221	1.306959	6.962372
H	0.783597	-1.211279	6.190512
H	1.648574	-0.827584	6.570321
H	0.125221	-1.306959	6.962372
N	-0.980443	-4.610360	-1.533304
H	-0.349354	-5.217692	-2.050967
H	-1.781168	-5.168748	-1.244999
N	-0.992728	-4.774435	1.457525
H	-1.465467	-4.125044	2.085195
H	-1.688144	-5.418184	1.085151
N	-1.046441	1.058714	-6.046486
H	-0.977880	0.662440	-6.981631
H	-2.024238	1.028658	-5.752343
N	1.046441	-1.058714	-6.046486
H	0.977880	-0.662440	-6.981631
H	2.024238	-1.028658	-5.752343
H	-0.745730	2.029254	-6.097297
H	-0.329571	-5.316795	2.007634
H	0.984161	-2.148960	5.846547
H	-0.984161	2.148960	5.846547
H	0.329571	5.316795	2.007634
H	1.296326	3.856548	-2.148154
H	0.745730	-2.029254	-6.097297
H	-1.296326	-3.856548	-2.148154
C	-2.376652	0.951904	-3.178260
O	-2.953684	0.215568	-4.044779

H	-2.833459	3.050056	-0.546103
H	2.711547	-0.892581	4.352598
C	2.234263	-3.188070	1.900846
O	2.746534	-4.176512	1.284262

**Pt-U-IVc1 (M11L, SMD water)**

Pt	0.000000	4.013165	0.137635
Pt	0.000000	0.000000	4.472926
Pt	0.000000	-4.013165	0.137635
Pt	0.000000	0.000000	-4.386764
C	-2.317000	0.933605	2.935644
C	3.050476	-1.681540	2.070810
H	-2.776892	0.189815	3.586290
C	-3.050476	1.681540	2.070810
C	-2.541098	3.056074	-3.103021
C	2.541098	-3.056074	-3.103021
C	-2.025698	1.872193	-3.525469
C	2.025698	-1.872193	-3.525469
H	2.555934	-1.255765	-4.251168
H	-2.555934	1.255765	-4.251168
H	-3.477359	3.440771	-3.493325
H	3.477359	-3.440771	-3.493325
H	-4.127031	1.574374	1.996947
N	0.824274	-1.390254	-3.111942
N	0.737285	-3.170824	-1.566332
N	-0.824274	1.390254	-3.111942
N	-0.737285	3.170824	-1.566332
N	-1.016059	2.714571	1.360239
N	-0.979851	1.077344	3.065201
N	1.016059	-2.714571	1.360239
N	0.979851	-1.077344	3.065201
C	2.317000	-0.933605	2.935644
H	2.776892	-0.189815	3.586290
H	4.127031	-1.574374	1.996947
C	-1.794488	3.811949	-2.159684
O	-2.059832	5.012871	-1.846883
C	-2.389227	2.658951	1.278523
O	-3.011523	3.472855	0.534030
C	2.389227	-2.658951	1.278523
O	3.011523	-3.472855	0.534030
C	1.794488	-3.811949	-2.159684
O	2.059832	-5.012871	-1.846883
C	-0.320775	1.961109	2.260111
O	0.939405	2.097791	2.373385
C	0.320775	-1.961109	2.260111
O	-0.939405	-2.097791	2.373385
C	0.198589	-2.021483	-2.068196
O	-0.875875	-1.554838	-1.582964
C	-0.198589	2.021483	-2.068196
O	0.875875	1.554838	-1.582964
H	1.070010	4.113914	2.437042
H	1.572123	5.489371	1.658240
H	0.074136	5.441819	2.337157
H	0.257103	5.727580	-1.737533
H	1.427431	6.109437	-0.637202
H	1.657756	4.857903	-1.682742
H	-0.304374	1.630037	6.489768
H	-1.647395	1.728753	5.548207
H	-1.463967	0.467390	6.586321
H	1.647395	-1.728753	5.548207

H	1.463967	-0.467390	6.586321
H	0.304374	-1.630037	6.489768
H	-1.572123	-5.489371	1.658240
H	-0.074136	-5.441819	2.337157
H	-1.070010	-4.113914	2.437042
H	-1.427431	-6.109437	-0.637202
H	-1.657756	-4.857903	-1.682742
H	-0.257103	-5.727580	-1.737533
H	-0.710160	2.242686	-5.576056
H	0.108379	1.297389	-6.637307
H	-1.474376	0.987944	-6.320331
N	0.770819	4.889583	1.843035
N	0.963708	5.338434	-1.114062
N	-0.966620	1.081490	5.943711
N	0.966620	-1.081490	5.943711
N	-0.770819	-4.889583	1.843035
N	-0.963708	-5.338434	-1.114062
N	-0.594393	1.283171	-5.898850
N	0.594393	-1.283171	-5.898850
H	1.474376	-0.987944	-6.320331
H	0.710160	-2.242686	-5.576056
H	-0.108379	-1.297389	-6.637307

**Pt-U-IVc2 (M11L, SMD water)**

Pt	0.026024	-3.579894	0.503787
Pt	4.693196	0.036687	0.007960
Pt	-0.030002	3.579399	-0.509215
Pt	-4.688497	-0.036825	-0.002755
C	2.466140	2.391381	2.764833
C	2.603135	-2.475547	-2.724064
C	-2.475379	-2.391677	-2.770778
C	-2.603032	2.481144	2.727661
H	-2.538398	-2.613648	-3.830041
H	-2.703340	2.742001	3.775037
H	2.701866	-2.735653	-3.771774
N	-3.341060	1.263992	0.816295
N	-1.537006	2.782325	0.620001
N	-3.292994	-1.272439	-0.835437
N	-1.446508	-2.741662	-0.649132
N	1.536493	-2.775174	-0.615920
N	3.345943	-1.263302	-0.811808
N	1.444822	2.736766	0.638223
N	3.294349	1.272613	0.834048
H	2.523881	2.614546	3.824145
C	-1.561438	-3.001248	-1.968792
C	1.692313	-3.086430	-1.919906
C	1.554038	2.997482	1.958288
C	-1.694459	3.095133	1.923214
C	2.416718	-1.893026	-0.041038
O	2.366214	-1.695206	1.211825
C	2.356588	1.886682	0.062426
O	2.330070	1.702452	-1.193556
C	-2.414097	1.896738	0.045131
O	-2.361901	1.697964	-1.207336
C	-2.353872	-1.890154	-0.068229
O	-2.321082	-1.707105	1.187678
H	2.169126	-3.623424	1.848574
H	1.176615	-4.725207	2.590314
H	1.987876	-5.153009	1.222869
H	-1.996066	-5.110012	1.139317

H	-1.170749	-4.787906	2.524663
H	-2.122983	-3.610207	1.843461
H	7.104411	-0.809537	-0.689913
H	6.152487	-2.103628	-0.345319
H	5.945506	-1.285016	-1.773653
H	6.033717	2.248968	0.344819
H	5.877019	1.436735	1.782215
H	7.059358	1.015540	0.703619
H	1.162991	4.710784	-2.576130
H	1.957313	5.133750	-1.197851
H	2.136851	3.602108	-1.821231
H	-1.186054	4.789127	-2.556332
H	-2.158403	3.627529	-1.875866
H	-2.023500	5.130625	-1.181827
H	-6.026965	-2.249894	-0.339872
H	-7.056250	-1.017351	-0.691097
H	-5.877967	-1.433876	-1.775946
N	1.507087	-4.386419	1.688701
N	-1.488586	-4.387129	1.644667
N	6.162815	-1.184429	-0.781088
N	6.097392	1.336322	0.790522
N	1.478558	4.369922	-1.670219
N	-1.517524	4.399046	-1.676243
N	-6.094145	-1.336252	-0.783068
N	-6.156756	1.182672	0.791423
H	-5.938865	1.279880	1.784182
H	-6.145980	2.103306	0.358710
H	-7.098667	0.808785	0.699456
C	-3.364659	-1.452524	-2.194567
O	-4.237481	-0.809404	-2.864965
C	3.438263	-1.476337	-2.165710
O	4.282576	-0.808900	-2.848624
H	1.060189	-3.885445	-2.298478
H	-0.889221	-3.754093	-2.371446
H	-1.065867	3.897270	2.301224
C	-3.433242	1.477227	2.170280
O	-4.273476	0.805771	2.854321
H	0.877948	3.748764	2.357160
C	3.360443	1.454231	2.193247
O	4.232713	0.814573	2.867608

**Pt-U-Id (M11L, SMD water)**

Pt	0.829789	3.944587	0.439016
Pt	-3.944587	0.829789	-0.439016
Pt	3.944587	-0.829789	-0.439016
Pt	-0.829789	-3.944587	0.439016
C	0.554632	-1.646746	-2.903798
C	-0.176144	-2.453100	-2.082422
H	0.180995	-1.348663	-3.877502
H	-1.156241	-2.825100	-2.370784
N	0.267128	-2.849430	-0.871278
N	2.227550	-1.580750	-1.216229
C	-0.554632	1.646746	-2.903798
C	0.176144	2.453100	-2.082422
H	-0.180995	1.348663	-3.877502
H	1.156241	2.825100	-2.370784
N	-0.267128	2.849430	-0.871278
N	-2.227550	1.580750	-1.216229
C	1.646746	0.554632	2.903798
C	-1.646746	-0.554632	2.903798

N	-2.849430	-0.267128	0.871278
N	-1.580750	-2.227550	1.216229
C	-2.453100	0.176144	2.082422
H	-1.348663	-0.180995	3.877502
H	-2.825100	1.156241	2.370784
H	1.348663	0.180995	3.877502
C	2.453100	-0.176144	2.082422
N	2.849430	0.267128	0.871278
N	1.580750	2.227550	1.216229
H	2.825100	-1.156241	2.370784
C	-1.814436	1.168004	-2.455872
O	-2.570218	0.404216	-3.139247
C	-1.168004	-1.814436	2.455872
O	-0.404216	-2.570218	3.139247
C	1.814436	-1.168004	-2.455872
O	2.570218	-0.404216	-3.139247
C	1.168004	1.814436	2.455872
O	0.404216	2.570218	3.139247
C	-1.496711	2.431956	-0.444925
O	-1.955960	2.849430	0.661226
C	-2.431956	-1.496711	0.444925
O	-2.849430	-1.955960	-0.661226
C	1.496711	-2.431956	-0.444925
O	1.955960	-2.849430	0.661226
C	2.431956	1.496711	0.444925
O	2.849430	1.955960	-0.661226
N	5.670562	-0.032844	0.379804
H	5.959014	-0.566351	1.197759
H	6.452204	-0.018112	-0.272131
N	4.993548	-1.910855	-1.850156
H	4.515633	-1.788083	-2.742738
H	5.957784	-1.605776	-1.967110
N	1.910855	4.993548	1.850156
H	1.605776	5.957784	1.967110
H	1.788083	4.515633	2.742738
N	0.032844	5.670562	-0.379804
H	0.018112	6.452204	0.272131
H	0.566351	5.959014	-1.197759
N	-4.993548	1.910855	-1.850156
H	-4.515633	1.788083	-2.742738
H	-5.957784	1.605776	-1.967110
N	-5.670562	0.032844	0.379804
H	-5.959014	0.566351	1.197759
H	-6.452204	0.018112	-0.272131
N	-0.032844	-5.670562	-0.379804
H	0.925793	-5.500639	-0.678727
H	-0.018112	-6.452204	0.272131
N	-1.910855	-4.993548	1.850156
H	-2.904107	-5.005887	1.628899
H	-1.605776	-5.957784	1.967110
H	-5.005887	2.904107	-1.628899
H	-5.500639	-0.925793	0.678727
H	-0.566351	-5.959014	-1.197759
H	-1.788083	-4.515633	2.742738
H	5.005887	-2.904107	-1.628899
H	5.500639	0.925793	0.678727
H	2.904107	5.005887	1.628899
H	-0.925793	5.500639	-0.678727

**Pt-U-IId (M11L, SMD water)**

Pt	0.015539	4.116313	-0.112918
Pt	4.236297	0.042113	-0.057760
Pt	0.046303	-4.039720	0.055392
Pt	-4.147086	0.019153	0.107839
C	-1.517165	-1.504948	3.119861
C	-0.768096	-2.385679	2.397939
H	-1.349792	-1.355622	4.180660
H	0.027340	-2.971378	2.858403
N	-0.966074	-2.603292	1.081084
N	-2.696321	-0.996300	1.115294
C	1.776337	1.763365	2.966748
C	0.992135	2.604151	2.235964
H	1.648896	1.656960	4.038137
H	0.207142	3.201261	2.699421
N	1.138531	2.766354	0.904114
N	2.876216	1.175952	0.938884
C	-1.714295	1.566402	-3.051696
C	1.670446	-1.593733	-3.044765
N	2.786238	-1.001070	-1.025252
N	1.132352	-2.682148	-0.998916
C	2.573148	-0.846534	-2.349632
H	1.525230	-1.460653	-4.110903
H	3.183238	-0.087184	-2.837977
H	-1.596622	1.404113	-4.117184
N	-2.798580	1.078582	-0.988460
N	-1.064504	2.676086	-1.050006
C	-0.925302	2.444963	-2.372533
H	-0.144907	3.019309	-2.871698
C	2.782961	1.019707	2.298053
O	3.598858	0.239163	2.888009
C	0.923532	-2.580898	-2.349417
O	0.102009	-3.375907	-2.911187
C	-2.551865	-0.788918	2.462278
O	-3.349696	0.007719	3.056846
C	-2.720270	0.860094	-2.339222
O	-3.547288	0.062464	-2.888522
C	-2.014520	1.988790	-0.347314
O	-2.172969	2.220680	0.889364
C	2.096269	2.049047	0.244102
O	2.265940	2.218150	-1.001782
C	2.054995	-1.929763	-0.337826
O	2.255726	-2.105086	0.901578
C	-1.937474	-1.895310	0.428011
O	-2.139907	-2.098463	-0.806182
N	-1.130904	5.494506	-1.138569
H	-1.071132	6.437440	-0.758064
H	-0.842894	5.538293	-2.115203
N	1.098701	5.595711	0.837431
H	0.980045	6.515925	0.416814
H	0.818708	5.666133	1.814650
N	-5.505899	-1.022221	1.263068
H	-6.460585	-0.675350	1.195096
H	-5.515373	-2.011399	1.023545
N	-5.623991	0.993887	-0.957161
H	-6.549500	0.586944	-0.838204
H	-5.682094	1.979330	-0.711131
N	-1.053219	-5.423770	1.131504
H	-0.826338	-6.391996	0.910113
H	-0.900663	-5.295921	2.130777
N	1.027696	-5.493665	-1.030446

H	0.616401	-6.421610	-0.951246
H	0.971223	-5.201709	-2.007350
N	5.631564	-1.107968	-1.060232
H	6.122126	-0.565746	-1.768915
H	6.330285	-1.493398	-0.427213
N	5.706502	1.067049	0.963969
H	5.432981	1.041895	1.947537
H	6.634115	0.656604	0.877286
H	2.092921	5.375196	0.817038
H	-2.110931	5.216519	-1.118620
H	-5.195327	-0.924797	2.230527
H	-5.362340	0.917093	-1.940839
H	-2.047059	-5.292471	0.951813
H	2.007879	-5.563267	-0.766808
H	5.175074	-1.889657	-1.528465
H	5.765226	2.038152	0.666464

**Pt-U-III d (M11L, SMD water)**

Pt	2.756568	3.170015	0.066130
Pt	0.000000	0.000000	-3.918694
Pt	-2.756568	-3.170015	0.066130
Pt	0.000000	0.000000	4.059246
C	1.298132	-3.079252	1.389076
H	2.230763	-3.574103	1.141552
N	-1.047576	-2.807300	1.098298
N	0.100948	-1.444931	2.639150
C	3.152094	-0.914069	-1.162221
C	3.291574	0.286788	-0.531899
H	3.759160	-1.770790	-0.888658
H	4.010634	0.428100	0.274280
N	2.565130	1.374177	-0.865095
N	1.456157	0.081315	-2.501766
C	-1.298132	3.079252	1.389076
C	-3.152094	0.914069	-1.162221
N	-1.456157	-0.081315	-2.501766
N	-2.565130	-1.374177	-0.865095
H	-3.759160	1.770790	-0.888658
H	-2.230763	3.574103	1.141552
C	-1.252723	2.057278	2.290967
N	-0.100948	1.444931	2.639150
N	1.047576	2.807300	1.098298
H	-2.150755	1.696486	2.791437
C	1.252723	-2.057278	2.290967
C	-3.291574	-0.286788	-0.531899
H	2.150755	-1.696486	2.791437
H	-4.010634	-0.428100	0.274280
C	2.217428	-1.025900	-2.228566
O	2.070439	-2.074208	-2.933884
C	-2.217428	1.025900	-2.228566
O	-2.070439	2.074208	-2.933884
C	0.086878	-3.510925	0.783105
O	0.000000	-4.498692	-0.013384
C	-0.086878	3.510925	0.783105
O	0.000000	4.498692	-0.013384
C	1.626843	1.266784	-1.854369
O	0.934569	2.277561	-2.180295
C	1.062880	1.817447	2.029731
O	2.151086	1.249445	2.350263
C	-1.062880	-1.817447	2.029731
O	-2.151086	-1.249445	2.350263

C	-1.626843	-1.266784	-1.854369
O	-0.934569	-2.277561	-2.180295
N	4.506683	3.521025	-0.979843
H	5.232125	3.910339	-0.380548
H	4.870081	2.658236	-1.382512
N	2.866080	5.017915	0.978926
H	3.533165	5.652089	0.544023
H	1.935893	5.430832	0.903019
N	1.509849	0.031795	-5.331693
H	1.186715	-0.102326	-6.287817
H	2.015863	0.914358	-5.296655
N	-1.509849	-0.031795	-5.331693
H	-1.186715	0.102326	-6.287817
H	-2.015863	-0.914358	-5.296655
N	0.106378	-1.499558	5.477167
H	0.978255	-2.015436	5.368586
H	0.065734	-1.168052	6.439320
N	-0.106378	1.499558	5.477167
H	-0.978255	2.015436	5.368586
H	-0.065734	1.168052	6.439320
N	-2.866080	-5.017915	0.978926
H	-3.533165	-5.652089	0.544023
H	-1.935893	-5.430832	0.903019
N	-4.506683	-3.521025	-0.979843
H	-5.232125	-3.910339	-0.380548
H	-4.870081	-2.658236	-1.382512
H	0.659176	2.158184	5.345603
H	-0.659176	-2.158184	5.345603
H	4.351514	4.176850	-1.743276
H	3.105453	4.943135	1.964942
H	-2.168050	0.715539	-5.115530
H	2.168050	-0.715539	-5.115530
H	-4.351514	-4.176850	-1.743276
H	-3.105453	-4.943135	1.964942

**Pt-U-IVd (M11L, SMD water)**

Pt	0.000000	3.968603	0.000000
Pt	-4.288977	0.000000	0.000000
Pt	4.288977	0.000000	0.000000
Pt	0.000000	-3.968603	0.000000
C	-1.717323	-1.537462	3.047562
C	-0.921246	-2.375969	2.326420
H	-1.575839	-1.398528	4.113524
H	-0.112449	-2.939472	2.791458
N	-1.087289	-2.577720	1.002612
N	-2.874175	-1.039023	1.027050
C	1.717323	1.537462	3.047562
C	0.921246	2.375969	2.326420
H	1.575839	1.398528	4.113524
H	0.112449	2.939472	2.791458
N	1.087289	2.577720	1.002612
N	2.874175	1.039023	1.027050
C	-1.717323	1.537462	-3.047562
C	1.717323	-1.537462	-3.047562
N	2.874175	-1.039023	-1.027050
N	1.087289	-2.577720	-1.002612
H	1.575839	-1.398528	-4.113524
H	-1.575839	1.398528	-4.113524
N	-2.874175	1.039023	-1.027050
N	-1.087289	2.577720	-1.002612

C	-0.921246	2.375969	-2.326420
C	0.921246	-2.375969	-2.326420
H	-0.112449	2.939472	-2.791458
H	0.112449	-2.939472	-2.791458
C	2.762555	-0.846122	-2.379410
O	3.594787	-0.082609	-2.968953
C	2.762555	0.846122	2.379410
O	3.594787	0.082609	2.968953
C	-2.762555	0.846122	-2.379410
O	-3.594787	0.082609	-2.968953
C	-2.762555	-0.846122	2.379410
O	-3.594787	-0.082609	2.968953
C	2.073997	1.900984	0.341061
O	2.248871	2.102029	-0.898603
C	-2.073997	1.900984	-0.341061
O	-2.248871	2.102029	0.898603
C	-2.073997	-1.900984	0.341061
O	-2.248871	-2.102029	-0.898603
C	2.073997	-1.900984	-0.341061
O	2.248871	-2.102029	0.898603
H	-1.009439	6.331199	-0.612756
H	-0.800390	5.448816	-1.983839
H	-2.085331	5.150915	-1.001527
H	1.009439	6.331199	0.612756
H	0.800390	5.448816	1.983839
H	2.085331	5.150915	1.001527
H	-5.416426	0.962505	-2.069624
H	-6.648785	0.625510	-1.018955
H	-5.766461	2.000166	-0.826559
H	-5.416426	-0.962505	2.069624
H	-6.648785	-0.625510	1.018955
H	-5.766461	-2.000166	0.826559
H	-2.085331	-5.150915	1.001527
H	-1.009439	-6.331199	0.612756
H	-0.800390	-5.448816	1.983839
H	2.085331	-5.150915	-1.001527
H	1.009439	-6.331199	-0.612756
H	0.800390	-5.448816	-1.983839
H	5.416426	-0.962505	-2.069624
H	6.648785	-0.625510	-1.018955
H	5.766461	-2.000166	-0.826559
H	5.416426	0.962505	2.069624
H	6.648785	0.625510	1.018955
H	5.766461	2.000166	0.826559
N	1.096796	5.397444	1.010191
N	-1.096796	5.397444	-1.010191
N	-5.713476	1.020082	-1.094574
N	-5.713476	-1.020082	1.094574
N	1.096796	-5.397444	-1.010191
N	-1.096796	-5.397444	1.010191
N	5.713476	-1.020082	-1.094574
N	5.713476	1.020082	1.094574

<b>Pd-C-Ia (M11L, SMD water)</b>			
Pd	0.000206	3.646915	0.000257
Pd	-4.442351	0.000173	-0.000014
Pd	-0.000154	-3.646937	-0.000317
Pd	4.442269	-0.000145	0.000126
C	-1.544200	0.964889	2.947867
C	-2.664006	0.520896	2.302671
H	-1.290891	0.627873	3.946835
H	-3.343196	-0.187787	2.773966
N	-2.990584	0.912900	1.057195
N	-1.049152	2.249991	1.004858
C	1.544088	-0.965427	2.947850
C	2.663872	-0.521229	2.302747
H	1.290752	-0.628623	3.946883
H	3.342998	0.187428	2.774174
N	2.990503	-0.912993	1.057218
N	1.049166	-2.250204	1.004595
C	2.205931	-1.828542	0.418763
O	2.551456	-2.298300	-0.705122
C	1.544404	0.965309	-2.947902
C	-2.205879	1.828424	0.418881
O	-2.551362	2.298452	-0.704905
C	-1.544224	-0.964670	-2.947909
C	-2.206118	-1.828342	-0.419021
O	-2.551652	-2.298332	0.704763
H	1.710439	-4.692692	1.623602
H	0.405603	-5.698028	1.505269
H	1.542866	-5.675397	0.308102
H	-0.406141	-5.697740	-1.506203
H	-1.543567	-5.675029	-0.309189
H	-1.710763	-4.692130	-1.624592
H	-5.493244	-1.383764	-1.900969
H	-6.307098	-1.692096	-0.499999
H	-6.626034	-0.316250	-1.352881
H	-6.625877	0.316821	1.353031
H	-5.492888	1.384165	1.901090
H	-6.306830	1.692687	0.500205
N	1.036498	-5.098403	0.976796
N	-1.036989	-5.098052	-0.977742
N	-5.888583	-0.956412	-1.065662
N	-5.888378	0.956917	1.065800
N	-1.049359	-2.249905	-1.004939
N	-2.990742	-0.912737	-1.057334
C	-2.664053	-0.520667	-2.302761
H	-3.343198	0.188051	-2.774072
H	-1.290846	-0.627629	-3.946851
H	1.291129	0.628537	-3.946962
C	2.664109	0.521036	-2.302717
N	1.049392	2.250077	-1.004667
N	2.990663	0.912756	-1.057153
C	2.206080	1.828333	-0.418752
O	2.551534	2.298048	0.705176
H	3.343239	-0.187642	-2.774107
H	-1.542889	5.675243	0.309010
H	-1.710423	4.692309	1.624351
H	-0.405638	5.697737	1.506198
H	0.406191	5.698054	-1.505273
H	1.543473	5.675119	-0.308125
H	1.710848	4.692500	-1.623717
H	5.493040	1.385026	-1.899969

H	6.308493	1.690855	-0.499371
H	6.625005	0.315537	-1.354052
H	6.308382	-1.691304	0.500037
H	6.624752	-0.315883	1.354607
H	5.492657	-1.385285	1.900426
N	5.888609	0.956308	-1.065485
N	5.888397	-0.956673	1.065963
N	1.036990	5.098272	-0.976862
N	-1.036502	5.098167	0.977619
C	0.684421	-1.818690	2.232333
C	-0.684590	-1.818134	-2.232582
C	0.684716	1.818606	-2.232449
C	-0.684472	1.818255	2.232541
N	0.478413	2.241932	2.717595
N	-0.478101	2.242492	-2.717466
N	-0.478452	-2.242546	2.717252
N	0.478274	-2.241885	-2.717590
H	-1.187317	-2.594415	2.078084
H	-0.792590	-1.884933	3.605360
H	0.792442	-1.884061	-3.605600
H	1.187091	-2.594018	-2.078522
H	0.792480	1.884098	3.605641
H	1.187360	2.593801	2.078515
H	-1.186992	2.594433	-2.078371
H	-0.792178	1.884912	-3.605608

<b>Pd-C-IIa (M11L, SMD water)</b>			
Pd	3.833994	1.948921	-0.198096
Pd	1.751739	-3.394224	-0.786121
Pd	-3.753140	-1.792347	-0.323358
Pd	-1.703049	3.560569	-0.693885
C	-0.310089	2.993430	1.834071
C	-4.769131	1.863049	1.697159
C	0.717163	2.697656	2.681790
H	-1.295669	3.253858	2.216939
C	4.759978	-0.420200	1.302697
C	-0.666999	-2.604565	2.609519
H	5.453624	0.320461	1.701255
C	4.830931	-1.727225	1.689431
C	0.356208	-2.904501	1.760658
H	1.333796	-3.193838	2.142430
H	-0.541732	-2.632830	3.685796
H	5.568543	-2.073324	2.404230
H	0.589934	2.708649	3.758090
H	-5.499100	2.213057	2.418003
N	3.006376	-2.163889	0.217467
N	3.847670	0.031982	0.423271
N	0.217957	-2.879915	0.421362
N	-2.045550	-2.230963	0.697630
N	-3.830573	0.098534	0.392906
N	-2.942099	2.280181	0.236637
N	-0.168570	3.003776	0.495188
N	2.097585	2.375703	0.764012
C	3.906822	-2.616642	1.113998
C	-1.912989	-2.278848	2.040280
C	-3.842401	2.698795	1.142151
C	1.968928	2.410291	2.106863
C	2.962598	-0.844396	-0.138767
O	2.119327	-0.450316	-0.989513
C	1.036607	2.664995	-0.048323



O	1.191260	2.638409	-1.304465
C	-0.980104	-2.509706	-0.115533
O	-1.124699	-2.440697	-1.371131
C	-2.924161	0.971950	-0.148526
O	-2.090987	0.568638	-1.003957
N	3.837996	3.880433	-0.834980
H	4.605052	4.110299	-1.462829
H	2.957605	4.021569	-1.329963
N	5.575739	1.535869	-1.169562
H	6.008604	2.351156	-1.598536
H	6.247181	1.132247	-0.518490
N	0.527538	-4.668238	-1.801164
H	0.932298	-5.027022	-2.663070
H	0.276321	-5.460554	-1.214025
N	3.331948	-3.890505	-1.970915
H	3.140559	-4.675357	-2.590077
H	3.571035	-3.082371	-2.543576
N	-5.411385	-1.395621	-1.434135
H	-5.684039	-0.417717	-1.355868
H	-5.215719	-1.588381	-2.415523
N	-3.712834	-3.685958	-1.071455
H	-3.809697	-4.372987	-0.327407
H	-4.441617	-3.857779	-1.761162
N	-0.485077	4.896588	-1.633274
H	-0.882978	5.279275	-2.488068
H	-0.255061	5.670708	-1.014498
N	-3.287691	4.102774	-1.851974
H	-3.098312	4.905493	-2.448386
H	-3.541506	3.315616	-2.446518
H	-6.199139	-1.974097	-1.146953
H	-4.089508	4.326881	-1.264900
H	0.365098	4.379378	-1.860611
H	-2.802909	-3.800608	-1.518480
H	4.145386	-4.128220	-1.405744
H	3.874740	4.517047	-0.042066
H	5.393788	0.851670	-1.901796
H	-0.311344	-4.128191	-2.019698
C	-4.758901	0.522227	1.275246
H	-3.802007	3.754804	1.407577
N	-2.968194	-2.027218	2.803147
N	-5.644305	-0.360366	1.735833
N	3.892679	-3.909659	1.420150
N	3.042790	2.181178	2.852873
H	-3.871189	-1.818967	2.411421
H	-2.883063	-2.052994	3.805112
H	-5.700617	-1.297875	1.365850
H	-6.360288	-0.063685	2.377858
H	3.201884	-4.530922	1.025787
H	4.554665	-4.283568	2.079107
H	2.977134	2.198621	3.856254
H	3.949261	2.047319	2.434761

**Pd-C-IIIa (M1 1L, SMD water)**

Pd	-2.744546	-2.861342	-0.507847
Pd	2.995425	-2.729190	-0.584453
Pd	2.952865	2.963613	-0.328529
Pd	-2.803027	2.963107	-0.544410
C	0.229369	-2.590406	2.631795
C	-1.014261	-2.687669	1.979100
C	1.350899	-2.599249	1.856893

H	0.284027	-2.536840	3.713044
H	2.342019	-2.561248	2.305685
C	-5.257800	0.077552	1.341304
C	-4.655104	1.222377	0.908567
H	-6.158804	0.094038	1.944012
C	4.581640	-1.135995	1.399065
C	5.017328	0.061516	1.996263
C	4.517525	1.228663	1.492739
H	5.723293	0.046955	2.818417
H	4.814062	2.194320	1.899928
N	3.639679	1.259160	0.474816
N	1.303669	-2.671418	0.513020
N	-1.061701	-2.732437	0.630717
N	-3.542099	-1.139821	0.210516
N	-3.534817	1.222062	0.164507
C	0.005601	2.734842	2.716039
H	-0.009540	2.688511	3.798852
N	-1.153469	2.896538	0.635646
N	1.207586	2.784282	0.665184
H	-4.579486	2.120279	-2.178905
H	-5.274086	3.242034	-1.186221
H	-4.379330	3.728536	-2.482664
H	-1.153144	4.597016	-1.517818
H	-2.640377	5.085694	-2.060345
H	-2.171817	5.457382	-0.524375
H	2.845842	5.047553	-1.904602
H	1.336625	4.455477	-1.553945
H	2.142819	5.411606	-0.458542
H	5.501980	3.046197	-0.614792
H	4.830026	2.383068	-1.966206
H	4.860655	4.021738	-1.777978
H	-4.930674	-3.829112	-1.504034
H	-4.939479	-2.188427	-1.707927
H	-4.030961	-3.135694	-2.701719
H	-1.109972	-4.436143	-1.614524
H	-1.944192	-5.306408	-0.472074
H	-2.622043	-5.032084	-1.950272
H	2.269745	-5.174847	-0.933172
H	1.335417	-4.138699	-1.840649
H	2.827049	-4.628615	-2.385445
H	4.876910	-1.814764	-2.043628
H	5.520331	-2.967740	-1.054082
H	4.723704	-3.410671	-2.425491
N	4.729354	-2.744988	-1.656047
N	2.288647	-4.374291	-1.560489
N	-2.033028	-4.628117	-1.225191
N	-4.355836	-3.022390	-1.742564
N	-4.447429	3.031669	-1.743599
N	-2.126422	4.746354	-1.250439
N	2.251155	4.685576	-1.163071
N	4.743166	3.137334	-1.287621
N	3.694560	-1.097416	0.383551
C	0.036980	2.836553	-0.031295
O	0.047560	2.857008	-1.297939
C	-2.965995	0.034837	-0.202953
O	-1.935483	0.010520	-0.926440
C	0.089941	-2.683725	-0.107846
C	0.018225	-2.673156	-1.372047
O	3.217979	0.091809	-0.090311
O	2.401479	0.103527	-1.052530

H	5.684291	-2.393202	2.555116
H	4.680746	-3.172140	1.376642
H	-3.038478	-2.846819	2.205942
H	-2.133155	-2.724392	3.669912
N	-2.148051	-2.747390	2.664709
N	5.014196	-2.323377	1.808391
C	1.171987	2.697826	2.007914
C	-4.666751	-1.137521	0.956031
C	-1.188469	2.885576	1.985069
H	2.135189	2.617036	2.510717
N	-5.188697	-2.307866	1.320817
N	-2.362609	3.033134	2.584986
H	-4.825196	-3.184428	0.975934
H	-6.039945	-2.331232	1.857894
H	-3.196291	3.228974	2.054420
H	-2.424640	3.030925	3.588636
H	-5.070568	2.200218	1.151773

**Pd-C-IVa (M11L, SMD water)**

Pd	-2.849910	3.205460	-0.255767
Pd	2.880465	2.531224	-0.755487
Pd	2.849910	-3.205460	-0.255767
Pd	-2.880465	-2.531224	-0.755487
C	-4.558388	-0.988847	1.105990
C	-0.321541	-2.569746	2.615579
C	-5.127888	0.108060	1.684311
H	-4.894292	-1.995857	1.351014
C	5.127888	-0.108060	1.684311
C	0.321541	2.569746	2.615579
C	4.558388	0.988847	1.105990
H	4.894292	1.995857	1.351014
H	5.934891	-0.023369	2.402868
H	0.450471	2.488358	3.688799
H	-5.934891	0.023369	2.402868
H	-0.450471	-2.488358	3.688799
N	1.238539	2.582222	0.421516
N	-1.090316	2.908225	0.723003
N	3.570012	0.898271	0.199061
N	3.629354	-1.455163	0.403071
N	1.090316	-2.908225	0.723003
N	-1.238539	-2.582222	0.421516
N	-3.570012	-0.898271	0.199061
N	-3.629354	1.455163	0.403071
C	1.374104	2.466315	1.756180
C	4.644301	-1.368327	1.288353
C	-1.374104	-2.466315	1.756180
C	-4.644301	1.368327	1.288353
C	-0.006746	2.777461	-0.102905
O	-0.170064	2.856901	-1.356085
C	-3.094033	0.327909	-0.163883
O	-2.180755	0.428360	-1.026454
C	3.094033	-0.327909	-0.163883
O	2.180755	-0.428360	-1.026454
C	0.006746	-2.777461	-0.102905
O	0.170064	-2.856901	-1.356085
N	-4.558388	3.544025	-1.310277
H	-5.000853	4.416900	-1.028006
H	-4.328805	3.611030	-2.300811
N	-2.090816	4.968670	-0.928265
H	-2.731962	5.485886	-1.525993

H	-1.830896	5.563981	-0.145141
N	4.578669	2.455412	-1.875596
H	4.599975	3.130751	-2.636294
H	5.386322	2.626740	-1.279048
N	2.257508	4.225371	-1.701696
H	2.717407	4.381640	-2.595475
H	1.255140	4.107327	-1.857345
N	2.090816	-4.968670	-0.928265
H	1.252505	-4.733700	-1.460263
H	2.731962	-5.485886	-1.525993
N	4.558388	-3.544025	-1.310277
H	5.234629	-2.791377	-1.197160
H	5.000853	-4.416900	-1.028006
N	-4.578669	-2.455412	-1.875596
H	-4.599975	-3.130751	-2.636294
H	-5.386322	-2.626740	-1.279048
N	-2.257508	-4.225371	-1.701696
H	-2.717407	-4.381640	-2.595475
H	-1.255140	-4.107327	-1.857345
H	1.830896	-5.563981	-0.145141
H	-2.421255	-5.037192	-1.111144
H	-4.671586	-1.523625	-2.275792
H	4.328805	-3.611030	-2.300811
H	2.421255	5.037192	-1.111144
H	-5.234629	2.791377	-1.197160
H	-1.252505	4.733700	-1.460263
H	4.671586	1.523625	-2.275792
C	0.946309	-2.826534	2.062452
H	-2.383427	-2.297800	2.126209
C	-0.946309	2.826534	2.062452
H	2.383427	2.297800	2.126209
N	2.008008	-3.008355	2.837385
N	5.166831	-2.492653	1.771991
N	-2.008008	3.008355	2.837385
N	-5.166831	2.492653	1.771991
H	1.916796	-2.960501	3.837967
H	2.906209	-3.249904	2.454238
H	4.876718	-3.400440	1.440314
H	5.925979	-2.452476	2.431233
H	-2.906209	3.249904	2.454238
H	-1.916796	2.960501	3.837967
H	-5.925979	2.452476	2.431233
H	-4.876718	3.400440	1.440314

**Pd-C-Ib (M11L, SMD water)**

Pd	2.008180	3.516783	0.258749
Pd	3.798029	-1.858902	-0.018760
Pd	-1.707607	-3.531233	-0.276338
Pd	-3.483680	2.055514	-0.690023
C	2.575177	0.927688	-3.056924
C	-0.911837	1.452504	2.634087
C	-1.999926	1.585195	1.819194
H	-2.983637	1.243997	2.138810
C	1.844973	-1.522764	2.149620
C	-5.223641	-1.509774	0.888678
H	2.735091	-1.130493	2.637304
C	0.656135	-1.620576	2.810286
C	-4.260686	-2.424732	0.583036
H	-4.386019	-3.476857	0.840113
H	-6.141618	-1.789579	1.391980

H	0.545966	-1.301962	3.840803
H	-0.987643	0.997240	3.615632
N	-0.283307	-2.574844	0.830300
N	1.990233	-1.910037	0.869219
N	-3.102915	-2.095703	-0.025069
N	-3.831026	0.149737	-0.115041
N	-1.928071	2.135816	0.591775
N	0.385741	2.493671	0.927427
N	3.256231	-0.237589	-1.089292
N	2.546962	2.004572	-0.940704
C	2.324657	2.013045	-2.266526
H	1.932406	2.939825	-2.682769
H	2.396457	0.944891	-4.125798
C	-4.963164	-0.170924	0.546890
C	0.325147	1.908725	2.142882
C	3.028982	-0.243133	-2.419423
C	-0.430305	-2.184583	2.114492
C	3.061384	0.891598	-0.348380
O	3.368163	0.905635	0.877102
C	0.917740	-2.405131	0.189535
O	1.032441	-2.733864	-1.025883
C	-2.888369	-0.801012	-0.411472
O	-1.853805	-0.485985	-1.056492
C	-0.720570	2.586515	0.136099
O	-0.617554	3.106873	-1.013226
N	1.466056	5.071783	1.456888
H	1.399113	5.936170	0.922431
H	0.561900	4.895501	1.890809
N	3.600261	4.600144	-0.397745
H	3.321677	5.539827	-0.674010
H	4.299068	4.676979	0.338745
N	4.364821	-3.476221	1.082687
H	4.624529	-4.252598	0.477170
H	5.166432	-3.244981	1.667081
N	5.652889	-1.822479	-0.861472
H	5.802882	-0.953062	-1.369091
H	6.370921	-1.898307	-0.142990
N	-0.397211	-5.078108	-0.466182
H	-0.085433	-5.388916	0.451277
H	-0.782824	-5.880488	-0.958531
N	-3.059521	-4.552937	-1.405057
H	-3.471887	-5.310426	-0.863020
H	-3.809145	-3.941276	-1.721454
N	-3.225062	4.006242	-1.216695
H	-3.696689	4.255574	-2.082620
H	-3.565686	4.617121	-0.478583
N	-5.038116	1.938301	-2.002415
H	-5.404832	0.990081	-2.056794
H	-5.799542	2.560328	-1.736633
H	0.402556	-4.710727	-0.980651
H	3.606117	-3.783785	1.687745
H	5.770516	-2.597816	-1.510958
H	4.030718	4.144695	-1.199900
H	2.154333	5.205321	2.195319
H	-2.216068	4.121962	-1.325815
H	-2.614694	-4.956646	-2.227822
H	-4.722407	2.204926	-2.933753
N	-5.813614	0.802629	0.853571
N	1.456703	1.812165	2.833025
N	-1.600732	-2.370278	2.712940

N	3.251053	-1.365252	-3.094973
H	-6.667828	0.593398	1.342547
H	-5.597168	1.768841	0.660609
H	-2.366030	-2.817909	2.238008
H	-1.721046	-2.112231	3.677545
H	3.462527	-2.227249	-2.616717
H	3.074958	-1.401663	-4.084639
H	1.453862	1.333747	3.719455
H	2.334013	1.868703	2.325488

<b>Pd-C-IIb1 (M11L, SMD water)</b>			
Pd	-0.848513	3.605796	0.130786
Pd	-4.397665	-0.861801	-0.092923
Pd	0.751490	-3.489914	-0.614337
Pd	4.331179	1.103615	-0.316026
C	1.356014	0.970055	2.676271
C	-2.421249	-1.213633	2.139882
C	-1.213677	-1.673989	2.695556
C	-0.323808	-2.279153	1.854980
H	-1.000667	-1.541223	3.750482
H	0.628044	-2.653105	2.229288
N	-0.561055	-2.455620	0.540013
N	0.499633	2.324832	0.913083
N	2.727376	1.558419	0.818482
C	3.159305	-3.256604	1.082619
C	4.400305	-2.716191	1.464749
C	4.739987	-1.505272	0.935801
H	5.054425	-3.246840	2.146382
H	5.684900	-1.024676	1.186661
N	3.937956	-0.825749	0.095568
N	2.365987	-2.584864	0.218807
H	3.775616	3.485002	-0.813478
H	5.138569	3.510461	0.146152
H	5.283543	3.241941	-1.476549
H	6.754556	1.168208	-1.208959
H	6.196481	-0.381492	-1.310457
H	5.736119	0.734306	-2.432972
H	2.118179	-5.505760	-1.462523
H	1.773241	-4.519932	-2.740808
H	2.994921	-4.126195	-1.706320
H	-0.484829	-5.084665	-2.272558
H	-1.123294	-5.233494	-0.759041
H	-1.494769	-3.896354	-1.677953
H	-2.690671	5.402144	0.133162
H	-1.662051	5.698935	-1.123049
H	-2.815928	4.527115	-1.261503
H	0.745350	4.712265	1.824193
H	0.310894	5.834893	0.693665
H	-0.727154	5.452924	1.919437
H	-5.240971	-3.227345	0.400775
H	-4.984803	-2.475490	1.844453
H	-6.362209	-2.171919	0.993662
H	-6.556600	-1.206702	-1.468043
H	-6.802448	0.004594	-0.374965
H	-5.974645	0.307770	-1.768037
N	-6.135308	-0.384705	-1.038987
N	-5.363856	-2.352496	0.907031
N	-0.033031	5.074863	1.277128
N	-2.159948	4.966988	-0.619289
N	4.698973	3.074583	-0.660885

N	5.946346	0.595824	-1.446230
N	2.064043	-4.534548	-1.764325
N	-0.764643	-4.569076	-1.441200
N	-2.659862	-1.382793	0.822929
C	2.734728	-1.361935	-0.272382
O	1.974978	-0.750702	-1.072609
C	1.699622	2.267752	0.273281
O	1.855663	2.893747	-0.819641
C	-1.737238	-1.987991	0.013826
O	-1.990479	-2.123288	-1.215687
C	-2.127589	1.056134	-3.064555
H	-1.895001	0.884425	-4.109264
N	-3.403581	0.549981	-1.120238
N	-1.710048	2.181870	-1.007663
C	-2.736238	1.507072	-0.419259
O	-3.069285	1.780896	0.771145
H	3.306005	-4.959981	2.180328
H	-3.203277	-0.477320	3.862720
N	-3.359441	-0.632007	2.880525
N	2.737761	-4.430180	1.540785
H	1.835704	-4.798628	1.278194
H	-4.145774	-0.172163	2.446875
C	2.542785	0.942428	2.003428
H	1.223039	0.458797	3.623440
C	-3.114031	0.364943	-2.421928
C	-1.358907	1.946243	-2.290186
C	0.291228	1.669547	2.077054
H	-3.701969	-0.391800	-2.938635
H	3.402885	0.410630	2.407082
N	-0.919012	1.732936	2.615712
H	-1.101871	1.227224	3.467356
H	-1.714557	2.019256	2.046836
N	-0.287746	2.574623	-2.759956
H	0.379403	2.985908	-2.111206
H	0.004801	2.412441	-3.709371

**Pd-C-IIb2 (M11L, SMD water)**

Pd	4.299140	-1.177823	-0.090702
Pd	1.259504	3.630612	0.277832
Pd	-3.956248	1.362396	-0.511558
Pd	-0.871336	-3.668610	-0.471419
C	2.354559	-1.346226	2.122971
C	1.223220	-1.731632	2.781999
H	3.177774	-0.861446	2.646540
C	-0.062489	1.713610	2.141470
C	-1.187306	1.043566	2.662087
C	-2.340430	1.094357	1.931999
H	-1.125408	0.494242	3.595447
H	-3.240768	0.586730	2.273500
N	-2.441534	1.761139	0.764504
N	2.527093	-1.548705	0.804655
N	0.391221	-2.573420	0.706332
C	-4.775381	-1.207029	0.679525
C	-4.679705	-2.578490	0.976360
C	-3.538187	-3.213936	0.588610
H	-5.474104	-3.094139	1.504010
H	-3.391150	-4.275385	0.793424
N	-2.525032	-2.587579	-0.043724
N	-3.792221	-0.594382	-0.013642
H	1.080800	-5.278237	0.003028

H	0.466370	-5.673210	-1.475125
H	1.414432	-4.315405	-1.306723
H	-1.589146	-4.974739	-2.572152
H	-2.174251	-5.749304	-1.236252
H	-2.946766	-4.413353	-1.825815
H	-5.172715	1.214999	-2.762156
H	-5.638157	-0.079967	-1.856657
H	-6.307359	1.404449	-1.579436
H	-4.672476	3.480949	-1.849274
H	-4.699006	3.809481	-0.230682
H	-3.235553	3.695108	-1.026671
H	6.046221	-0.008677	-1.577243
H	6.825813	-0.699832	-0.297529
H	6.353532	-1.631004	-1.575455
H	4.419484	-3.546305	0.888715
H	5.963097	-3.096625	0.519517
H	5.238807	-2.519755	1.884811
H	0.306414	5.931397	0.924637
H	-0.265110	4.807564	1.989899
H	1.269245	5.396844	2.154563
H	2.268003	5.696140	-0.884951
H	3.269660	5.237200	0.344992
H	3.292036	4.416825	-1.087225
N	2.690862	4.895333	-0.419447
N	0.560389	5.116212	1.479811
N	5.080376	-2.772591	0.910973
N	6.092486	-0.839351	-0.990286
N	0.704085	-4.896464	-0.862268
N	-2.034756	-4.836440	-1.666388
N	-5.446606	0.919463	-1.826237
N	-4.187987	3.330021	-0.967995
N	-0.186848	2.420852	0.997196
C	-2.650361	-1.265030	-0.371177
O	-1.743772	-0.671956	-1.014264
C	1.527826	-2.130090	0.078554
O	1.654695	-2.287969	-1.169277
C	-1.355640	2.446087	0.302066
O	-1.425654	3.128222	-0.765007
C	2.334571	1.113174	-3.023341
C	3.204810	0.271947	-2.392126
H	2.110130	1.018802	-4.079548
N	1.996223	2.185262	-0.921325
N	3.475225	0.361037	-1.076876
C	2.921828	1.367873	-0.345507
O	3.268196	1.555358	0.857798
H	-6.581690	-0.914969	1.560081
H	1.249833	1.152328	3.567686
N	1.124476	1.704541	2.734907
N	-5.820510	-0.483449	1.062893
H	-5.857993	0.510416	0.895452
H	1.953226	1.945437	2.193503
H	1.096615	-1.564131	3.845867
C	1.656718	2.051968	-2.222063
C	0.229601	-2.391027	2.034621
N	-0.864828	-2.867380	2.616264
N	0.680039	2.822233	-2.687704
H	3.704467	-0.532698	-2.930230
H	-1.002574	-2.757967	3.606444
H	-1.555968	-3.374320	2.090336
H	0.030573	3.248490	-2.031603

H	0.400301	2.733323	-3.650550
<b>Pd-C-IIb3 (M11L, SMD water)</b>			
Pd	-2.239041	3.408163	0.257838
Pd	-3.844423	-2.099372	0.069547
Pd	1.728382	-3.350147	-0.632719
Pd	3.340695	2.321962	-0.513712
C	-0.415364	2.425670	2.359917
C	0.775604	2.105119	2.943685
H	-1.345676	2.419785	2.925621
C	-1.865910	-2.183093	2.242794
C	-0.673966	-2.423149	2.860126
H	-0.561379	-2.349843	3.935769
N	0.265650	-2.865254	0.708760
N	-0.509281	2.788616	1.068211
N	1.819426	2.468505	0.826495
C	4.194841	-2.225910	0.556262
C	5.135838	-1.230769	0.868036
C	4.815167	0.050242	0.529588
H	6.078117	-1.482162	1.340243
H	5.505853	0.870988	0.724614
N	3.651841	0.381244	-0.061400
N	3.020902	-1.896891	-0.025656
H	3.394605	4.874219	-0.153129
H	3.650061	4.596218	-1.759832
H	2.122631	4.425273	-1.127571
H	4.438185	2.324180	-2.832505
H	5.531812	2.918837	-1.749563
H	5.291894	1.291367	-1.873373
H	3.489519	-4.767575	-1.902190
H	2.630055	-3.852014	-2.971606
H	3.849138	-3.166515	-2.103555
H	0.947425	-5.369400	-2.079180
H	0.479903	-5.598928	-0.513883
H	-0.339194	-4.510439	-1.470618
H	-4.690847	4.193823	0.217865
H	-3.866180	4.983785	-0.973271
H	-4.370782	3.429977	-1.207786
H	-1.411326	5.033655	2.091063
H	-1.954410	5.905688	0.801373
H	-3.030431	5.261265	1.875439
H	-4.755091	-4.491910	0.414716
H	-3.724693	-4.146406	1.652580
H	-5.258748	-3.541905	1.665750
H	-5.924993	-2.798658	-1.284837
H	-6.408822	-1.833846	-0.036184
H	-5.752261	-1.161873	-1.391781
N	-5.700607	-1.956644	-0.757772
N	-4.465522	-3.766255	1.067435
N	-2.149000	5.099173	1.392004
N	-3.997307	4.081353	-0.519767
N	3.118325	4.298368	-0.944739
N	4.828337	2.197505	-1.899953
N	3.090278	-3.843916	-2.062301
N	0.574906	-4.906674	-1.253138
N	-2.023128	-2.284942	0.910530
C	2.733484	-0.591893	-0.344397
O	1.644755	-0.307568	-0.909668
C	0.607027	2.800256	0.289942

O	0.528454	3.137576	-0.926807
C	-0.948857	-2.592329	0.129496
O	-1.071559	-2.661904	-1.126125
C	-2.583709	0.585788	-2.949916
H	-2.433357	0.553067	-4.022825
N	-3.267747	-0.457779	-0.927056
N	-2.414563	1.738320	-0.868544
C	-2.943402	0.660178	-0.217579
O	-3.146312	0.712385	1.028705
H	5.305345	-3.771979	1.261730
N	4.432856	-3.506700	0.835748
H	3.806228	-4.241412	0.542006
H	0.846260	1.836093	3.991210
C	-3.101402	-0.473584	-2.260833
C	1.929063	2.168442	2.138521
N	3.137712	1.956985	2.643573
H	3.248026	1.734410	3.618265
H	3.965848	2.082486	2.085447
C	0.411525	-2.806802	2.049477
C	-2.195592	1.711164	-2.200991
H	-2.752975	-1.908057	2.812448
H	-3.392897	-1.391234	-2.769466
N	-1.623095	2.777605	-2.752584
N	1.582651	-3.130877	2.583556
H	-1.081171	3.388514	-2.152419
H	-1.424254	2.776659	-3.739475
H	1.709657	-3.103740	3.581030
H	2.353502	-3.442426	2.016602

<b>Pd-C-IIb4 (M11L, SMD water)</b>			
Pd	-3.231872	2.603931	-0.142725
Pd	-2.764327	-3.003922	0.412532
Pd	2.884736	-2.933655	-0.697049
Pd	2.493513	2.895579	-0.336001
C	-0.298626	2.003284	2.855467
C	-0.707179	-1.675991	2.153560
C	0.618962	-1.497136	2.593103
C	1.616896	-1.960287	1.783162
H	0.831367	-1.005706	3.536492
H	2.662210	-1.864727	2.072630
N	1.379752	-2.555598	0.598517
N	-1.484407	2.307050	0.819921
N	0.879679	2.448158	0.824978
C	4.856425	-1.123970	0.436254
C	5.400483	0.022257	0.936490
H	6.350949	0.028062	1.456482
N	3.490979	1.184906	0.094312
N	3.680828	-1.148921	-0.218929
H	2.173731	5.280720	-1.346849
H	0.741060	4.435784	-1.272496
H	1.357493	5.167689	0.082400
H	4.479529	4.269842	-1.271385
H	4.729379	2.682076	-1.648821
H	3.644551	3.569669	-2.511129
H	4.854364	-4.168481	-1.828831
H	4.033350	-3.295210	-2.962631
H	5.105487	-2.543498	-1.962566
H	1.141358	-4.652356	-1.192253
H	2.523897	-5.196895	-1.953526
H	2.341871	-5.426888	-0.329684

H	-5.749126	3.095294	-0.365549
H	-4.968643	3.766269	-1.656719
H	-5.290874	2.146984	-1.633748
H	-2.608533	4.593824	1.387365
H	-3.684671	5.121955	0.254000
H	-4.214733	4.260378	1.557160
H	-1.686943	-4.483407	2.225182
H	-3.326643	-4.517228	2.420733
H	-2.615100	-5.437823	1.250472
H	-4.492744	-4.740963	-0.406469
H	-5.253342	-3.638632	0.559116
H	-4.890384	-3.254357	-1.004009
N	-4.560786	-3.751012	-0.178808
N	-2.576470	-4.541885	1.733034
N	-3.458196	4.352577	0.881198
N	-5.019112	2.942736	-1.059456
N	1.597656	4.669507	-0.771652
N	4.022831	3.412203	-1.577799
N	4.400006	-3.275928	-2.012752
N	2.149505	-4.790544	-1.099255
N	-0.941409	-2.325630	0.993155
C	2.983022	0.012709	-0.406124
O	1.896580	0.018470	-1.041486
C	-0.311419	2.463655	0.144393
O	-0.316558	2.651111	-1.104138
C	0.086856	-2.729027	0.192425
O	-0.172885	-3.282880	-0.915300
C	-2.696266	-0.534557	-3.041457
H	-2.528872	-0.644992	-4.106637
N	-2.951218	-1.487642	-0.883123
N	-3.053598	0.854816	-1.135762
C	-3.167566	-0.253612	-0.348928
O	-3.482526	-0.134542	0.869304
H	-1.616921	-0.728342	3.690326
N	-1.761077	-1.256263	2.844911
H	-2.641939	-1.143202	2.352845
H	-0.289921	1.811616	3.922688
C	-2.738508	-1.612311	-2.204326
C	-2.826055	0.741096	-2.461575
C	-1.460870	2.070079	2.144237
H	-2.599809	-2.625338	-2.577569
N	-2.745042	1.849275	-3.189747
H	-2.719955	2.757221	-2.753244
H	-2.558795	1.791419	-4.176566
C	0.904092	2.225483	2.156322
C	4.670812	1.208278	0.749892
N	2.068795	2.239875	2.793514
N	5.113287	2.373817	1.217235
H	4.627537	3.239857	1.037153
H	5.993590	2.418568	1.703575
H	2.101366	2.087556	3.787185
H	2.931130	2.445172	2.317564
H	-2.429604	1.944376	2.626360
H	5.361716	-2.082629	0.551300

**Pd-C-IIIb1 (M11L, SMD water)**

Pd	-4.087431	1.052196	-0.449927
Pd	-0.370023	-3.586901	-0.557530
Pd	4.579335	-0.710630	0.111083
Pd	0.938615	3.633178	0.192042

C	-0.211683	1.695339	2.115047
C	2.357586	1.117144	-2.967050
H	0.779775	1.778537	2.559363
C	-1.212948	0.993267	2.723237
C	2.548964	-1.059158	2.211639
C	-4.365815	-3.081840	0.614405
H	3.312411	-0.526282	2.776641
C	1.397326	-1.489977	2.802199
C	-3.106520	-3.509349	0.325398
H	-2.812242	-4.544067	0.506716
H	-5.117522	-3.743069	1.029776
H	1.191280	-1.315037	3.852350
H	-1.065408	0.491353	3.673664
N	0.751622	-2.417173	0.693829
N	2.820121	-1.280270	0.912569
N	-2.151438	-2.702017	-0.179881
N	-3.704726	-0.918946	-0.156536
N	-2.611218	1.527406	0.861470
N	-0.397088	2.341576	0.949745
N	3.576592	0.635973	-0.981648
N	1.829508	2.210138	-0.919337
C	3.347337	0.457650	-2.294530
H	2.171060	0.948383	-4.021512
H	3.988112	-0.265231	-2.796349
C	-4.650340	-1.726949	0.368965
C	-2.464514	0.958250	2.077671
C	1.532994	1.974393	-2.213917
C	0.497151	-2.224876	2.006349
C	-2.444753	-1.389808	-0.438205
O	-1.584850	-0.628269	-0.952679
C	-1.584808	2.231035	0.299489
O	-1.742083	2.797139	-0.824436
C	1.896472	-1.908545	0.130646
O	2.104707	-2.057555	-1.106768
C	2.839991	1.549823	-0.288339
O	3.094543	1.802234	0.924068
N	1.307445	-4.685411	-0.915549
H	1.668669	-5.075410	-0.047337
H	1.154498	-5.450315	-1.569014
N	-1.374404	-4.806168	-1.841848
H	-0.881689	-4.871276	-2.731252
H	-1.454488	-5.744270	-1.452681
N	-5.456812	0.589638	-1.888664
H	-5.473607	-0.408227	-2.090883
H	-6.398139	0.880814	-1.629188
N	-4.531364	3.023508	-0.673156
H	-3.631468	3.474934	-0.842406
H	-5.163501	3.217355	-1.446464
N	2.301172	4.945370	-0.563746
H	2.261409	5.864632	-0.128395
H	3.237259	4.567820	-0.428908
N	0.085367	5.101337	1.317666
H	0.752042	5.468716	1.994482
H	-0.229374	5.871280	0.730634
N	6.356593	-0.133193	-0.693205
H	6.239762	0.726987	-1.223977
H	7.052798	0.028466	0.032274
N	5.565542	-2.082607	1.254669
H	6.263840	-2.590005	0.714810
H	6.039622	-1.607971	2.021433

H	-2.311760	-4.454890	-2.027514
H	1.992388	-4.035108	-1.301634
H	-4.942948	3.393732	0.180275
H	-5.202098	1.078802	-2.745623
H	2.146358	5.058760	-1.563632
H	-0.717811	4.736467	1.825674
H	4.916243	-2.759059	1.651518
H	6.712436	-0.851393	-1.320912
N	-3.520512	0.385587	2.640396
N	0.458980	2.573671	-2.715720
N	-5.847146	-1.221533	0.652194
N	-0.596255	-2.763125	2.532569
H	-6.054761	-0.241424	0.537345
H	-6.563676	-1.816915	1.032485
H	-0.798117	-2.646213	3.511025
H	-1.209184	-3.339327	1.981936
H	0.203966	2.415558	-3.676298
H	-0.236855	2.961314	-2.083931
H	-4.428583	0.429234	2.206720
H	-3.444579	-0.041550	3.547785

**Pd-C-IIIb2 (M11L, SMD water)**

Pd	-0.588186	3.636425	-0.536849
Pd	-4.263249	-0.920867	-0.380703
Pd	0.809738	-3.602337	0.064154
Pd	4.444199	0.790319	-0.035714
C	2.108986	-0.972747	-3.060722
C	1.240696	1.618138	2.724593
C	-4.211684	2.936968	1.484739
C	-1.371188	-1.019494	2.687914
H	-4.826663	3.502323	2.175296
H	-1.236282	-0.546905	3.655080
H	1.007556	1.459230	3.771730
N	-2.740499	-1.516535	0.802360
N	-0.529041	-2.333419	0.888278
N	-3.828739	0.973814	0.180915
N	-2.238140	2.719019	0.170400
N	0.646735	2.480733	0.584743
N	2.717701	1.359929	0.869574
N	1.686687	-2.161640	-1.041151
N	3.402517	-0.551956	-1.108971
H	1.871774	-0.760263	-4.097115
C	-3.019633	3.411160	1.021715
C	0.378641	2.267368	1.887838
C	3.108387	-0.317032	-2.400997
C	-2.554897	-0.951095	2.012466
C	-2.631537	1.481767	-0.252500
O	-1.915131	0.815471	-1.048567
C	1.824636	2.013560	0.065875
O	2.107654	2.199653	-1.151496
C	-1.720929	-2.227360	0.241778
O	-1.876693	-2.809117	-0.875117
C	2.725375	-1.521976	-0.436442
O	3.059784	-1.839716	0.743148
N	-4.689652	-2.839876	-0.906027
H	-5.222127	-3.305978	-0.175442
H	-5.206944	-2.911057	-1.779286
N	-5.764669	-0.281964	-1.598150
H	-5.524637	-0.496126	-2.565261
H	-6.639805	-0.753430	-1.377578

N	-1.805184	4.838497	-1.641581
H	-2.786933	4.658940	-1.439794
H	-1.616727	5.821537	-1.453193
N	0.999786	4.730850	-1.190902
H	1.730473	4.058990	-1.429786
H	0.776574	5.298234	-2.005690
N	6.154456	0.224278	-0.983513
H	6.954853	0.810538	-0.754180
H	6.380304	-0.735600	-0.729889
N	5.476216	2.202258	1.009127
H	6.134266	1.771340	1.656302
H	6.002446	2.796546	0.370474
N	2.158886	-4.885610	-0.758580
H	3.092352	-4.491540	-0.654187
H	2.157549	-5.813554	-0.340960
N	-0.061185	-5.060354	1.189041
H	-1.036772	-5.154028	0.912859
H	0.382199	-5.972365	1.099329
H	-5.915400	0.722233	-1.528132
H	-3.777050	-3.288159	-1.011655
H	1.330125	5.347535	-0.452454
H	-1.650425	4.668523	-2.633934
H	6.012158	0.258950	-1.991312
H	4.847129	2.797973	1.544154
H	-0.034175	-4.790609	2.171029
H	1.967640	-4.985076	-1.753874
H	3.703690	0.448553	-2.895364
C	1.331733	-1.877297	-2.312579
C	-0.312041	-1.709547	2.067383
H	-3.409975	-0.425367	2.433927
H	-0.572889	2.652778	2.252460
C	2.453165	1.158177	2.177943
C	-4.611267	1.664812	1.036058
H	-2.644842	4.388098	1.325985
N	-5.748176	1.109630	1.441201
N	0.900368	-1.792264	2.598083
N	3.367757	0.542946	2.919285
N	0.248342	-2.471746	-2.797944
H	-6.007886	0.177484	1.157354
H	-6.356574	1.604251	2.071381
H	-0.425530	-2.887501	-2.159074
H	-0.046958	-2.268425	-3.738636
H	1.691748	-2.072161	2.020457
H	1.090812	-1.307019	3.459962
H	4.179501	0.120942	2.495451
H	3.195660	0.368474	3.895302

**Pd-C-IVb (M11L, SMD water)**

Pd	-3.914701	-1.758614	-0.470652
Pd	1.476583	-3.563352	0.356099
Pd	4.191791	1.422882	-0.157767
Pd	-1.182607	3.453241	-0.533967
C	2.293759	1.552750	2.088481
C	2.337601	-1.054936	-3.014348
H	3.162827	1.147067	2.604928
C	1.162485	1.897073	2.768208
C	-4.897509	2.034679	1.052761
C	-1.128330	-1.034536	2.633317
C	-4.895247	0.744636	0.610276
C	-2.279846	-1.200742	1.918268

H	-3.207928	-0.730863	2.239384
H	-5.729399	0.075946	0.820333
H	-5.723748	2.448859	1.618179
H	-1.099369	-0.434268	3.536861
H	1.080177	1.773916	3.842496
N	-2.342306	-1.934317	0.788284
N	-0.048838	-2.434044	1.040279
N	-3.881793	0.220210	-0.102142
N	-2.741100	2.283852	0.049962
N	0.207755	2.582631	0.687311
N	2.412556	1.707659	0.757961
N	2.112936	-2.109170	-0.889539
N	3.458029	-0.188878	-1.104571
C	3.160118	-0.144695	-2.415891
H	3.594914	0.680158	-2.978234
H	2.088008	-0.995345	-4.067505
C	-3.773620	2.815216	0.740279
C	0.105038	2.460626	2.028613
C	1.741077	-2.023123	-2.185457
C	0.035524	-1.658398	2.142457
C	-2.785922	0.986952	-0.394213
O	-1.832328	0.520832	-1.072066
C	1.351692	2.178776	0.040224
O	1.423657	2.267698	-1.217606
C	2.981766	-1.212528	-0.343998
O	3.348918	-1.342158	0.860589
C	-1.215917	-2.568770	0.354391
O	-1.245020	-3.307027	-0.676533
H	-4.488672	-4.041410	-1.600514
H	-3.016362	-4.060960	-0.820694
H	-4.438384	-4.230073	0.038126
H	-5.981493	-2.363172	-1.947626
H	-6.148766	-0.830190	-1.371459
H	-5.131576	-1.128638	-2.633690
H	-0.083027	5.493215	-1.742567
H	0.666459	5.222022	-0.298708
H	0.978494	4.217448	-1.580799
H	-2.608832	5.319426	-1.630425
H	-2.073900	4.267304	-2.783158
H	-3.372305	3.869936	-1.851236
H	4.664572	3.030569	1.794025
H	5.867349	3.250098	0.690986
H	4.379948	3.910434	0.430038
H	5.882059	0.659641	-1.943077
H	6.477086	2.027506	-1.241390
H	6.593813	0.579678	-0.459144
H	3.893815	-4.200522	-0.165345
H	3.087654	-5.613090	0.106301
H	2.920582	-4.833212	-1.336885
H	-0.133928	-5.290628	1.322605
H	1.385123	-5.860642	1.625007
H	0.753469	-4.656537	2.559289
N	-3.994186	-3.771624	-0.753878
N	-5.480459	-1.498958	-1.750993
N	3.021036	-4.697480	-0.332774
N	0.805821	-5.023201	1.610709
N	5.997398	1.148781	-1.057511
N	4.866662	3.095421	0.797791
N	0.259362	4.769863	-1.114208
N	-2.465904	4.333669	-1.844739

N	0.812607	-2.864992	-2.624356
N	-3.682319	4.085914	1.132085
N	-0.988054	2.904119	2.637799
N	1.220062	-1.540547	2.728744
H	2.062813	-1.752964	2.197512
H	1.310742	-0.932887	3.526797
H	-1.726191	3.370413	2.136127
H	-1.070681	2.832498	3.637713
H	-2.920354	4.678254	0.834030
H	-4.444416	4.512497	1.633002
H	0.515894	-2.810448	-3.584818
H	0.201816	-3.327255	-1.956068

**Pd-C-Ic (M1 1L, SMD water)**

Pd	0.660702	3.997654	-0.173656
Pd	0.310629	0.055965	4.181774
Pd	-0.660702	-3.997654	0.173656
Pd	-0.310629	-0.055965	-4.181774
C	2.635125	-3.209881	2.797347
C	-2.554396	2.127447	1.855427
C	-1.749943	2.961072	1.136544
H	-2.177702	3.766621	0.544016
C	1.749943	-2.961072	-1.136544
C	-2.635125	3.209881	-2.797347
H	2.177702	-3.766621	-0.544016
C	2.554396	-2.127447	-1.855427
C	-2.199907	2.030521	-3.330280
H	-2.861532	1.420108	-3.943930
H	-3.631465	3.590905	-2.989519
H	3.634122	-2.221786	-1.839936
H	-3.634122	2.221786	1.839936
N	0.577061	-1.050651	-2.640077
N	0.407511	-2.846978	-1.110163
N	-0.949914	1.559436	-3.149382
N	-0.528794	3.375821	-1.698003
N	-0.407511	2.846978	1.110163
N	-0.577061	1.050651	2.640077
N	0.528794	-3.375821	1.698003
N	0.949914	-1.559436	3.149382
C	2.199907	-2.030521	3.330280
H	2.861532	-1.420108	3.943930
H	3.631465	-3.590905	2.989519
C	-1.733645	3.912993	-1.977843
C	-1.926596	1.113535	2.596416
C	1.733645	-3.912993	1.977843
C	1.926596	-1.113535	-2.596416
C	-0.089519	2.254515	-2.347724
O	1.103364	1.878270	-2.201583
C	0.191881	1.899789	1.895853
O	1.454087	1.813043	1.949098
C	0.089519	-2.254515	2.347724
O	-1.103364	-1.878270	2.201583
C	-0.191881	-1.899789	-1.895853
O	-1.454087	-1.813043	-1.949098
N	1.677820	5.145389	-1.513170
H	2.542628	5.533821	-1.142247
H	1.903841	4.573780	-2.325421
N	1.857660	4.582785	1.362473
H	2.743678	4.975278	1.051726
H	1.388471	5.270181	1.946547



N	-1.080006	0.804155	-5.862842
H	-0.526508	0.558170	-6.682300
H	-2.034844	0.485590	-6.019977
N	0.279481	-1.672961	-5.271777
H	0.027992	-2.522877	-4.770185
H	-0.145904	-1.715055	-6.196064
N	-1.857660	-4.582785	-1.362473
H	-1.388471	-5.270181	-1.946547
H	-2.743678	-4.975278	-1.051726
N	-1.677820	-5.145389	1.513170
H	-1.903841	-4.573780	2.325421
H	-2.542628	-5.533821	1.142247
N	1.080006	-0.804155	5.862842
H	2.034844	-0.485590	6.019977
H	0.526508	-0.558170	6.682300
N	-0.279481	1.672961	5.271777
H	0.145904	1.715055	6.196064
H	-0.027992	2.522877	4.770185
H	-1.291063	1.662316	5.391570
H	1.088344	-1.819454	5.787238
H	-2.035936	-3.734032	-1.902684
H	-1.086583	-5.916015	1.818389
H	-1.088344	1.819454	-5.787238
H	1.291063	-1.662316	-5.391570
H	1.086583	5.916015	-1.818389
H	2.035936	3.734032	1.902684
N	-2.611415	0.220295	3.304224
N	-2.029994	5.093767	-1.445155
N	2.611415	-0.220295	-3.304224
N	2.029994	-5.093767	1.445155
H	-2.152511	-0.653515	3.527733
H	-3.617592	0.239444	3.280064
H	-1.352810	5.589279	-0.884733
H	-2.927917	5.518410	-1.604446
H	3.617592	-0.239444	-3.280064
H	2.152511	0.653515	-3.527733
H	2.927917	-5.518410	1.604446
H	1.352810	-5.589279	0.884733

**Pd-C-IIc1 (M11L, SMD water)**

Pd	3.913057	1.531786	-0.496839
Pd	1.313117	-3.667748	-0.340589
Pd	-3.995413	-1.435316	0.952099
Pd	-1.465850	3.689715	-0.101757
C	-1.770011	-1.933158	-2.599777
C	-2.762197	-1.844232	-1.669314
H	-1.958704	-1.783779	-3.656831
H	-3.789721	-1.651500	-1.970685
N	-2.547320	-1.994862	-0.347708
C	-4.473314	1.497524	-2.112268
C	-3.426554	2.304192	-1.772332
H	-5.005317	1.614214	-3.049235
H	-3.080994	3.074391	-2.460344
N	-2.771984	2.215376	-0.596069
N	-4.090333	0.316280	-0.081471
H	0.619352	5.165592	-0.291830
H	-0.606536	6.149759	0.202615
H	0.130428	5.149992	1.284650
H	-2.824318	5.888388	-0.218627
H	-2.698836	5.257022	-1.735346

H	-3.807016	4.651643	-0.670640
H	-5.418331	-1.284119	3.127017
H	-5.297255	0.198031	2.412623
H	-6.361706	-0.917766	1.823002
H	-4.281106	-3.949273	1.421170
H	-2.802947	-3.385299	1.950609
H	-4.166964	-3.190244	2.882593
H	2.923249	3.637563	-1.425752
H	4.229812	4.084104	-0.492600
H	4.465153	3.561832	-2.040789
H	5.232136	1.272848	-2.682140
H	6.306570	1.612340	-1.475850
H	5.710605	0.080229	-1.650037
H	3.718301	-4.608519	-0.091456
H	2.686276	-5.508911	0.834126
H	2.768821	-5.751259	-0.794036
H	0.471097	-6.069842	-0.914411
H	-0.810111	-5.039451	-0.847909
H	0.167898	-5.051483	-2.175705
N	0.155099	-5.132989	-1.159868
N	2.796631	-5.040683	-0.064406
N	5.478268	1.069289	-1.714435
N	3.899757	3.436689	-1.204202
N	-0.192167	5.227004	0.321688
N	-2.863388	5.024158	-0.756939
N	-5.438870	-0.794429	2.235166
N	-3.808988	-3.206066	1.930654
N	-0.281510	-2.479699	-0.814091
C	-3.115480	1.213011	0.271777
O	-2.546735	1.094618	1.387973
C	1.113971	2.057052	2.744888
C	-1.297991	-2.344408	0.088304
O	-1.085096	-2.567774	1.316152
C	3.299878	-2.638556	1.555812
C	4.393630	-1.932485	1.965751
H	2.983073	-3.532648	2.091004
H	4.994419	-2.248902	2.810823
N	2.567183	-2.298564	0.475236
N	3.893413	-0.351421	0.258048
C	2.868251	-1.141810	-0.188388
O	2.223806	-0.795964	-1.213688
C	1.164346	2.349550	0.009003
O	1.189597	2.506525	-1.246602
N	2.309139	1.990728	0.674604
N	0.010613	2.559744	0.702350
H	1.100314	1.950391	3.823556
C	-4.820151	0.482909	-1.201927
C	-0.478437	-2.219040	-2.127329
C	4.712674	-0.771130	1.242740
C	-0.000499	2.397334	2.039083
N	-5.825693	-0.356472	-1.424276
N	0.576593	-2.293100	-2.930977
N	5.791446	-0.043939	1.520322
H	1.493832	-2.187227	-2.513187
H	0.467075	-2.099121	-3.913007
H	6.417751	-0.326534	2.255505
H	6.055155	0.745405	0.949993
H	-6.045469	-1.083595	-0.760897
H	-6.374234	-0.286021	-2.264415
C	2.310775	1.892069	2.023130

H	-0.952995	2.569183	2.532208
N	3.454560	1.660005	2.650893
H	3.470522	1.577310	3.653281
H	4.331766	1.605604	2.159662

**Pd-C-IIc2 (M11L, SMD water)**

Pd	0.403123	3.646446	0.771144
Pd	-4.416420	0.379606	-0.089304
Pd	-0.430355	-3.778499	-0.646689
Pd	4.445763	-0.571356	-0.159043
C	-2.683791	-2.359290	2.687835
C	-1.652119	2.290931	-2.699557
C	-0.844238	2.930015	-1.807379
H	-0.059373	3.595343	-2.157107
C	3.204464	2.796846	-2.346094
C	2.151003	-2.827747	2.601190
C	3.651894	1.578505	-1.928370
H	4.283110	0.972271	-2.577231
H	3.486335	3.214642	-3.305480
H	2.231873	-3.096912	3.647819
H	-1.521679	2.402251	-3.769855
N	2.942374	-1.614433	0.706768
N	1.094542	-3.067969	0.481260
N	3.369458	1.058527	-0.715294
N	1.939314	2.903961	-0.332660
N	-0.964156	2.792707	-0.472186
N	-2.819123	1.369513	-0.838539
N	-1.816944	-2.876916	0.530757
N	-3.285156	-1.040844	0.795233
H	-2.764084	-2.576924	3.746587
C	2.364203	3.499333	-1.465110
C	-2.650476	1.453580	-2.175724
C	-1.946282	-3.137800	1.844284
C	1.230918	-3.404348	1.776255
C	-1.980989	2.020111	0.023443
O	-2.159277	1.915861	1.270972
C	2.489551	1.721633	0.098287
O	2.177618	1.280197	1.235050
C	1.982357	-2.186769	-0.075022
O	1.927082	-1.920271	-1.310038
C	-2.549641	-1.858112	-0.016729
O	-2.565747	-1.684439	-1.266456
N	1.801670	4.466579	2.000199
H	1.442590	4.682761	2.928002
H	2.566472	3.801860	2.101379
N	-1.121089	4.455826	1.846459
H	-0.843174	4.770027	2.772910
H	-1.521791	5.245957	1.346714
N	-5.637145	1.770511	-0.947710
H	-6.223394	1.338171	-1.659456
H	-6.245330	2.178932	-0.239714
N	-6.090521	-0.575657	0.575897
H	-6.622331	0.023140	1.205578
H	-6.684347	-0.808592	-0.218867
N	-1.956673	-4.464693	-1.801286
H	-2.545661	-3.648053	-1.968324
H	-1.650994	-4.844895	-2.693908
N	0.982709	-4.623224	-1.841807
H	1.495975	-5.341485	-1.336124
H	0.612672	-5.034264	-2.695927

N	6.127190	0.352249	-0.867011
H	6.053952	1.366848	-0.819754
H	6.935656	0.076000	-0.311008
N	5.625365	-2.173264	0.277915
H	5.063010	-2.985659	0.525824
H	6.196299	-2.420099	-0.529524
H	-5.112131	2.525091	-1.385992
H	2.172434	5.322480	1.591496
H	-1.817409	3.712413	1.932702
H	6.308175	0.087960	-1.834621
H	6.247043	-1.964070	1.057246
H	-2.493804	-5.177720	-1.313921
H	1.617602	-3.859728	-2.079969
H	-5.874166	-1.440648	1.067554
C	3.003762	-1.866017	2.032748
H	0.575344	-4.188335	2.145265
C	-3.323651	-1.238513	2.130404
H	-1.439005	-4.024628	2.214434
N	-3.464855	0.757160	-2.959670
N	1.948377	4.735904	-1.718414
N	3.910427	-1.218783	2.756821
N	-4.001778	-0.375128	2.878199
H	1.366424	5.228067	-1.056387
H	2.223680	5.205239	-2.564587
H	-4.045834	0.030636	-2.570178
H	-3.357902	0.799072	-3.959347
H	-4.051815	-0.502722	3.874791
H	-4.367287	0.479223	2.485781
H	4.465607	-0.477999	2.355631
H	3.993023	-1.399782	3.743134

**Pd-C-IIIc1 (M11L, SMD water)**

Pd	-1.640696	-3.666005	-0.957480
Pd	-3.979655	1.532500	0.010051
Pd	1.479375	3.552802	0.649663
Pd	3.822520	-1.814339	0.137001
C	-1.089120	2.732955	-2.739388
H	-1.061262	2.843533	-3.817227
N	-0.070411	3.066915	-0.597624
C	4.145914	1.665225	-2.150765
H	4.716879	1.926669	-3.034787
N	3.351519	0.021254	-0.611859
N	2.753881	2.297422	-0.326700
H	4.945048	-3.556652	1.673721
H	3.662497	-4.270958	0.916178
H	5.081172	-4.056529	0.106198
H	6.388692	-1.845559	0.375051
H	6.018966	-1.801131	-1.230073
H	5.975149	-0.417890	-0.326834
H	2.687041	4.540934	2.747665
H	3.337758	3.084158	2.328972
H	3.751417	4.445442	1.494626
H	-0.120660	5.534210	0.993102
H	-0.611156	4.198234	1.854939
H	0.564124	5.209986	2.459097
H	0.427976	-4.273882	-2.218942
H	-0.296986	-5.706546	-1.772294
H	-0.828966	-4.900643	-3.111885
H	-2.971722	-4.084138	-3.164311
H	-3.947334	-4.383800	-1.865472

H	-3.579826	-2.817340	-2.283780
H	-6.132497	1.766841	1.418960
H	-6.535745	1.309500	-0.113885
H	-5.989814	0.188909	0.961295
H	-5.418630	3.695827	-0.200587
H	-3.849778	4.028672	-0.582355
H	-4.825890	3.278820	-1.681217
N	-4.597457	3.345499	-0.690397
N	-5.878593	1.151142	0.648472
N	-3.221562	-3.771370	-2.229111
N	-0.455588	-4.785144	-2.172665
N	4.449359	-3.637833	0.787402
N	5.776553	-1.417009	-0.317871
N	2.983085	3.965974	1.961237
N	0.186517	4.789091	1.613547
N	-2.182408	2.012332	-0.760817
C	0.709297	-3.334910	2.559631
C	-3.517935	-1.936165	2.438287
H	-3.751195	-2.223712	3.457131
N	-3.425001	-0.277593	0.725174
N	-2.777072	-2.500601	0.249047
N	-0.069178	-3.457470	0.311097
N	1.989509	-2.397010	0.780628
H	0.588821	-3.569972	3.610733
C	3.997356	0.372955	-1.744859
C	-3.099076	-2.843392	1.508937
C	-0.180120	-3.760881	1.617877
C	-2.122709	2.120336	-2.101496
H	-1.023682	-4.385394	1.899806
H	-3.016425	-3.898521	1.759442
H	-2.965287	1.705725	-2.652800
H	4.429914	-0.442096	-2.323416
C	-3.027777	-1.224861	-0.176973
O	-2.906138	-0.932003	-1.398410
C	-1.145446	2.455182	0.001799
O	-1.171806	2.318548	1.259314
C	2.678869	0.988798	0.086416
O	1.994938	0.710057	1.105896
C	1.054415	-2.807178	-0.124296
O	1.238200	-2.599322	-1.358559
C	3.571339	2.658457	-1.336498
C	-0.067730	3.272569	-1.934308
N	3.810828	3.949264	-1.544901
N	0.895754	4.002695	-2.474161
H	4.406842	4.237359	-2.302639
H	3.486868	4.654530	-0.900023
H	0.916714	4.154892	-3.468444
H	1.603426	4.446842	-1.914833
C	1.805218	-2.581715	2.106060
C	-3.598889	-0.594060	2.028118
N	2.706794	-2.080155	2.941543
N	-3.872773	0.385415	2.881950
H	-3.845483	1.351730	2.594022
H	-4.021090	0.181357	3.856034
H	3.445877	-1.481747	2.605062
H	2.607712	-2.213558	3.933847

**Pd-C-IIIc2 (M11L, SMD water)**

Pd	0.068276	3.758243	-0.760426
Pd	-4.418435	0.077311	0.003160

Pd	-0.074215	-3.736820	0.770489
Pd	4.513440	-0.073874	-0.010964
C	3.527132	1.904940	1.842465
C	2.865408	-3.172685	-2.295863
H	4.247250	1.355831	2.448002
C	2.987268	3.072308	2.296408
C	-1.226343	-2.873315	-1.804453
C	-1.846886	2.174524	2.692495
H	-0.488300	-3.588732	-2.157626
C	-1.979881	-2.169158	-2.695949
H	-1.708899	2.264164	3.763960
H	-1.853681	-2.286719	-3.766163
H	3.267932	3.502649	3.250647
N	-3.064391	-1.158962	-0.836997
N	-1.348097	-2.745509	-0.467916
N	-2.959580	1.215598	0.819863
N	-1.227010	2.790252	0.472857
N	1.652107	3.098927	0.325184
N	3.241515	1.375671	0.634108
N	1.532425	-3.140283	-0.322461
N	3.185355	-1.479304	-0.642744
H	3.129516	-3.618113	-3.247789
C	-1.098462	2.895902	1.810387
C	2.063803	3.713853	1.452475
C	3.449061	-2.024190	-1.849081
C	-2.911954	-1.256865	-2.173193
C	2.267097	1.958239	-0.127057
O	1.929559	1.476830	-1.242390
C	-2.192993	1.960402	-0.031082
O	-2.392492	1.884816	-1.276944
C	-2.302767	-1.896534	0.024240
O	-2.500533	-1.791257	1.267821
C	2.192135	-2.021591	0.123895
O	1.877012	-1.523529	1.238337
N	1.404249	4.703612	-1.967726
H	2.084085	4.019309	-2.294456
H	0.978447	5.143239	-2.781003
N	-1.493869	4.474547	-1.846691
H	-1.934426	5.255630	-1.366134
H	-1.228362	4.780637	-2.779654
N	6.030618	1.214629	0.439397
H	6.429679	0.994415	1.350811
H	6.770615	1.134747	-0.256752
N	5.978709	-1.416059	-0.477441
H	6.378814	-1.207035	-1.391135
H	6.726994	-1.367162	0.212599
N	-1.652176	-4.391798	1.871880
H	-2.114065	-5.168734	1.404596
H	-1.390524	-4.690447	2.808364
N	1.234408	-4.719548	1.976887
H	1.928568	-4.053393	2.311130
H	0.795464	-5.156249	2.784783
N	-5.825716	1.300846	0.825584
H	-6.347049	0.807827	1.548644
H	-5.399562	2.123956	1.246559
N	-5.922928	-1.058482	-0.772452
H	-6.436033	-0.548817	-1.489672
H	-5.556907	-1.913071	-1.187589
H	-6.484538	1.616341	0.115737
H	1.714932	-5.443302	1.445816

H	5.632970	-2.373587	-0.492264
H	5.721234	2.184700	0.452711
H	1.899033	5.420776	-1.440878
H	-2.151239	3.695916	-1.919696
H	-6.576309	-1.319940	-0.036371
H	-2.289174	-3.595558	1.935237
C	-2.780579	1.271946	2.156617
H	-0.355419	3.602407	2.171684
H	4.187358	-1.504874	-2.458979
C	1.919811	-3.774965	-1.447771
N	1.558843	4.909676	1.739434
N	-3.521821	0.480866	2.922872
N	1.372456	-4.952530	-1.731707
N	-3.671450	-0.499595	-2.955445
H	-4.000019	-0.306325	2.510151
H	-3.401914	0.495284	3.922002
H	0.921972	5.366499	1.103415
H	1.827158	5.388903	2.582316
H	1.623173	-5.442065	-2.574135
H	0.719450	-5.386503	-1.096456
H	-3.570123	-0.547952	-3.955284
H	-4.220102	0.252117	-2.568242

**Pd-C-IVc1 (M11L, SMD water)**

Pd	4.047519	1.350146	-0.743146
Pd	1.230825	-3.752714	-0.165821
Pd	-4.047529	-1.350109	0.743156
Pd	-1.230828	3.752730	0.165837
C	3.398985	-2.716533	1.488567
C	-1.482793	-1.899205	-2.671478
H	3.079203	-3.571854	2.082479
C	4.544671	-2.048465	1.807781
C	1.482700	1.898996	2.671492
C	-4.544608	2.048500	-1.807876
C	0.331411	2.271230	2.046751
C	-3.398966	2.716594	-1.488570
H	-3.079171	3.571948	-2.082427
H	-0.591957	2.416772	2.601615
H	1.530410	1.741791	3.742949
H	-5.180100	2.363416	-2.627636
H	5.180193	-2.363385	2.627517
N	-2.614907	2.388618	-0.440176
N	-4.013032	0.509718	-0.074273
N	0.268216	2.506654	0.721660
N	2.548863	1.901865	0.530265
N	4.013027	-0.509728	0.074166
N	2.614860	-2.388556	0.440229
N	-2.548931	-1.902012	-0.530232
N	-0.268249	-2.506679	-0.721632
C	-0.331472	-2.271334	-2.046739
H	0.591898	-2.416849	-2.601606
H	-1.530522	-1.742056	-3.742944
C	2.635118	1.770393	1.872871
C	4.872320	-0.931218	1.022350
C	-2.635208	-1.770588	-1.872851
C	-4.872287	0.931241	-1.022470
C	2.920891	-1.263922	-0.280382
O	2.224866	-0.906632	-1.264767
C	-1.370508	-2.300636	0.051523
O	-1.319900	-2.493254	1.301484

C	-2.920928	1.263941	0.280355
O	-2.224933	0.906614	1.264747
C	1.370468	2.300589	-0.051505
O	1.319904	2.493306	-1.301441
H	5.689337	-0.209125	-1.974328
H	5.177430	0.962952	-3.014059
H	6.358232	1.300362	-1.911573
H	4.434039	3.895733	-0.874611
H	4.563338	3.295322	-2.407361
H	3.062444	3.428571	-1.700706
H	2.528672	-5.934887	-0.578333
H	3.581740	-4.854648	0.072310
H	2.505821	-5.645234	1.045015
H	-1.004408	-5.018838	-0.340678
H	-0.169562	-5.203039	-1.750768
H	0.200122	-6.137123	-0.441475
H	-4.563304	-3.295248	2.407477
H	-4.434032	-3.895664	0.874724
H	-3.062418	-3.428457	1.700772
H	-5.176956	-0.962241	3.014201
H	-5.689456	0.209262	1.974136
H	-6.357914	-1.300441	1.912103
H	1.004338	5.018979	0.339933
H	-0.200197	6.137154	0.441788
H	0.170283	5.202658	1.750563
N	5.492460	0.785789	-2.061634
N	4.048767	3.222524	-1.532604
N	2.629586	-5.210341	0.131258
N	-0.083963	-5.204081	-0.735416
N	-4.048755	-3.222449	1.532707
N	-5.492255	-0.785563	2.061780
N	0.084105	5.204028	0.735260
N	-2.629569	5.210380	-0.131197
H	-2.505798	5.645328	-1.044929
H	-3.581743	4.854736	-0.072268
H	-2.528619	5.934880	0.578438
N	5.999744	-0.249367	1.210111
N	3.818960	1.541306	2.421273
N	-5.999711	0.249398	-1.210314
N	-3.819052	-1.541609	-2.421275
H	-6.652343	0.538305	-1.919366
H	-6.264742	-0.509382	-0.601565
H	-3.898791	-1.419605	-3.416664
H	-4.662204	-1.506861	-1.871727
H	6.264646	0.509524	0.601446
H	6.652424	-0.538256	1.919126
H	4.662107	1.506785	1.871701
H	3.898728	1.419330	3.416661

**Pd-C-IVc2 (M11L, SMD water)**

Pd	-0.015754	-3.802447	-0.640399
Pd	-4.408195	0.000949	-0.000758
Pd	-0.013736	3.802092	0.641570
Pd	4.403101	-0.001024	-0.000376
C	-2.299483	2.505796	-2.713563
C	-2.302668	-2.504675	2.713728
C	2.401797	-2.643042	2.649077
C	2.404056	2.643951	-2.648380
H	2.494567	-2.911623	3.694876
H	2.497415	2.913373	-3.693904

H	-2.343409	-2.716856	3.775841
N	3.052193	1.285262	-0.794480
N	1.462476	3.008720	-0.494459
N	3.051851	-1.286601	0.794198
N	1.460703	-3.008865	0.495126
N	-1.441717	-2.973763	0.544250
N	-3.050741	-1.260429	0.820431
N	-1.439919	2.974249	-0.543390
N	-3.049653	1.261869	-0.820902
H	-2.339282	2.718071	-3.775698
C	1.615252	-3.349025	1.787295
C	-1.529089	-3.235174	1.860954
C	-1.526190	3.235831	-1.860136
C	1.617846	3.349901	-1.786270
C	-2.251681	-2.011054	0.002823
O	-2.275579	-1.828831	-1.246719
C	-2.250821	2.011996	-0.002620
O	-2.275931	1.829796	1.246913
C	2.235177	2.007764	0.029790
O	2.207730	1.771037	1.269922
C	2.234425	-2.009005	-0.029718
O	2.207626	-1.773239	-1.270050
H	-2.125252	-3.784980	-1.979343
H	-1.199948	-5.000186	-2.641887
H	-2.036942	-5.275762	-1.247728
H	1.955289	-5.287952	-1.386392
H	1.097601	-4.895775	-2.743103
H	2.064368	-3.753663	-2.019449
H	-6.506841	-1.467173	-0.057118
H	-5.509202	-2.074052	1.105301
H	-6.429652	-0.742021	1.424667
H	-5.507666	2.076230	-1.107973
H	-6.428346	0.744399	-1.427552
H	-6.506222	1.470002	0.053972
H	-1.197391	4.998882	2.643769
H	-2.034067	5.276195	1.249720
H	-2.123468	3.784820	1.980120
H	1.100313	4.894150	2.744640
H	2.066825	3.752516	2.020116
H	1.957525	5.287102	1.387855
H	5.514193	-2.103568	1.055263
H	6.501962	-1.465984	-0.097862
H	6.430816	-0.775935	1.401062
N	-1.515656	-4.577469	-1.772366
N	1.440117	-4.543995	-1.851509
N	-5.882492	-1.214385	0.707173
N	-5.881473	1.216790	-0.709846
N	-1.513355	4.577106	1.773873
N	1.442506	4.542892	1.852720
N	5.880933	-1.232774	0.675557
N	5.881417	1.229968	-0.676744
H	6.430198	0.773061	-1.403050
H	5.515091	2.101330	-1.055567
H	6.503416	1.462198	0.096196
C	3.084507	-1.532074	2.124253
C	-3.041384	-1.445567	2.159769
H	-0.954189	-4.081553	2.227004
H	1.079820	-4.234810	2.120649
H	1.083256	4.236403	-2.119075
C	3.085512	1.531855	-2.124306

H	-0.950640	4.081980	-2.225678
C	-3.039137	1.447014	-2.160228
N	3.804967	-0.727881	2.896830
N	-3.769027	-0.633731	2.917645
N	-3.766614	0.635549	-2.918657
N	3.805411	0.727572	-2.897304
H	4.212216	0.119321	2.530393
H	3.862412	-0.897434	3.886890
H	3.863255	0.897753	-3.887231
H	4.211739	-0.120320	-2.531396
H	-4.213636	0.183596	2.528941
H	-3.789686	-0.760684	3.915523
H	-4.211875	-0.181592	-2.530313
H	-3.786702	0.762651	-3.916532

**Pd-C-Id (M11L, SMD water)**

Pd	-1.825388	3.576669	-0.359404
Pd	3.576669	1.825388	0.359404
Pd	-3.576669	-1.825388	0.359404
Pd	1.825388	-3.576669	-0.359404
C	-0.117499	-1.681918	2.905096
C	0.784020	-2.325277	2.105645
H	0.159590	-1.287640	3.876143
H	1.818232	-2.462327	2.413566
N	0.452959	-2.826290	0.902812
N	-1.750037	-2.037763	1.201906
C	0.117499	1.681918	2.905096
C	-0.784020	2.325277	2.105645
H	-0.159590	1.287640	3.876143
H	-1.818232	2.462327	2.413566
N	-0.452959	2.826290	0.902812
N	1.750037	2.037763	1.201906
C	-1.681918	0.117499	-2.905096
C	1.681918	-0.117499	-2.905096
N	2.826290	0.452959	-0.902812
N	2.037763	-1.750037	-1.201906
C	2.325277	0.784020	-2.105645
H	1.287640	0.159590	-3.876143
H	2.462327	1.818232	-2.413566
H	-1.287640	-0.159590	-3.876143
C	-2.325277	-0.784020	-2.105645
N	-2.826290	-0.452959	-0.902812
N	-2.037763	1.750037	-1.201906
H	-2.462327	-1.818232	-2.413566
C	1.417439	1.504280	2.396269
C	1.504280	-1.417439	-2.396269
C	-1.417439	-1.504280	2.396269
C	-1.504280	1.417439	-2.396269
C	0.834668	2.730604	0.460582
O	1.185416	3.281522	-0.619912
C	2.730604	-0.834668	-0.460582
O	3.281522	-1.185416	0.619912
C	-0.834668	-2.730604	0.460582
O	-1.185416	-3.281522	-0.619912
C	-2.730604	0.834668	-0.460582
O	-3.281522	1.185416	0.619912
N	-5.399861	-1.587472	-0.514616
H	-5.329221	-1.801828	-1.507468
H	-6.121078	-2.181312	-0.110542
N	-4.320959	-3.228126	1.632594

H	-4.951317	-2.807542	2.312807
H	-4.835767	-3.943299	1.121716
N	-3.228126	4.320959	-1.632594
H	-3.943299	4.835767	-1.121716
H	-2.807542	4.951317	-2.312807
N	-1.587472	5.399861	0.514616
H	-2.181312	6.121078	0.110542
H	-1.801828	5.329221	1.507468
N	4.320959	3.228126	1.632594
H	4.951317	2.807542	2.312807
H	4.835767	3.943299	1.121716
N	5.399861	1.587472	-0.514616
H	5.329221	1.801828	-1.507468
H	6.121078	2.181312	-0.110542
N	1.587472	-5.399861	0.514616
H	0.617327	-5.692319	0.419828
H	2.181312	-6.121078	0.110542
N	3.228126	-4.320959	-1.632594
H	3.683446	-3.561757	-2.136038
H	3.943299	-4.835767	-1.121716
H	3.561757	3.683446	2.136038
H	5.692319	0.617327	-0.419828
H	1.801828	-5.329221	1.507468
H	2.807542	-4.951317	-2.312807
H	-3.561757	-3.683446	2.136038
H	-5.692319	-0.617327	-0.419828
H	-3.683446	3.561757	-2.136038
H	-0.617327	5.692319	0.419828
N	-2.351885	-0.834668	3.061578
N	-0.834668	2.351885	-3.061578
N	2.351885	0.834668	3.061578
N	0.834668	-2.351885	-3.061578
H	3.234409	0.623313	2.621065
H	2.128788	0.380892	3.931076
H	-0.380892	2.128788	-3.931076
H	-0.623313	3.234409	-2.621065
H	-2.128788	-0.380892	3.931076
H	-3.234409	-0.623313	2.621065
H	0.623313	-3.234409	-2.621065
H	0.380892	-2.128788	-3.931076

**Pd-C-IIId (M11L, SMD water)**

Pd	-4.535435	0.065215	-0.107408
Pd	-0.038688	3.638897	-0.125626
Pd	4.375952	0.019200	0.186414
Pd	-0.100671	-3.569748	0.052335
C	1.365650	-0.864901	3.022987
C	2.523712	-0.459226	2.423040
H	1.069622	-0.495669	3.998585
H	3.191825	0.252145	2.905859
N	2.903111	-0.894172	1.206962
N	0.940609	-2.192070	1.092125
C	-1.749310	1.152161	2.909579
C	-2.851514	0.698040	2.240105
H	-1.567415	0.896790	3.947944
H	-3.589966	0.066182	2.732247
N	-3.086501	0.983761	0.946539
N	-1.093421	2.248950	0.898034
C	-1.523802	-0.858149	-2.931918
C	1.661464	1.028946	-3.008476

N	1.076914	2.262536	-1.066821
N	2.956729	0.833243	-1.011620
C	0.846702	1.896801	-2.340508
H	1.474718	0.744971	-4.038452
H	-0.025541	2.339867	-2.819401
H	-1.223296	-0.508665	-3.913394
N	-1.113655	-2.163888	-0.980615
N	-3.078396	-0.870466	-1.131257
C	-2.695006	-0.458116	-2.353112
H	-3.369199	0.229798	-2.858786
C	-0.820717	1.916799	2.178132
C	2.739947	0.470452	-2.294079
C	0.523805	-1.718550	2.286954
C	-0.689167	-1.704766	-2.179127
C	-2.301884	-1.759555	-0.450168
O	-2.685552	-2.224988	0.664094
C	-2.220636	1.798860	0.272672
O	-2.465341	2.156800	-0.913344
C	2.160847	1.766046	-0.407149
O	2.443239	2.173509	0.756309
C	2.133132	-1.810238	0.554738
O	2.523486	-2.314987	-0.537958
N	-5.943594	-0.917744	-1.201533
H	-6.899051	-0.647334	-0.976801
H	-5.787449	-0.739434	-2.192027
N	-5.968720	1.032172	0.969769
H	-6.773697	1.289946	0.401581
H	-6.291490	0.431172	1.725700
N	0.930884	-4.995029	1.076968
H	0.854681	-5.922284	0.663584
H	1.916404	-4.738900	1.101306
N	-1.157352	-4.967020	-0.986214
H	-1.096281	-5.898792	-0.580543
H	-2.138682	-4.695400	-1.009326
N	5.753697	-0.829567	1.423388
H	6.669836	-0.389115	1.366306
H	5.435672	-0.774223	2.389350
N	5.851785	1.000903	-0.822606
H	6.444592	1.513269	-0.171974
H	6.436833	0.344463	-1.336119
N	1.013031	5.046541	-1.156819
H	0.859174	4.914745	-2.154997
H	0.766065	6.005687	-0.920838
N	-1.177065	5.040038	0.819028
H	-0.894108	5.109393	1.794897
H	-1.107697	5.966334	0.402102
H	-5.584806	1.881080	1.379803
H	-5.850271	-1.918368	-1.041362
H	0.592504	-5.044605	2.035977
H	-0.819130	-5.014154	-1.945430
H	5.859990	-1.812840	1.182952
H	5.461043	1.667875	-1.485294
H	2.005479	4.918764	-0.968309
H	-2.154653	4.755486	0.792423
N	0.324539	2.352594	2.693816
N	0.506331	-2.096496	-2.605724
N	3.567358	-0.403850	-2.854047
N	-0.671824	-2.100004	2.723954
H	1.073015	2.626859	2.061976
H	0.577879	2.072120	3.627358

H	-1.023535	-1.704412	3.581337
H	-1.354255	-2.467754	2.064993
H	0.857394	-1.735207	-3.478593
H	1.181371	-2.480184	-1.948026
H	4.256747	-0.889026	-2.302023
H	3.425167	-0.697807	-3.805613

**Pd-C-III d (M11L, SMD water)**

Pd	0.000000	3.603500	0.156718
Pd	0.000000	0.000000	-4.291803
Pd	0.000000	-3.603500	0.156718
Pd	0.000000	0.000000	4.587262
C	2.923538	-0.823781	1.624918
H	3.908367	-0.460180	1.354458
N	1.003325	-2.156191	1.152046
N	1.075942	-0.859110	3.122342
C	3.008077	1.056891	-1.407712
C	2.274613	1.893192	-0.616991
H	4.021724	0.768637	-1.150913
H	2.679095	2.301169	0.308816
N	1.026790	2.275566	-0.940569
N	1.106679	0.879220	-2.841112
C	-2.923538	0.823781	1.624918
C	-3.008077	-1.056891	-1.407712
N	-1.106679	-0.879220	-2.841112
N	-1.026790	-2.275566	-0.940569
H	-4.021724	-0.768637	-1.150913
H	-3.908367	0.460180	1.354458
C	-2.301028	0.426346	2.774827
N	-1.075942	0.859110	3.122342
N	-1.003325	2.156191	1.152046
H	-2.775386	-0.271979	3.462106
C	2.301028	-0.426346	2.774827
C	-2.274613	-1.893192	-0.616991
H	2.775386	0.271979	3.462106
H	-2.679095	-2.301169	0.308816
C	2.376868	0.526198	-2.550394
C	-2.376868	-0.526198	-2.550394
C	2.215071	-1.694632	0.774482
C	-2.215071	1.694632	0.774482
C	0.449849	1.805799	-2.081706
O	-0.682677	2.230032	-2.448349
C	-0.425110	1.751288	2.319775
O	0.698612	2.218573	2.660061
C	0.425110	-1.751288	2.319775
O	-0.698612	-2.218573	2.660061
C	-0.449849	-1.805799	-2.081706
O	0.682677	-2.230032	-2.448349
N	1.033304	5.066884	-0.816263
H	0.919624	5.991271	-0.404763
H	2.025661	4.836971	-0.806457
N	-1.051787	4.936485	1.281553
H	-0.859047	5.911354	1.061081
H	-2.047406	4.771726	1.144448
N	1.083424	0.922593	-5.748302
H	1.599663	0.245374	-6.307124
H	0.455815	1.432873	-6.367488
N	-1.083424	-0.922593	-5.748302
H	-1.599663	-0.245374	-6.307124
H	-0.455815	-1.432873	-6.367488

N	1.135129	-0.923962	6.006569
H	2.109178	-0.941059	5.709270
H	1.088821	-0.464832	6.914108
N	-1.135129	0.923962	6.006569
H	-2.109178	0.941059	5.709270
H	-1.088821	0.464832	6.914108
N	1.051787	-4.936485	1.281553
H	0.859047	-5.911354	1.061081
H	2.047406	-4.771726	1.144448
N	-1.033304	-5.066884	-0.816263
H	-0.919624	-5.991271	-0.404763
H	-2.025661	-4.836971	-0.806457
H	-0.823098	1.886149	6.120030
H	0.823098	-1.886149	6.120030
H	0.727645	5.108657	-1.786737
H	-0.838263	4.784915	2.265744
H	-1.748087	-1.586395	-5.355289
H	1.748087	1.586395	-5.355289
H	-0.727645	-5.108657	-1.786737
H	0.838263	-4.784915	2.265744
N	-2.696256	2.107589	-0.393464
N	-3.006755	0.310666	-3.366950
N	3.006755	-0.310666	-3.366950
N	2.696256	-2.107589	-0.393464
H	3.579050	-1.744052	-0.715895
H	2.058072	-2.484852	-1.089808
H	-2.058072	2.484852	-1.089808
H	-3.579050	1.744052	-0.715895
H	3.944707	-0.608609	-3.157294
H	2.514682	-0.779946	-4.110683
H	-2.514682	0.779946	-4.110683
H	-3.944707	0.608609	-3.157294

**Pd-C-IV d (M11L, SMD water)**

Pd	0.000206	3.646915	0.000257
Pd	-4.442351	0.000173	-0.000014
Pd	-0.000154	-3.646937	-0.000317
Pd	4.442269	-0.000145	0.000126
C	-1.544200	0.964889	2.947867
C	-2.664006	0.520896	2.302671
H	-1.290891	0.627873	3.946835
H	-3.343196	-0.187787	2.773966
N	-2.990584	0.912900	1.057195
N	-1.049152	2.249991	1.004858
C	1.544088	-0.965427	2.947850
C	2.663872	-0.521229	2.302747
H	1.290752	-0.628623	3.946883
H	3.342998	0.187428	2.774174
N	2.990503	-0.912993	1.057218
N	1.049166	-2.250204	1.004595
C	2.205931	-1.828542	0.418763
O	2.551456	-2.298300	-0.705122
C	1.544404	0.965309	-2.947902
C	-2.205879	1.828424	0.418881
O	-2.551362	2.298452	-0.704905
C	-1.544224	-0.964670	-2.947909
C	-2.206118	-1.828342	-0.419021
O	-2.551652	-2.298332	0.704763
H	1.710439	-4.692692	1.623602
H	0.405603	-5.698028	1.505269

H	1.542866	-5.675397	0.308102
H	-0.406141	-5.697740	-1.506203
H	-1.543567	-5.675029	-0.309189
H	-1.710763	-4.692130	-1.624592
H	-5.493244	-1.383764	-1.900969
H	-6.307098	-1.692096	-0.499999
H	-6.626034	-0.316250	-1.352881
H	-6.625877	0.316821	1.353031
H	-5.492888	1.384165	1.901090
H	-6.306830	1.692687	0.500205
N	1.036498	-5.098403	0.976796
N	-1.036989	-5.098052	-0.977742
N	-5.888583	-0.956412	-1.065662
N	-5.888378	0.956917	1.065800
N	-1.049359	-2.249905	-1.004939
N	-2.990742	-0.912737	-1.057334
C	-2.664053	-0.520667	-2.302761
H	-3.343198	0.188051	-2.774072
H	-1.290846	-0.627629	-3.946851
H	1.291129	0.628537	-3.946962
C	2.664109	0.521036	-2.302717
N	1.049392	2.250077	-1.004667
N	2.990663	0.912756	-1.057153
C	2.206080	1.828333	-0.418752
O	2.551534	2.298048	0.705176
H	3.343239	-0.187642	-2.774107
H	-1.542889	5.675243	0.309010
H	-1.710423	4.692309	1.624351
H	-0.405638	5.697737	1.506198
H	0.406191	5.698054	-1.505273
H	1.543473	5.675119	-0.308125
H	1.710848	4.692500	-1.623717
H	5.493040	1.385026	-1.899969
H	6.308493	1.690855	-0.499371
H	6.625005	0.315537	-1.354052
H	6.308382	-1.691304	0.500037
H	6.624752	-0.315883	1.354607
H	5.492657	-1.385285	1.900426
N	5.888609	0.956308	-1.065485
N	5.888397	-0.956673	1.065963
N	1.036990	5.098272	-0.976862
N	-1.036502	5.098167	0.977619
C	0.684421	-1.818690	2.232333
C	-0.684590	-1.818134	-2.232582
C	0.684716	1.818606	-2.232449
C	-0.684472	1.818255	2.232541
N	0.478413	2.241932	2.717595
N	-0.478101	2.242492	-2.717466
N	-0.478452	-2.242546	2.717252
N	0.478274	-2.241885	-2.717590
H	-1.187317	-2.594415	2.078084
H	-0.792590	-1.884933	3.605360
H	0.792442	-1.884061	-3.605600
H	1.187091	-2.594018	-2.078522
H	0.792480	1.884098	3.605641
H	1.187360	2.593801	2.078515
H	-1.186992	2.594433	-2.078371
H	-0.792178	1.884912	-3.605608

<b>Pd-U-Ia (M11L, SMD water)</b>			
Pd	3.180835	2.779311	-0.273176
Pd	2.623762	-3.020005	-0.614082
Pd	-3.180779	-2.779337	-0.273058
Pd	-2.623829	3.019981	-0.614028
C	-1.036920	2.502216	1.801912
C	-5.148788	0.467108	1.615243
C	0.061265	2.407781	2.603077
H	-2.045699	2.454887	2.212527
C	-4.722898	-0.761602	1.203728
H	-5.170571	-1.675453	1.595008
C	4.722896	0.761554	1.203663
C	-0.061125	-2.407683	2.603128
H	5.170625	1.675401	1.594889
C	5.148681	-0.467151	1.615298
C	1.037017	-2.502131	1.801898
H	2.045825	-2.454908	2.212455
H	0.031102	-2.278516	3.676139
H	5.947774	-0.578588	2.340298
H	-0.030907	2.278584	3.676091
H	-5.947938	0.578539	2.340176
N	3.512704	-1.401753	0.166930
N	3.739958	0.934095	0.296660
N	0.955430	-2.680247	0.464510
N	-1.395312	-2.640271	0.650319
N	-3.739900	-0.934139	0.296779
N	-3.512681	1.401697	0.167015
N	-0.955403	2.680364	0.464520
N	1.395351	2.640380	0.650198
C	4.514660	-1.615987	1.073976
O	4.825863	-2.815887	1.374106
C	-1.350801	-2.523297	2.015727
O	-2.433387	-2.544114	2.681003
C	-4.514826	1.615952	1.073855
O	-4.826231	2.815853	1.373764
C	1.350912	2.523555	2.015621
O	2.433512	2.544400	2.680872
C	3.127605	-0.162932	-0.238721
O	2.221669	-0.026785	-1.117729
C	0.277526	2.710926	-0.117181
O	0.382625	2.836699	-1.383534
C	-0.277566	-2.710820	-0.117120
O	-0.382789	-2.836762	-1.383451
C	-3.127525	0.162881	-0.238579
O	-2.221681	0.026738	-1.117671
N	2.622084	4.650215	-0.862291
H	3.215752	5.047674	-1.586553
H	1.677580	4.544603	-1.233753
N	4.995130	2.938596	-1.206069
H	5.132471	3.831148	-1.675434
H	5.744426	2.822572	-0.526265
N	1.754166	-4.697780	-1.395044
H	2.255352	-5.083478	-2.191507
H	1.675437	-5.421903	-0.685023
N	4.373786	-3.362552	-1.598647
H	4.382542	-4.212929	-2.157134
H	4.590581	-2.574199	-2.204039
N	-4.994790	-2.938517	-1.206519
H	-5.081187	-2.199212	-1.900826
H	-5.131995	-3.831076	-1.675907



N	-2.621920	-4.650261	-0.862161
H	-2.604065	-5.293075	-0.074354
H	-3.215646	-5.047861	-1.586287
N	-1.754427	4.697842	-1.395059
H	-2.255755	5.083593	-2.191408
H	-1.675554	5.421924	-0.685013
N	-4.373868	3.362261	-1.598550
H	-4.382765	4.212765	-2.156837
H	-4.590399	2.574001	-2.204157
H	-5.744299	-2.822447	-0.526961
H	-5.095160	3.430276	-0.881413
H	-0.820665	4.405631	-1.687571
H	-1.677511	-4.544464	-1.233808
H	5.094994	-3.430934	-0.881460
H	2.604503	5.293112	-0.074541
H	5.081791	2.199283	-1.900337
H	0.820361	-4.405515	-1.687363

**Pd-U-IIa (M11L, SMD water)**

Pd	3.870971	1.911528	-0.145624
Pd	1.745747	-3.454205	-0.770910
Pd	-3.822699	-1.789708	-0.245590
Pd	-1.661131	3.600000	-0.680901
C	-0.269017	2.955187	1.835788
C	-4.752573	1.891043	1.649803
C	0.756566	2.626540	2.670249
H	-1.257613	3.202761	2.221941
C	4.664939	-0.478678	1.389879
C	-0.702865	-2.533103	2.559863
H	5.332569	0.257748	1.837986
C	4.700032	-1.789282	1.766587
C	0.320217	-2.861963	1.722863
H	1.303033	-3.137102	2.105561
H	-0.572639	-2.525494	3.636675
H	5.389566	-2.143953	2.525090
H	0.624352	2.599828	3.746455
H	-5.485138	2.247201	2.366219
N	2.959426	-2.181903	0.196461
N	3.819078	-0.007868	0.450411
N	0.185847	-2.895915	0.378272
N	-2.060155	-2.217536	0.633660
N	-3.809894	0.133724	0.347927
N	-2.901554	2.300628	0.211229
N	-0.131453	3.012955	0.493175
N	2.117805	2.348589	0.741610
C	3.811134	-2.698709	1.134809
O	3.765009	-3.946970	1.388042
C	-1.970606	-2.212011	2.001188
O	-2.999889	-1.941731	2.696256
C	-3.814257	2.720326	1.111929
C	2.028808	2.328391	2.108883
O	3.062764	2.063918	2.798719
C	2.951215	-0.869963	-0.155920
O	2.154204	-0.450022	-1.051192
C	1.074188	2.686779	-0.057864
O	1.227753	2.723775	-1.323661
C	-1.016755	-2.551916	-0.168815
O	-1.168185	-2.568057	-1.435685
C	-2.895323	0.991058	-0.178776
O	-2.051736	0.593188	-1.040060

N	3.904847	3.850639	-0.771992
H	4.669809	4.079984	-1.402184
H	3.019133	3.987827	-1.259634
N	5.649326	1.476203	-1.059145
H	6.097590	2.283992	-1.486198
H	6.299127	1.077963	-0.383384
N	0.547300	-4.776727	-1.767614
H	0.942355	-5.098519	-2.648106
H	0.343760	-5.589925	-1.191669
N	3.381138	-4.006042	-1.854662
H	3.193789	-4.708306	-2.567036
H	3.773255	-3.183925	-2.308797
N	-5.626178	-1.373283	-1.104675
H	-5.518781	-0.663013	-1.824895
H	-6.095536	-2.178011	-1.512041
N	-3.837690	-3.731502	-0.878218
H	-3.852602	-4.362736	-0.080790
H	-4.616004	-3.967828	-1.489243
N	-0.445614	4.970506	-1.578793
H	-0.838740	5.357615	-2.433639
H	-0.232989	5.738038	-0.946512
N	-3.217669	4.206530	-1.849813
H	-3.009311	4.045249	-2.833462
H	-4.057265	3.682030	-1.612466
H	-6.195830	-0.997131	-0.346551
H	-3.409796	5.198134	-1.722462
H	0.409991	4.456538	-1.794810
H	-2.962477	-3.860502	-1.385588
H	4.078972	-4.378188	-1.212762
H	3.945313	4.482325	0.024189
H	5.488018	0.782381	-1.786778
H	-0.314098	-4.258309	-1.947792
C	-4.775397	0.533329	1.232088
O	-5.645733	-0.311312	1.624970
H	-3.761944	3.775605	1.382564

**Pd-U-IIIa (M11L, SMD water)**

Pd	3.060937	2.892838	-0.359232
Pd	2.911535	-2.895352	-0.470080
Pd	-2.911685	-2.818226	-0.490250
Pd	-2.715113	3.067227	-0.457604
C	-5.194776	0.203602	1.401232
C	0.131416	2.674195	2.701563
C	4.594018	1.079240	1.386932
C	0.026814	-2.417505	2.585620
H	4.933019	2.038341	1.779996
C	5.074034	-0.100823	1.873582
C	1.172177	-2.471159	1.850862
H	2.155068	-2.407277	2.318792
H	0.049469	-2.304213	3.664144
H	5.809623	-0.129806	2.669598
H	0.127438	2.595046	3.783314
H	-6.059001	0.240267	2.055752
N	3.652558	-1.207333	0.319789
N	3.682644	1.143087	0.394270
N	1.171857	-2.629693	0.508772
N	-1.187457	-2.649020	0.550194
N	-3.615667	-1.029242	0.113547
N	-3.474153	1.319677	0.188917
N	-1.030346	2.891257	0.634471

N	1.323662	2.757395	0.643852
C	4.596964	-1.312220	1.304843
O	4.995234	-2.471012	1.655204
C	-1.222971	-2.551393	1.918503
O	-2.338245	-2.605009	2.523212
C	-4.541066	1.334893	1.013690
C	1.291551	2.638510	1.988427
C	3.199519	-0.014737	-0.146500
O	2.347385	0.030551	-1.086476
C	0.148085	2.856861	-0.038909
O	0.162149	2.942266	-1.312258
C	-0.022320	-2.681638	-0.146831
O	-0.040268	-2.792961	-1.419176
C	-3.001837	0.122657	-0.273028
O	-2.016319	0.095685	-1.075385
N	2.438043	4.679518	-1.124353
H	3.045031	5.040906	-1.856463
H	1.510699	4.497187	-1.510953
N	4.833539	3.055455	-1.354307
H	5.304916	3.930920	-1.136626
H	5.450324	2.286734	-1.100107
N	2.153745	-4.611756	-1.282396
H	2.698497	-4.960083	-2.067413
H	2.090053	-5.348722	-0.584445
N	4.724973	-3.168610	-1.358817
H	4.832916	-4.073725	-1.811342
H	4.885900	-2.440581	-2.051264
N	-4.667027	-3.024736	-1.509769
H	-4.761208	-2.303005	-2.219803
H	-4.793267	-3.931902	-1.952159
N	-2.236177	-4.642468	-1.110602
H	-2.190664	-5.294208	-0.331275
H	-2.801579	-5.060484	-1.845518
N	-1.988299	4.847714	-1.132378
H	-2.540468	5.250584	-1.885808
H	-1.927481	5.527248	-0.378384
N	-4.397295	3.308429	-1.596463
H	-4.863113	4.186565	-1.376320
H	-4.153369	3.318379	-2.585413
H	-5.383007	-2.890751	-0.794435
H	-5.058158	2.549733	-1.441752
H	-1.049684	4.638102	-1.475100
H	-1.294658	-4.475892	-1.467039
H	5.426515	-3.083289	-0.624599
H	2.364393	5.382584	-0.393012
H	4.675863	3.019226	-2.359370
H	1.216562	-4.363307	-1.603798
C	-4.728015	-1.044461	0.913400
O	-5.294297	-2.158660	1.170203
H	-4.862076	2.321003	1.349694
H	2.260396	2.526856	2.476803
C	-1.097439	2.846594	2.004099
O	-2.221770	2.974854	2.580424

**Pd-U-IVa (M11L, SMD water)**

Pd	0.000000	4.459474	-0.081058
Pd	3.616501	0.000000	-0.919675
Pd	0.000000	-4.459474	-0.081058
Pd	-3.616501	0.000000	-0.919675
C	-3.503462	1.724916	1.503833

C	-3.092207	-2.753570	2.296955
C	-3.092207	2.753570	2.296955
H	-4.316445	1.068561	1.810971
C	3.092207	-2.753570	2.296955
C	3.092207	2.753570	2.296955
C	3.503462	-1.724916	1.503833
H	4.316445	-1.068561	1.810971
H	3.555543	-2.950162	3.257720
H	3.555543	2.950162	3.257720
H	-3.555543	2.950162	3.257720
H	-3.555543	-2.950162	3.257720
N	2.963415	1.474137	0.294182
N	1.489672	3.289149	0.619730
N	2.963415	-1.474137	0.294182
N	1.489672	-3.289149	0.619730
N	-1.489672	-3.289149	0.619730
N	-2.963415	-1.474137	0.294182
N	-2.963415	1.474137	0.294182
N	-1.489672	3.289149	0.619730
C	3.503462	1.724916	1.503833
C	2.037988	-3.590874	1.839559
O	1.601942	-4.592343	2.491041
C	-3.503462	-1.724916	1.503833
C	-2.037988	3.590874	1.839559
O	-1.601942	4.592343	2.491041
C	1.970538	2.293978	-0.169693
O	1.516963	2.122195	-1.344806
C	-1.970538	2.293978	-0.169693
O	-1.516963	2.122195	-1.344806
C	1.970538	-2.293978	-0.169693
O	1.516963	-2.122195	-1.344806
C	-1.970538	-2.293978	-0.169693
O	-1.516963	-2.122195	-1.344806
N	-1.491547	5.671329	-0.779303
H	-1.168811	6.400904	-1.410657
H	-2.177850	5.102262	-1.269713
N	1.491547	5.671329	-0.779303
H	1.168811	6.400904	-1.410657
H	1.953594	6.113722	0.012926
N	4.252786	-1.479326	-2.170582
H	4.622727	-1.146719	-3.058210
H	4.962210	-2.054606	-1.723810
N	4.252786	1.479326	-2.170582
H	4.622727	1.146719	-3.058210
H	3.422413	2.046216	-2.344342
N	-1.491547	-5.671329	-0.779303
H	-2.177850	-5.102262	-1.269713
H	-1.168811	-6.400904	-1.410657
N	1.491547	-5.671329	-0.779303
H	1.953594	-6.113722	0.012926
H	1.168811	-6.400904	-1.410657
N	-4.252786	1.479326	-2.170582
H	-4.622727	1.146719	-3.058210
H	-4.962210	2.054606	-1.723810
N	-4.252786	-1.479326	-2.170582
H	-4.622727	-1.146719	-3.058210
H	-3.422413	-2.046216	-2.344342
H	-1.953594	-6.113722	0.012926
H	-4.962210	-2.054606	-1.723810
H	-3.422413	2.046216	-2.344342

H	2.177850	-5.102262	-1.269713
H	4.962210	2.054606	-1.723810
H	-1.953594	6.113722	0.012926
H	2.177850	5.102262	-1.269713
H	3.422413	-2.046216	-2.344342
C	-2.037988	-3.590874	1.839559
O	-1.601942	-4.592343	2.491041
H	-4.316445	-1.068561	1.810971
C	2.037988	3.590874	1.839559
O	1.601942	4.592343	2.491041
H	4.316445	1.068561	1.810971

**Pd-U-Ib (M11L, SMD water)**

Pd	-2.570451	-3.227389	0.368990
Pd	-3.384789	2.391977	-0.138350
Pd	2.267322	3.298682	-0.139408
Pd	3.098799	-2.502615	-0.789365
C	-2.667075	-0.638241	-3.025536
C	0.669869	-1.572934	2.576562
C	1.694628	-1.767542	1.698995
H	2.714743	-1.484461	1.957093
C	-1.564552	1.738079	2.132710
C	5.271746	0.597792	1.059394
H	-2.496961	1.403706	2.584800
C	-0.394904	1.751224	2.832821
C	4.469512	1.676823	0.834593
H	4.706869	2.655273	1.253505
H	6.175300	0.672801	1.654280
H	-0.349887	1.422189	3.865757
H	0.839155	-1.126786	3.551398
N	0.672840	2.587163	0.877050
N	-1.646205	2.144895	0.848569
N	3.346185	1.618398	0.090829
N	3.727263	-0.680240	-0.224268
N	1.529539	-2.334404	0.482192
N	-0.774630	-2.538499	0.959358
N	-3.159242	0.639713	-1.084440
N	-2.810097	-1.679745	-0.889002
C	-2.589290	-1.736090	-2.217368
H	-2.346147	-2.719920	-2.616945
H	-2.499511	-0.708723	-4.094707
C	4.887875	-0.648680	0.503356
O	5.553215	-1.728241	0.651004
C	-0.636910	-1.998784	2.210340
O	-1.649592	-1.934863	2.977341
C	-2.954068	0.622841	-2.436689
O	-3.037711	1.715520	-3.089465
C	0.787647	2.220025	2.193249
O	1.906642	2.336967	2.785563
C	-3.141038	-0.483360	-0.321235
O	-3.446244	-0.431038	0.908028
C	-0.514383	2.557566	0.214013
O	-0.578584	2.940374	-1.000971
C	2.967760	0.426473	-0.458902
O	1.939875	0.358792	-1.199820
C	0.268152	-2.702166	0.105629
O	0.068259	-3.219625	-1.041003
N	-2.313099	-4.751174	1.698848
H	-3.104013	-5.389035	1.752556
H	-1.481313	-5.286569	1.460189

N	-4.376394	-3.968306	-0.233438
H	-4.320642	-4.959685	-0.457504
H	-5.075423	-3.845779	0.496669
N	-3.606013	4.182752	0.825113
H	-3.757241	4.940797	0.162918
H	-4.397973	4.155041	1.463965
N	-5.100885	2.674335	-1.200250
H	-5.834966	2.039064	-0.899334
H	-5.456622	3.625903	-1.151352
N	1.237061	5.041835	-0.373216
H	1.123860	5.526900	0.512998
H	1.669552	5.679985	-1.036879
N	3.835608	4.097036	-1.182080
H	4.200532	4.922272	-0.710252
H	4.592757	3.423810	-1.277737
N	2.551568	-4.399760	-1.316112
H	2.893244	-4.666522	-2.236284
H	2.892350	-5.075679	-0.637214
N	4.743402	-2.618600	-1.982296
H	5.521477	-2.401912	-1.357991
H	4.889188	-3.534130	-2.400957
H	0.323504	4.754801	-0.726953
H	-2.766944	4.390345	1.363306
H	-4.839846	2.459800	-2.163875
H	-4.689915	-3.467977	-1.062555
H	-2.172375	-4.325883	2.614304
H	1.529961	-4.384219	-1.321613
H	3.539122	4.371391	-2.117010
H	4.702648	-1.925984	-2.725504

**Pd-U-IIb1 (M11L, SMD water)**

Pd	-1.657442	-3.697676	-0.365588
Pd	3.817979	-1.709087	0.039197
Pd	1.764086	3.738489	0.015139
Pd	-3.689154	1.720589	-0.629964
C	2.419335	0.858469	-3.036297
C	-1.179849	2.338829	2.726914
C	-2.209824	2.047033	1.882993
H	-3.157205	1.655697	2.255002
C	-4.689228	-1.628759	1.770898
C	0.742648	-2.412694	2.892967
C	-3.798426	-2.555592	1.314975
C	-0.273534	-2.848476	2.096087
H	-1.245331	-3.117878	2.510394
H	-3.775028	-3.569188	1.716262
H	-5.404698	-1.863533	2.551107
H	0.621639	-2.318557	3.966617
H	-1.262085	2.184744	3.797178
N	-0.144263	-2.989640	0.761215
N	2.070545	-2.194665	0.927986
N	-2.897489	-2.290507	0.347540
N	-3.735443	-0.097967	0.218935
N	-2.142144	2.243442	0.548549
N	0.067438	3.017090	0.818970
N	3.037344	-0.153776	-0.974061
N	2.173060	2.036746	-0.980570
C	2.048317	1.958852	-2.320881
H	1.636271	2.841350	-2.810021
H	2.320820	0.822116	-4.115819
C	-4.670812	-0.331151	1.191245

O	-5.464162	0.610153	1.520431
C	0.021046	2.860947	2.178926
O	1.033013	3.199335	2.875516
C	2.959470	-0.253215	-2.336513
O	3.387288	-1.312048	-2.904702
C	1.985330	-2.080355	2.290402
O	3.011524	-1.704903	2.947086
C	-2.855282	-1.042377	-0.203353
O	-2.007110	-0.778016	-1.111321
C	1.042736	-2.655844	0.168971
O	1.180103	-2.803127	-1.087276
C	-0.987032	2.738100	0.010134
O	-0.908556	2.946364	-1.242731
C	2.685696	0.971610	-0.296434
O	2.845194	1.045221	0.961902
N	-3.656691	3.571276	-1.500729
H	-4.157259	3.616868	-2.385327
H	-4.043445	4.274533	-0.876378
N	-5.267027	1.124523	-1.774295
H	-5.728602	1.890441	-2.259978
H	-4.935787	0.456069	-2.466762
N	-0.409036	-5.139650	-1.088106
H	-0.221194	-5.851137	-0.386293
H	-0.760199	-5.598640	-1.924861
N	-3.219128	-4.382670	-1.488702
H	-3.382407	-3.728899	-2.252282
H	-3.063407	-5.306260	-1.887606
N	4.659391	-3.241896	1.095679
H	5.675210	-3.259885	1.049651
H	4.369374	-3.078193	2.060273
N	5.567596	-1.247140	-0.903563
H	6.332128	-1.891381	-0.717727
H	5.343632	-1.268460	-1.898702
N	1.368704	5.458320	1.032661
H	2.095830	6.166040	0.961907
H	0.491950	5.864093	0.715098
N	3.490705	4.484028	-0.787139
H	3.711833	5.428387	-0.478304
H	4.263742	3.874957	-0.527201
H	4.306715	-4.143590	0.784484
H	5.865285	-0.308107	-0.650575
H	1.272060	5.171017	2.006707
H	3.422377	4.492094	-1.803012
H	-2.664475	3.757410	-1.659277
H	-5.952945	0.659783	-1.183183
H	-4.064007	-4.421501	-0.921478
H	0.450765	-4.635595	-1.312011

**Pd-U-Iib2 (M11L, SMD water)**

Pd	4.084030	1.447343	-0.328419
Pd	-1.194507	3.777218	-0.098454
Pd	-4.193301	-1.092363	0.340104
Pd	1.009600	-3.575125	-0.664324
C	-2.713647	1.068143	-3.001711
C	-0.680589	-1.603739	2.700514
C	0.152110	-2.194989	1.796936
C	4.675052	-2.472696	1.112801
C	1.067569	1.487773	2.666723
C	4.789322	-1.162474	0.755308
H	5.427379	-2.967139	1.717047

H	0.937131	1.114565	3.677032
H	-0.349914	-1.379319	3.708884
N	2.422951	1.831794	0.741945
N	0.183994	2.569411	0.740154
N	3.875657	-0.524145	-0.003813
N	2.613344	-2.508483	-0.077880
N	-0.227854	-2.505000	0.536756
N	-2.342586	-1.553169	1.004756
N	-2.128296	2.266264	-1.029729
N	-3.458347	0.332915	-0.867095
C	-2.054275	2.077721	-2.362873
C	0.042434	2.078631	1.990164
C	2.771888	-1.204231	-0.436070
O	1.923203	-0.635722	-1.189384
C	1.381422	2.428432	0.105475
O	1.522718	2.880007	-1.079034
C	-1.488634	-2.152447	0.134953
O	-1.869833	-2.404740	-1.052812
C	-2.864064	1.399915	-0.273525
O	-3.008829	1.610413	0.969623
N	-0.532811	-4.788298	-1.236892
H	-0.370937	-5.237349	-2.135115
H	-0.692803	-5.512230	-0.540698
N	2.303230	-4.666880	-1.794480
H	1.889029	-5.494839	-2.216231
H	2.700721	-4.091764	-2.532694
N	4.303287	3.445916	-0.663067
H	4.576519	3.945036	0.179306
H	4.976678	3.655994	-1.396025
N	5.765016	1.075029	-1.433430
H	5.575912	1.244933	-2.419476
H	6.532990	1.679203	-1.148063
N	-0.236948	5.311056	0.851115
H	-0.689215	6.214513	0.726800
H	-0.197984	5.107761	1.848108
N	-2.555687	5.064792	-0.905527
H	-3.164076	5.439370	-0.180310
H	-2.091940	5.845143	-1.367265
N	-4.909468	-2.503298	1.630444
H	-5.919179	-2.472598	1.750410
H	-4.648501	-3.439718	1.331255
N	-6.033911	-0.667030	-0.430441
H	-6.755094	-1.341172	-0.186739
H	-6.343736	0.258768	-0.146069
H	0.717606	5.379447	0.504034
H	-3.136444	4.586826	-1.591187
H	-4.462944	-2.305370	2.525792
H	-5.883431	-0.676045	-1.440230
H	-1.346194	-4.173274	-1.304082
H	3.044884	-4.955358	-1.157053
H	6.066270	0.107869	-1.333142
H	3.373682	3.750632	-0.956686
C	2.339495	1.389071	2.038102
O	3.379051	0.944813	2.617651
C	3.529918	-3.188394	0.680256
O	3.317139	-4.417904	0.949587
C	-2.006246	-1.283092	2.303756
C	-2.884385	-0.786417	3.082454
O	-3.468577	0.149330	-2.222402
O	-4.145296	-0.813730	-2.713373

H	-0.945957	2.191442	2.434106
H	5.642389	-0.561394	1.072528
H	1.173552	-2.465694	2.064702
H	-2.662822	0.949229	-4.078552
H	-1.441627	2.795624	-2.907967

**Pd-U-IIb3 (M11L, SMD water)**

Pd	-0.958045	-3.789835	-0.465211
Pd	4.165257	-1.176767	0.208682
Pd	1.373931	3.934859	0.153937
Pd	-3.784427	1.417677	-0.637843
C	2.580721	1.243256	-2.881306
C	-1.367772	2.101841	2.814845
C	-4.667579	-2.398816	0.968146
C	1.042027	-2.127154	2.922178
C	-3.529888	-3.095666	0.693944
H	-5.499202	-2.848384	1.499681
H	0.867614	-2.021835	3.987509
H	-1.426737	1.919830	3.882453
N	0.360542	-2.898971	0.777251
N	2.410791	-1.754904	1.009381
N	-2.485804	-2.565885	0.022826
N	-3.662241	-0.529134	-0.110569
N	-2.327080	1.990453	0.637246
N	-0.172207	2.903736	0.921821
N	3.305597	0.323778	-0.810442
N	2.103017	2.342722	-0.825091
C	2.019191	2.260737	-2.168222
C	-0.259540	2.651132	2.245148
C	2.157703	-1.618183	2.328641
C	-2.544060	-1.259969	-0.378646
O	-1.572617	-0.746297	-1.015637
C	1.490462	-2.381324	0.221941
O	1.702524	-2.505958	-1.027438
C	-1.210812	2.560056	0.109210
O	-1.137065	2.794408	-1.141201
C	2.764307	1.370069	-0.133150
O	2.887442	1.461676	1.128608
N	-3.932996	3.378282	-1.189494
H	-4.547555	3.542483	-1.982815
H	-4.251462	3.949952	-0.411288
N	-5.278372	0.853059	-1.907764
H	-5.759121	1.627800	-2.358632
H	-4.924182	0.229434	-2.628284
N	0.530415	-5.094337	-0.955964
H	0.758837	-5.693313	-0.166692
H	0.313985	-5.683797	-1.756336
N	-2.251838	-4.695867	-1.768458
H	-2.282740	-4.154519	-2.630760
H	-1.975709	-5.647622	-2.002534
N	5.062963	-2.710493	1.224646
H	6.056255	-2.546018	1.375519
H	4.623126	-2.841588	2.133804
N	5.922982	-0.622855	-0.659244
H	6.695597	-1.261302	-0.486501
H	5.709352	-0.611805	-1.657566
N	0.614727	5.577114	1.102698
H	1.135782	6.432672	0.921177
H	-0.345462	5.718287	0.795714
N	2.940435	4.997068	-0.610921

H	3.197041	5.798212	-0.037659
H	3.751364	4.386994	-0.689014
H	4.960483	-3.576420	0.699236
H	6.201238	0.310097	-0.365336
H	0.604444	5.421260	2.108939
H	2.704615	5.332788	-1.542783
H	-2.976764	3.640855	-1.433895
H	-5.934656	0.346452	-1.312635
H	-3.194490	-4.728900	-1.385436
H	1.331967	-4.502174	-1.178762
C	-2.482004	1.790385	1.985153
O	-3.591161	1.364741	2.435236
C	0.110107	-2.847997	2.123790
O	-0.904435	-3.448661	2.598018
C	-4.755307	-1.053809	0.524562
O	-5.793961	-0.328226	0.680476
C	3.275058	0.225544	-2.175590
O	3.874962	-0.747961	-2.739396
H	2.513573	1.201483	-3.962838
H	1.479973	3.070388	-2.660318
H	0.612347	2.927077	2.839016
H	-3.412002	-4.133746	1.006269
H	2.915851	-1.084375	2.902141

**Pd-U-IIb4 (M11L, SMD water)**

Pd	3.635347	1.774165	-0.274858
Pd	-1.876575	3.666433	-0.115878
Pd	-3.904487	-1.766054	0.342723
Pd	1.519480	-3.673122	-0.817152
C	-2.689280	0.625009	-2.951567
C	-0.473113	-2.491249	2.734616
C	4.777442	-2.002945	1.289350
C	0.808974	2.319971	2.870962
H	5.574158	-2.385011	1.917780
H	0.785188	2.209598	3.949783
H	-0.200096	-2.394012	3.779364
N	1.969562	2.176002	0.796801
N	-0.277375	2.891188	0.830786
N	3.678849	-0.186295	0.207445
N	2.837408	-2.372025	-0.039527
N	0.110610	-3.063188	0.494457
N	-2.067171	-2.296478	0.980125
N	-2.383095	1.921324	-0.979979
N	-3.188653	-0.282297	-0.808480
C	-3.108748	-0.394337	-2.148472
C	-0.286265	2.728087	2.170826
C	2.750328	-1.035475	-0.312087
O	1.823359	-0.601786	-1.063427
C	0.860663	2.605251	0.135485
O	0.890204	2.765644	-1.127780
C	-1.155797	-2.751174	0.081176
O	-1.483540	-2.905643	-1.137531
C	-2.846564	0.897962	-0.214166
O	-2.979502	1.034553	1.042359
N	0.227480	-5.061444	-1.564920
H	0.480332	-5.393127	-2.492186
H	0.160958	-5.861560	-0.941457
N	2.993739	-4.270355	-2.098220
H	2.733631	-5.059711	-2.685887
H	3.239487	-3.489002	-2.702897

N	3.622122	3.740808	-0.822660
H	3.847771	4.340837	-0.033368
H	4.260775	3.957864	-1.584020
N	5.357286	1.394973	-1.302716
H	5.197607	0.699286	-2.027470
H	5.783797	2.213660	-1.729841
N	-1.409957	5.469547	0.731232
H	-2.241846	6.018619	0.939401
H	-0.893095	5.336516	1.598055
N	-3.483729	4.457519	-1.088323
H	-3.628776	5.452482	-0.934509
H	-3.293716	4.286656	-2.076357
N	-4.635478	-3.244458	1.541408
H	-5.645083	-3.228519	1.662277
H	-4.366612	-4.163119	1.198801
N	-5.759486	-1.191923	-0.300757
H	-6.527252	-1.662531	0.173900
H	-5.856291	-0.189508	-0.151706
H	-0.825006	6.008624	0.095663
H	-4.330542	3.960425	-0.823772
H	-4.185409	-3.073218	2.442404
H	-5.843060	-1.373313	-1.299052
H	-0.670276	-4.574703	-1.608125
H	3.823650	-4.531581	-1.568712
H	5.994862	1.008921	-0.605392
H	2.665579	3.924099	-1.127149
C	0.422252	-2.921003	1.800980
C	2.013958	2.057034	2.162082
O	3.106465	1.739966	2.729997
C	3.828986	-2.822988	0.757213
C	-2.311846	1.852401	-2.345684
O	-1.937001	2.881950	-2.998545
H	-2.643134	0.517206	-4.029741
H	-3.409066	-1.356818	-2.560939
H	-1.229734	2.953480	2.668316
C	-1.788091	-2.162071	2.314253
O	-2.709935	-1.768816	3.102963
C	4.723084	-0.617162	0.981043
O	5.598813	0.224041	1.369318
H	1.443272	-3.184114	2.077152
H	3.833171	-3.897299	0.945681

**Pd-U-IIIb1 (M11L, SMD water)**

Pd	2.593542	-2.934427	-0.481734
Pd	2.728132	2.974407	-0.639932
Pd	-3.023071	3.000553	0.184417
Pd	-3.161793	-2.798316	0.193802
C	-1.168600	-2.253332	2.288819
C	-2.932542	0.082148	-2.899620
H	-2.084835	-2.105516	2.860765
C	0.056669	-2.225582	2.883273
C	-0.972610	2.560623	2.244452
C	5.274593	0.013240	0.958093
H	-1.875697	2.420613	2.839008
C	0.263856	2.549937	2.815667
C	4.648251	1.169481	0.602208
H	5.074536	2.143411	0.844185
H	6.220319	0.016363	1.488386
H	0.394767	2.406079	3.882826
H	0.168114	-2.053007	3.948446

N	1.172399	2.877503	0.641479
N	-1.165489	2.756858	0.921597
N	3.475878	1.194074	-0.063770
N	3.460891	-1.161838	-0.044386
N	1.012138	-2.634747	0.740535
N	-1.331363	-2.477976	0.967537
N	-2.979201	1.274382	-0.840097
N	-3.144656	-1.069425	-0.827954
C	-2.877340	1.241590	-2.183613
H	-2.863078	0.077848	-3.981817
H	-2.757731	2.208069	-2.673746
C	4.663846	-1.218312	0.606710
O	5.184136	-2.357033	0.856044
C	1.210442	-2.472283	2.086856
O	2.381994	-2.568005	2.569295
C	-3.081335	-1.141051	-2.193392
O	-3.172518	-2.282280	-2.755282
C	1.402575	2.761752	1.988055
O	2.586623	2.863928	2.436038
C	2.865035	0.014477	-0.388069
O	1.763856	0.024623	-1.020586
C	-0.228497	-2.636771	0.181245
O	-0.363011	-2.815732	-1.072685
C	-0.079462	2.895747	0.109223
O	-0.239532	3.069777	-1.142178
C	-3.128099	0.107240	-0.149014
O	-3.265485	0.131471	1.113690
N	2.021191	4.792933	-1.229504
H	2.121544	5.480297	-0.486883
H	2.465814	5.159435	-2.067774
N	4.286475	3.065155	-1.964058
H	4.180266	2.320069	-2.649920
H	4.341393	3.950098	-2.463829
N	4.205400	-3.273853	-1.690665
H	5.012219	-3.101584	-1.089415
H	4.259337	-4.219706	-2.060144
N	1.742142	-4.731847	-0.958231
H	0.780593	-4.500469	-1.213519
H	2.190713	-5.209493	-1.736445
N	-4.991720	-3.156921	-0.624269
H	-5.319642	-4.112405	-0.508006
H	-5.694483	-2.525705	-0.248375
N	-3.170254	-4.560134	1.237563
H	-4.026212	-5.097395	1.117805
H	-2.386958	-5.135102	0.933965
N	-4.913618	3.240402	-0.543591
H	-5.466639	2.422475	-0.293737
H	-5.389571	4.067363	-0.189782
N	-3.124588	4.759442	1.222502
H	-2.669440	5.501394	0.694054
H	-4.083089	5.047300	1.409818
H	5.170805	2.923603	-1.479536
H	1.030022	4.628612	-1.414010
H	1.740167	-5.355973	-0.155567
H	4.217968	-2.621643	-2.470147
H	-4.861871	-2.967701	-1.618788
H	-3.053372	-4.368829	2.230871
H	-2.644911	4.671786	2.116674
H	-4.882880	3.302276	-1.559660

<b>Pd-U-IIIb2 (M11L, SMD water)</b>			
Pd	3.047597	-2.828372	-0.563247
Pd	2.658851	2.986642	-0.417241
Pd	-3.167805	2.673666	0.011932
Pd	-2.775553	-3.113690	0.065200
C	-2.637828	-0.221169	-3.051389
C	0.436614	-2.446490	2.750193
C	5.113042	0.180915	1.590807
C	0.003795	2.301050	2.811748
H	5.918029	0.209375	2.316622
H	0.104245	2.133810	3.878538
H	0.552458	-2.260314	3.812226
N	0.999768	2.665418	0.678238
N	-1.346682	2.568555	0.871466
N	3.489342	1.283292	0.245950
N	3.673174	-1.059539	0.152480
N	1.397802	-2.725689	0.587798
N	-0.939707	-2.864036	0.855605
N	-2.932273	0.947466	-0.999298
N	-2.693491	-1.395449	-0.980769
H	-2.545600	-0.226195	-4.131984
C	4.666472	-0.994637	1.063767
C	1.510141	-2.483575	1.911376
C	-2.568912	-1.372370	-2.322547
C	1.094913	2.441731	2.006215
C	3.071196	0.094847	-0.263136
O	2.147022	0.053201	-1.133358
C	0.153754	-2.914726	0.052476
O	0.028876	-3.155668	-1.190929
C	-0.237982	2.714313	0.100842
O	-0.342378	2.921219	-1.150782
C	-2.883336	-0.222251	-0.307312
O	-3.030071	-0.234245	0.953400
N	1.839707	4.728701	-1.104456
H	1.830945	5.439773	-0.377699
H	2.318896	5.107127	-1.917781
N	4.397726	3.298288	-1.434338
H	4.538422	2.547146	-2.106127
H	4.439648	4.186336	-1.929113
N	4.752971	-2.946061	-1.677655
H	5.516587	-2.468916	-1.201278
H	5.038002	-3.908260	-1.848765
N	2.430566	-4.643732	-1.254575
H	1.441578	-4.510344	-1.474044
H	2.927662	-4.953919	-2.086020
N	-4.650374	-3.351229	-0.713617
H	-5.132969	-4.179363	-0.371924
H	-5.207332	-2.534280	-0.469254
N	-2.900219	-4.828800	1.161499
H	-3.832844	-5.233456	1.193320
H	-2.255403	-5.535494	0.817044
N	-4.980212	2.832872	-0.913666
H	-5.615167	2.103158	-0.600650
H	-5.432139	3.734636	-0.781835
N	-3.434852	4.393191	1.079813
H	-2.796377	5.119988	0.767534
H	-4.383707	4.757145	1.040618
H	5.153274	3.269255	-0.751466
H	0.880260	4.483664	-1.357205
H	2.529114	-5.357131	-0.536281

H	4.610131	-2.491291	-2.577420
H	-4.601557	-3.407722	-1.729089
H	-2.626894	-4.551136	2.105052
H	-3.211899	4.137520	2.042511
H	-4.774371	2.700397	-1.904289
H	-2.417678	-2.340346	-2.801173
C	-2.844135	1.004540	-2.363293
O	-2.968816	2.133716	-2.944119
C	-1.287421	2.391581	2.228344
O	-2.374154	2.336055	2.892586
H	2.107693	2.395815	2.407277
H	2.524014	-2.331403	2.281331
C	-0.857884	-2.659497	2.208002
O	-1.925321	-2.685014	2.903007
C	4.502236	1.389256	1.160220
O	4.848320	2.547248	1.564030
H	5.102307	-1.950811	1.355795

<b>Pd-U-IVb (M11L, SMD water)</b>			
Pd	-0.568984	-3.615410	-0.612659
Pd	4.422221	-0.706415	0.324756
Pd	0.809311	3.738011	-0.085334
Pd	-4.261358	0.980042	-0.391039
C	-0.299973	1.903873	1.960619
C	2.616696	1.224951	-2.994781
H	0.677212	2.073018	2.412334
C	-1.283887	1.230046	2.620291
C	-4.317586	-2.950560	1.159581
C	1.015630	-1.540073	2.736230
C	-3.097298	-3.415180	0.774811
C	0.204972	-2.166127	1.835830
H	-0.796845	-2.495851	2.111681
H	-2.736620	-4.396805	1.085900
H	-4.980187	-3.535298	1.788476
H	0.686487	-1.344567	3.751214
H	-1.128710	0.841361	3.621433
N	0.583733	-2.435940	0.567052
N	2.647606	-1.370969	1.017047
N	-2.261113	-2.710190	-0.017491
N	-3.834214	-0.959857	-0.057278
N	-2.653903	1.514695	0.695709
N	-0.474617	2.415226	0.723145
N	3.489144	0.613304	-0.868996
N	1.877541	2.319891	-1.015855
C	1.821990	2.126285	-2.348836
H	1.106042	2.747199	-2.887281
H	2.572641	1.097519	-4.070900
C	-4.717358	-1.660255	0.718679
O	-5.846803	-1.142037	1.003041
C	-2.543191	1.053254	1.983205
O	-3.546741	0.517211	2.547713
C	3.506479	0.427697	-2.223489
O	4.306007	-0.432036	-2.720856
C	2.315469	-1.142065	2.325438
O	3.174680	-0.606650	3.099923
C	-2.631866	-1.465279	-0.445756
O	-1.867395	-0.811579	-1.220400
C	-1.657223	2.200420	0.079328
O	-1.822737	2.664716	-1.097286
C	2.742797	1.574622	-0.268384

O	2.862203	1.804019	0.974254
C	1.815983	-2.003423	0.148900
O	2.186336	-2.213280	-1.049754
H	0.914644	-5.264522	-1.995487
H	1.805082	-4.022509	-1.321112
H	1.337116	-5.335331	-0.401885
H	-1.338418	-4.958693	-2.690180
H	-1.836088	-5.745261	-1.325979
H	-2.663450	-4.422479	-1.866716
H	-5.346001	3.124465	-1.437992
H	-4.966498	3.415698	0.142616
H	-3.754527	3.342802	-0.997576
H	-6.531019	1.139516	-1.697311
H	-5.620172	-0.090436	-2.317662
H	-6.361131	-0.278811	-0.841016
H	-0.154533	5.083845	1.869002
H	-0.035297	6.128780	0.597683
H	-1.273957	5.043010	0.659699
H	2.255517	4.912905	-1.860438
H	1.840383	6.060533	-0.752598
H	3.026088	4.967757	-0.405585
H	6.415788	0.875732	-0.171553
H	6.981170	-0.673886	-0.249278
H	6.021699	-0.079847	-1.473625
H	5.170232	-2.977247	1.330085
H	6.321968	-1.858097	1.715498
H	4.861367	-1.845286	2.505880
N	1.066168	-4.710155	-1.156731
N	-1.736461	-4.830193	-1.761618
N	6.191520	-0.070883	-0.466908
N	5.322175	-2.011894	1.610515
N	2.126045	5.090262	-0.866085
N	-0.285633	5.178626	0.863661
N	-4.655652	2.957785	-0.709895
N	-5.893620	0.383472	-1.461078

**Pd-U-Ic (M11L, SMD water)**

Pd	0.784479	3.601641	-0.003596
Pd	0.213845	-0.071996	4.624779
Pd	-0.784479	-3.601641	0.003596
Pd	-0.213845	0.071996	-4.624779
C	2.465663	-3.058159	2.684856
C	-2.466974	2.264742	2.381113
C	-1.657952	2.851397	1.454846
H	-2.054262	3.543790	0.713498
C	1.657952	-2.851397	-1.454846
C	-2.465663	3.058159	-2.684856
H	2.054262	-3.543790	-0.713498
C	2.466974	-2.264742	-2.381113
C	-2.028443	1.985573	-3.402329
H	-2.672120	1.499767	-4.136382
H	-3.453760	3.479654	-2.837493
H	3.535264	-2.451144	-2.400011
H	-3.535264	2.451144	2.400011
N	0.528264	-1.214595	-3.265872
N	0.323789	-2.642629	-1.400282
N	-0.785717	1.466101	-3.278961
N	-0.400013	2.986861	-1.518443
N	-0.323789	2.642629	1.400282
N	-0.528264	1.214595	3.265872

N	0.400013	-2.986861	1.518443
N	0.785717	-1.466101	3.278961
C	2.028443	-1.985573	3.402329
H	2.672120	-1.499767	4.136382
H	3.453760	-3.479654	2.837493
C	-1.583599	3.635758	-1.734121
O	-1.843565	4.696439	-1.076903
C	-1.883749	1.397899	3.336163
O	-2.541373	0.803099	4.254100
C	1.583599	-3.635758	1.734121
O	1.843565	-4.696439	1.076903
C	1.883749	-1.397899	-3.336163
O	2.541373	-0.803099	-4.254100
C	0.048373	1.979732	-2.322845
O	1.232687	1.549092	-2.187427
C	0.248401	1.804901	2.322427
O	1.505336	1.599784	2.300372
C	-0.048373	-1.979732	2.322845
O	-1.232687	-1.549092	2.187427
C	-0.248401	-1.804901	-2.322427
O	-1.505336	-1.599784	-2.300372
N	1.861584	4.567122	-1.434563
H	2.625537	5.133827	-1.074583
H	2.242693	3.858203	-2.058672
N	2.004659	4.262494	1.495023
H	2.892936	4.628164	1.159542
H	1.543944	4.986038	2.041177
N	-0.869023	1.327453	-6.107771
H	-0.212258	1.334259	-6.885771
H	-1.774001	1.019700	-6.459821
N	0.335497	-1.307867	-6.021861
H	-0.161899	-2.182442	-5.875155
H	0.190406	-1.012647	-6.984419
N	-2.004659	-4.262494	-1.495023
H	-1.543944	-4.986038	-2.041177
H	-2.892936	-4.628164	-1.159542
N	-1.861584	-4.567122	1.434563
H	-2.242693	-3.858203	2.058672
H	-2.625537	-5.133827	1.074583
N	0.869023	-1.327453	6.107771
H	1.774001	-1.019700	6.459821
H	0.212258	-1.334259	6.885771
N	-0.335497	1.307867	6.021861
H	-0.190406	1.012647	6.984419
H	0.161899	2.182442	5.875155
H	-1.332183	1.456970	5.860010
H	0.965305	-2.284151	5.773721
H	-2.170088	-3.441037	-2.079726
H	-1.239752	-5.166931	1.972348
H	-0.965305	2.284151	-5.773721
H	1.332183	-1.456970	-5.860010
H	1.239752	5.166931	-1.972348
H	2.170088	3.441037	2.079726

**Pd-U-IIc1 (M11L, SMD water)**

Pd	-0.374520	-3.813354	-0.947735
Pd	-4.437505	0.310594	0.076540
Pd	0.236979	3.827005	0.590586
Pd	4.414489	-0.441829	0.225770
C	-2.008684	2.308523	-2.717237



C	-2.260902	-2.327486	2.558861
C	-1.531843	-3.029817	1.646647
H	-0.854165	-3.822726	1.957436
C	2.441756	-3.562855	2.191693
C	3.545290	3.023142	-1.911131
C	3.135133	-2.446475	1.838536
C	3.869029	1.758595	-1.530228
H	4.626640	1.188936	-2.069271
H	3.876253	-2.014298	2.511448
H	2.621481	-4.069890	3.133422
H	4.040969	3.510996	-2.743857
H	-2.178284	-2.525471	3.621891
N	3.313609	1.130873	-0.463720
N	1.869631	2.981128	-0.234145
N	2.973069	-1.808390	0.654556
N	1.223694	-3.311760	0.171510
N	-1.612866	-2.820267	0.314065
N	-3.209321	-1.136987	0.737174
N	-1.070442	2.811276	-0.581633
N	-2.937377	1.373563	-0.736802
C	-2.910459	1.515266	-2.079400
H	-3.672468	0.961093	-2.628544
H	-2.014027	2.426975	-3.795310
C	1.482072	-4.070478	1.278498
O	0.844391	-5.160600	1.450340
C	-3.138619	-1.317416	2.092703
O	-3.864630	-0.594342	2.851994
C	-1.070154	3.037996	-1.935840
O	-0.267312	3.883514	-2.435534
C	2.564282	3.719262	-1.154062
O	2.311421	4.957184	-1.291386
C	-2.488133	-1.873440	-0.147204
O	-2.636132	-1.702484	-1.399720
C	1.974231	-2.228235	-0.181420
O	1.749806	-1.634270	-1.278718
C	2.255964	1.736130	0.163779
O	1.645889	1.159789	1.116038
C	-1.995485	2.009289	0.018992
O	-1.999832	1.878613	1.285524
N	0.915418	-4.803702	-2.175141
H	0.469297	-5.217714	-2.990756
H	1.626982	-4.149106	-2.494347
N	-1.986065	-4.342726	-2.084863
H	-1.739858	-4.623456	-3.030884
H	-2.509766	-5.097731	-1.649683
N	-5.977952	-0.745994	0.890452
H	-6.872876	-0.263826	0.852529
H	-6.079196	-1.650817	0.437415
N	-5.740685	1.746440	-0.575811
H	-6.213970	2.187721	0.210766
H	-5.253038	2.472561	-1.097274
N	-1.392619	4.700616	1.455470
H	-1.996554	3.923194	1.724695
H	-1.168550	5.255234	2.278405
N	1.558030	4.878722	1.733061
H	2.167005	5.372114	1.081890
H	1.134575	5.552050	2.367150
N	5.748992	-1.907724	0.730171
H	5.335481	-2.834334	0.643758
H	6.558167	-1.869849	0.111908

N	6.043671	0.788369	0.047605
H	5.784251	1.772751	0.076780
H	6.695100	0.616445	0.812508
H	-5.705766	-0.885430	1.864226
H	1.376723	-5.545062	-1.651918
H	-2.554824	-3.492947	-2.114600
H	6.077703	-1.791480	1.687482
H	6.534458	0.614364	-0.828482
H	-1.881268	5.293408	0.789707
H	2.122830	4.230206	2.276832
H	-6.448894	1.339686	-1.183795

**Pd-U-IIc2 (M11L, SMD water)**

Pd	0.255217	3.555887	0.806862
Pd	-4.558300	0.221261	-0.117213
Pd	-0.262408	-3.706928	-0.591151
Pd	4.599432	-0.359609	-0.198288
C	-2.677939	-2.346155	2.671696
C	-1.887530	2.296909	-2.645548
C	-1.024688	2.865281	-1.757061
H	-0.219697	3.516293	-2.091888
C	3.023210	2.918293	-2.328922
C	2.441533	-2.712309	2.536101
C	3.606925	1.753433	-1.931507
H	4.297813	1.224856	-2.588391
H	3.250839	3.369716	-3.288398
H	2.557606	-2.976659	3.581106
H	-1.786517	2.456450	-3.713618
N	3.180118	-1.553230	0.594166
N	1.278732	-2.938700	0.467656
N	3.392319	1.183039	-0.723087
N	1.790750	2.862963	-0.302836
N	-1.118508	2.693506	-0.419408
N	-3.025528	1.349506	-0.786967
N	-1.665747	-2.811350	0.565082
N	-3.362451	-1.173561	0.717470
H	-2.770950	-2.549679	3.732777
C	2.112024	3.547548	-1.441695
O	1.570442	4.680816	-1.659503
C	-2.939674	1.491304	-2.146381
O	-3.809458	0.920729	-2.886644
C	-1.805675	-3.038650	1.886580
C	1.456653	-3.253103	1.766834
C	-2.140678	1.922993	0.071443
O	-2.270147	1.764094	1.328238
C	2.463023	1.749609	0.109706
O	2.231267	1.266117	1.257579
C	2.172584	-2.092724	-0.135164
O	2.061418	-1.842200	-1.378082
C	-2.488330	-1.892260	-0.034521
O	-2.435888	-1.739868	-1.295737
N	1.671001	4.400312	2.004513
H	1.298620	4.819357	2.853863
H	2.329652	3.668371	2.264355
N	-1.275853	4.311797	1.927571
H	-0.993710	4.590577	2.864087
H	-1.695688	5.114477	1.465414
N	-5.794974	1.614907	-0.953208
H	-6.777051	1.349982	-0.962005
H	-5.706421	2.508947	-0.477120

N	-6.138880	-0.886709	0.549136
H	-7.041167	-0.432529	0.430675
H	-6.170676	-1.792611	0.088635
N	-1.808347	-4.500843	-1.651118
H	-2.372768	-3.689465	-1.910323
H	-1.530715	-5.008618	-2.487310
N	1.144950	-4.554030	-1.797836
H	1.651177	-5.289590	-1.310669
H	0.767788	-4.937998	-2.661478
N	6.184964	0.762387	-0.858892
H	5.995619	1.757627	-0.758744
H	7.025224	0.550467	-0.323248
N	5.868853	-1.885975	0.263320
H	5.509165	-2.758547	-0.117563
H	6.822742	-1.758811	-0.066433
H	-5.463129	1.705721	-1.913791
H	2.174199	5.116354	1.485182
H	-1.954815	3.549807	1.988103
H	6.382887	0.572138	-1.840098
H	5.865872	-1.946200	1.281581
H	-2.362136	-5.122033	-1.066148
H	1.783588	-3.787385	-2.017795
H	-5.955636	-1.016563	1.544636
C	3.336979	-1.793129	1.934267
O	4.286402	-1.216312	2.559783
H	0.775219	-3.994837	2.177668
C	-3.476260	-1.339483	2.072634
O	-4.301133	-0.614336	2.721993
H	-1.194174	-3.833545	2.306534

**Pd-U-IIIc1 (M11L, SMD water)**

Pd	-0.535679	3.709790	0.622129
Pd	4.441411	0.599675	-0.002323
Pd	0.714430	-3.798800	-0.869790
Pd	-4.345232	-0.847828	0.074678
C	-3.937771	1.438061	-1.652824
C	-1.869838	-3.254235	2.455297
H	-4.611059	0.822341	-2.250114
C	-3.713399	2.739758	-1.979474
C	2.205419	-3.200022	1.657238
C	1.754167	2.341361	-2.714201
H	1.736417	-4.125327	1.983253
C	2.936069	-2.445847	2.525836
C	2.736304	1.630932	-2.098081
H	3.523977	1.132534	-2.664453
H	1.717379	2.448490	-3.792875
H	3.055186	-2.732030	3.564760
H	-4.214783	3.210170	-2.818749
N	3.425576	-0.994731	0.705252
N	2.038425	-2.874594	0.359197
N	2.814215	1.506813	-0.756018
N	0.845588	2.792974	-0.552338
N	-2.101518	2.782016	-0.244303
N	-3.378019	0.824480	-0.580209
N	-0.853782	-3.286139	0.299846
N	-2.764924	-1.958502	0.670546
C	-0.941700	-3.719092	1.574043
H	-1.911712	-3.609264	3.479019
H	-0.231517	-4.489603	1.864271
C	0.790554	3.008423	-1.908403

O	-0.083057	3.792116	-2.388675
C	-2.824873	3.491435	-1.162927
O	-2.676974	4.751696	-1.247670
C	-2.803108	-2.289753	2.000881
O	-3.690453	-1.758646	2.747797
C	3.545103	-1.259093	2.044777
O	4.211329	-0.456485	2.779128
C	-2.405658	1.502271	0.111998
O	-1.795214	0.959691	1.082269
C	1.846541	2.067872	0.023861
O	1.899895	1.938081	1.290848
C	2.713076	-1.788829	-0.136341
O	2.680375	-1.549535	-1.383712
C	-1.807024	-2.421160	-0.171478
O	-1.794205	-2.078116	-1.396470
N	-1.938310	4.677132	1.739014
H	-2.452203	4.003852	2.302179
H	-1.571979	5.402736	2.350103
N	1.026578	4.663698	1.527000
H	1.487577	5.297515	0.879391
H	0.762984	5.187497	2.358184
N	-6.120065	0.108564	-0.311217
H	-6.537776	-0.244370	-1.171219
H	-6.771557	-0.070829	0.451653
N	-5.434585	-2.474652	0.641869
H	-6.419203	-2.426134	0.389813
H	-5.037057	-3.316508	0.231283
N	2.292230	-4.304222	-2.055806
H	2.872005	-5.015461	-1.618466
H	2.023962	-4.630657	-2.980923
N	-0.631868	-4.660695	-2.131402
H	-1.368987	-3.961641	-2.236065
H	-0.250582	-4.884749	-3.047241
N	5.532654	2.181889	-0.702394
H	6.099555	1.896916	-1.499115
H	4.916218	2.934690	-1.001156
N	6.141477	-0.278149	0.705906
H	6.969355	0.307605	0.626847
H	5.946481	-0.461261	1.691200
H	6.155189	2.548316	0.015060
H	-1.023963	-5.508598	-1.729086
H	-5.342564	-2.527588	1.656174
H	-6.016127	1.117808	-0.397123
H	-2.577704	5.096370	1.064455
H	1.670095	3.913568	1.784274
H	6.322690	-1.156978	0.227825
H	2.820499	-3.433952	-2.143026

**Pd-U-IIIc2 (M11L, SMD water)**

Pd	0.000000	3.755588	0.011407
Pd	0.000000	0.000000	-4.512348
Pd	0.000000	-3.755588	0.011407
Pd	0.000000	0.000000	4.627555
C	-2.165412	1.570814	3.561655
C	2.842295	-2.558581	2.913741
H	-2.650989	0.970854	4.332069
C	-2.842295	2.558581	2.913741
C	2.332400	-2.444696	-1.234237
C	-3.048231	1.644473	-2.074135
H	2.820383	-3.041643	-0.465638

C	3.048231	-1.644473	-2.074135
H	-4.127192	1.564598	-1.996889
H	4.127192	-1.564598	-1.996889
H	-3.872554	2.796040	3.156588
N	0.995018	-1.066742	-3.121876
N	0.989919	-2.577204	-1.307800
N	-0.995018	1.066742	-3.121876
N	-0.989919	2.577204	-1.307800
N	-0.896984	2.875543	1.589575
N	-0.866769	1.276724	3.319573
N	0.896984	-2.875543	1.589575
N	0.866769	-1.276724	3.319573
H	3.872554	-2.796040	3.156588
C	-2.332400	2.444696	-1.234237
C	-2.154565	3.300284	1.918419
O	-2.650184	4.309099	1.317347
C	2.165412	-1.570814	3.561655
C	2.354842	-0.913836	-3.071217
O	2.925883	-0.152622	-3.921675
C	-0.224336	1.926703	2.301946
O	0.988018	1.670413	2.030325
C	-0.313486	1.880923	-2.274416
O	0.946823	2.018555	-2.388043
C	0.313486	-1.880923	-2.274416
O	-0.946823	-2.018555	-2.388043
C	0.224336	-1.926703	2.301946
O	-0.988018	-1.670413	2.030325
N	0.975186	4.911385	1.376092
H	1.459628	4.289856	2.021287
H	1.654645	5.552409	0.972536
N	0.882373	4.700617	-1.568897
H	0.211354	5.306176	-2.034362
H	1.695933	5.256163	-1.315633
N	-0.690095	1.231859	6.105513
H	-1.558301	0.869860	6.497976
H	-0.006783	1.300505	6.857931
N	0.690095	-1.231859	6.105513
H	1.558301	-0.869860	6.497976
H	0.006783	-1.300505	6.857931
N	-0.882373	-4.700617	-1.568897
H	-0.211354	-5.306176	-2.034362
H	-1.695933	-5.256163	-1.315633
N	-0.975186	-4.911385	1.376092
H	-1.459628	-4.289856	2.021287
H	-1.654645	-5.552409	0.972536
N	-1.032807	1.045425	-5.929524
H	-0.962631	0.646467	-6.862579
H	-2.004866	1.004742	-5.620713
N	1.032807	-1.045425	-5.929524
H	0.962631	-0.646467	-6.862579
H	2.004866	-1.004742	-5.620713
H	-0.728918	2.014832	-5.969739
H	-0.295493	-5.454150	1.904260
H	0.864123	-2.170810	5.752904
H	-0.864123	2.170810	5.752904
H	0.295493	5.454150	1.904260
H	1.160493	3.944081	-2.197263
H	0.728918	-2.014832	-5.969739
H	-1.160493	-3.944081	-2.197263
C	-2.354842	0.913836	-3.071217

O	-2.925883	0.152622	-3.921675
H	-2.820383	3.041643	-0.465638
H	2.650989	-0.970854	4.332069
C	2.154565	-3.300284	1.918419
O	2.650184	-4.309099	1.317347

**Pd-U-IVc1 (M11L, SMD water)**

Pd	-3.964114	0.496866	0.833190
Pd	-0.350869	-4.228390	-0.102669
Pd	4.031761	-0.164562	-0.676422
Pd	0.362731	4.342612	-0.103190
C	-2.545216	-3.198199	-1.630872
C	3.172759	-3.371791	1.907395
H	-2.109097	-3.934937	-2.306317
C	-3.805443	-2.730147	-1.835399
C	-2.176210	2.173866	-2.663196
C	2.429130	1.943349	2.670363
C	-1.180875	2.925393	-2.121277
C	1.592434	2.821871	2.055595
H	0.990753	3.532740	2.622193
H	-0.475153	3.475468	-2.744030
H	-2.313890	2.096462	-3.736213
H	2.537527	1.917528	3.749207
H	-4.419017	-3.088697	-2.654747
N	1.466606	2.885826	0.713817
N	2.993821	1.103160	0.509417
N	-1.015043	3.059424	-0.788459
N	-2.822176	1.584951	-0.441391
N	-3.420925	-1.236578	-0.037733
N	-1.760729	-2.821527	-0.587499
N	3.161870	-1.783351	0.146982
N	1.247461	-3.109973	0.507865
C	1.879684	-3.642359	1.584642
H	1.287588	-4.335483	2.183033
H	3.659984	-3.846098	2.752679
C	-3.079826	1.508582	-1.788951
O	-4.099842	0.877226	-2.199167
C	-4.319927	-1.773881	-0.917602
O	-5.534892	-1.402687	-0.884247
C	3.893071	-2.470269	1.077479
O	5.146638	-2.277140	1.161417
C	3.209858	1.067716	1.865194
O	4.091282	0.290695	2.342962
C	-2.185694	-1.768350	0.183641
O	-1.449901	-1.293853	1.101475
C	1.883260	-2.115275	-0.187539
O	1.299118	-1.515635	-1.141289
C	2.164821	2.014323	-0.068914
O	2.062247	2.077802	-1.337205
C	-1.833384	2.374105	0.061392
O	-1.687468	2.497706	1.321165
H	-4.575154	-1.215423	2.654699
H	-5.780306	-0.082942	2.638767
H	-5.693446	-1.217658	1.430350
H	-5.142813	2.785836	1.121590
H	-4.973430	2.118132	2.621969
H	-3.643720	2.754632	1.848784
H	-1.715838	-6.368548	0.276643
H	-2.749721	-5.247859	-0.342515
H	-1.715519	-6.056281	-1.344275

H	1.870328	-5.586351	0.039546
H	0.746945	-6.298525	1.016396
H	0.692070	-6.528251	-0.616699
H	5.902938	-1.021568	-2.299908
H	5.496857	-2.145185	-1.149663
H	4.537466	-1.934227	-2.485484
H	5.443032	1.276197	-2.349821
H	4.129072	2.098459	-1.747010
H	5.516063	1.944535	-0.842160
H	-1.647507	5.547103	-1.197388
H	-0.855274	6.624978	-0.232341
H	-0.252170	6.254777	-1.721159
N	-5.147452	-0.625403	2.055429
N	-4.521148	2.248460	1.720360
N	-1.810072	-5.631992	-0.422053
N	0.888479	-5.845298	0.114318
N	5.127923	-1.459338	-1.807733
N	4.906198	1.480837	-1.510292
N	-0.727648	5.872107	-0.905923
N	1.766110	5.664004	0.573820
H	1.611961	5.844758	1.564268
H	2.693174	5.257135	0.466463
H	1.747867	6.555460	0.082259

**Pd-U-IVc2 (M11L, SMD water)**

Pd	0.000000	3.692636	-0.013011
Pd	0.000000	0.000000	-4.571402
Pd	0.000000	-3.692636	-0.013011
Pd	0.000000	0.000000	4.581600
C	-3.061564	-2.040743	-2.492740
C	3.061564	2.040743	-2.492740
C	3.024453	2.121000	2.535106
C	-3.024453	-2.121000	2.535106
H	4.098459	2.230452	2.638056
H	-4.098459	-2.230452	2.638056
H	4.139654	2.120420	-2.579548
N	-0.961090	-1.158775	3.232084
N	-0.979145	-2.744153	1.483045
N	0.961090	1.158775	3.232084
N	0.979145	2.744153	1.483045
N	1.021928	2.709901	-1.458241
N	0.982574	1.137725	-3.220123
N	-1.021928	-2.709901	-1.458241
N	-0.982574	-1.137725	-3.220123
H	-4.139654	-2.120420	-2.579548
C	2.311745	2.867608	1.646266
C	2.359134	2.797095	-1.603603
C	-2.359134	-2.797095	-1.603603
C	-2.311745	-2.867608	1.646266
C	0.318354	1.894047	-2.308119
O	-0.951379	1.873482	-2.243141
C	-0.318354	-1.894047	-2.308119
O	0.951379	-1.873482	-2.243141
C	-0.286702	-1.909218	2.321975
O	0.982064	-1.864981	2.249010
C	0.286702	1.909218	2.321975
O	-0.982064	1.864981	2.249010
H	-1.321783	3.891933	-2.119266
H	-1.749420	5.232023	-1.225854
H	-0.324625	5.220743	-2.058008

H	-0.531157	5.331785	1.924073
H	-1.923725	5.090841	1.070715
H	-1.354675	3.889998	2.069410
H	0.703211	0.872472	-6.954217
H	0.732439	2.107539	-5.861911
H	1.934815	0.963736	-5.835772
H	-0.732439	-2.107539	-5.861911
H	-1.934815	-0.963736	-5.835772
H	-0.703211	-0.872472	-6.954217
H	1.749420	-5.232023	-1.225854
H	0.324625	-5.220743	-2.058008
H	1.321783	-3.891933	-2.119266
H	1.923725	-5.090841	1.070715
H	1.354675	-3.889998	2.069410
H	0.531157	-5.331785	1.924073
H	0.696003	2.125199	5.864965
H	0.676589	0.896950	6.964928
H	1.913467	0.997725	5.853814
N	-0.973645	4.646638	-1.525489
N	-1.085845	4.638773	1.428610
N	0.939641	1.121076	-5.996788
N	-0.939641	-1.121076	-5.996788
N	0.973645	-4.646638	-1.525489
N	1.085845	-4.638773	1.428610
N	0.915230	1.142367	6.007192
N	-0.915230	-1.142367	6.007192
H	-1.913467	-0.997725	5.853814
H	-0.696003	-2.125199	5.864965
H	-0.676589	-0.896950	6.964928
C	2.327833	1.182904	3.337898
O	2.902351	0.398699	4.164289
C	2.350139	1.131669	-3.315509
O	2.912610	0.345327	-4.148208
H	2.864043	3.525714	-0.973953
H	2.800044	3.620146	1.031237
H	-2.800044	-3.620146	1.031237
C	-2.327833	-1.182904	3.337898
O	-2.902351	-0.398699	4.164289
H	-2.864043	-3.525714	-0.973953
C	-2.350139	-1.131669	-3.315509
O	-2.912610	-0.345327	-4.148208

**Pd-U-Id (M11L, SMD water)**

Pd	-0.710934	-3.915887	0.441184
Pd	3.915887	-0.710934	-0.441184
Pd	-3.915887	0.710934	-0.441184
Pd	0.710934	3.915887	0.441184
C	-0.591059	1.614518	-2.923096
C	0.128441	2.430428	-2.098019
H	-0.216625	1.330579	-3.900789
H	1.099568	2.823295	-2.390295
N	-0.317701	2.809153	-0.884239
N	-2.248649	1.503654	-1.225424
C	0.591059	-1.614518	-2.923096
C	-0.128441	-2.430428	-2.098019
H	0.216625	-1.330579	-3.900789
H	-1.099568	-2.823295	-2.390295
N	0.317701	-2.809153	-0.884239
N	2.248649	-1.503654	-1.225424
C	-1.614518	-0.591059	2.923096

C	1.614518	0.591059	2.923096
N	2.809153	0.317701	0.884239
N	1.503654	2.248649	1.225424
C	2.430428	-0.128441	2.098019
H	1.330579	0.216625	3.900789
H	2.823295	-1.099568	2.390295
H	-1.330579	-0.216625	3.900789
C	-2.430428	0.128441	2.098019
N	-2.809153	-0.317701	0.884239
N	-1.503654	-2.248649	1.225424
H	-2.823295	1.099568	2.390295
C	1.834608	-1.101748	-2.465708
O	2.579254	-0.317701	-3.142549
C	1.101748	1.834608	2.465708
O	0.317701	2.579254	3.142549
C	-1.834608	1.101748	-2.465708
O	-2.579254	0.317701	-3.142549
C	-1.101748	-1.834608	2.465708
O	-0.317701	-2.579254	3.142549
C	1.538870	-2.371861	-0.458654
O	2.009675	-2.789359	0.644832
C	2.371861	1.538870	0.458654
O	2.789359	2.009675	-0.644832
C	-1.538870	2.371861	-0.458654
O	-2.009675	2.789359	0.644832
C	-2.371861	-1.538870	0.458654
O	-2.789359	-2.009675	-0.644832
N	-5.580272	-0.131632	0.400020
H	-5.679710	0.209521	1.353465
H	-6.443532	0.062298	-0.102635
N	-4.969482	1.702527	-1.877329
H	-4.469259	1.518296	-2.747105
H	-5.931605	1.387880	-1.975579
N	-1.702527	-4.969482	1.877329
H	-1.387880	-5.931605	1.975579
H	-1.518296	-4.469259	2.747105
N	0.131632	-5.580272	-0.400020
H	-0.062298	-6.443532	0.102635
H	-0.209521	-5.679710	-1.353465
N	4.969482	-1.702527	-1.877329
H	4.469259	-1.518296	-2.747105
H	5.931605	-1.387880	-1.975579
N	5.580272	0.131632	0.400020
H	5.679710	-0.209521	1.353465
H	6.443532	-0.062298	-0.102635
N	-0.131632	5.580272	-0.400020
H	-1.140498	5.449835	-0.435793
H	0.062298	6.443532	0.102635
N	1.702527	4.969482	1.877329
H	2.703980	4.973744	1.701782
H	1.387880	5.931605	1.975579
H	4.973744	-2.703980	-1.701782
H	5.449835	1.140498	0.435793
H	0.209521	5.679710	-1.353465
H	1.518296	4.469259	2.747105
H	-4.973744	2.703980	-1.701782
H	-5.449835	-1.140498	0.435793
H	-2.703980	-4.973744	1.701782
H	1.140498	-5.449835	-0.435793

<b>Pd-U-IIId (M11L, SMD water)</b>			
Pd	-0.178641	3.828383	-0.280248
Pd	4.386127	0.271608	0.024228
Pd	0.253312	-3.747299	0.015329
Pd	-4.268778	-0.174949	0.270161
C	-1.129687	-1.036296	2.999362
C	-0.342468	-1.853885	2.240826
H	-0.830677	-0.727187	3.995333
H	0.613847	-2.222895	2.609963
N	-0.699454	-2.271290	1.008476
N	-2.659158	-0.970087	1.180228
C	1.495468	1.510597	2.863732
C	0.652211	2.250306	2.087153
H	1.291507	1.334941	3.914569
H	-0.255044	2.693330	2.496795
N	0.889103	2.491480	0.781849
N	2.850382	1.197730	0.932833
C	-2.045237	1.220702	-3.076546
C	1.991481	-1.403699	-3.068876
N	3.106802	-0.855516	-1.036982
N	1.401333	-2.476686	-1.032340
C	2.908875	-0.684392	-2.359214
H	1.860299	-1.260082	-4.135810
H	3.536413	0.067812	-2.837201
H	-1.959238	0.993487	-4.133497
N	-3.076601	0.879955	-0.959844
N	-1.304678	2.418753	-1.159313
C	-1.205786	2.107096	-2.466883
H	-0.413969	2.615592	-3.017812
C	2.663846	0.964968	2.269517
O	3.540124	0.293667	2.908314
C	1.189122	-2.351178	-2.377575
O	0.309155	-3.085852	-2.936452
C	-2.366431	-0.589514	2.461545
O	-3.205221	0.124633	3.103793
C	-3.040124	0.573995	-2.292800
O	-3.887838	-0.254882	-2.761977
C	-2.270536	1.821276	-0.401558
O	-2.421072	2.165982	0.810161
C	2.004688	1.964829	0.195634
O	2.251399	2.215367	-1.025916
C	2.367269	-1.788551	-0.368900
O	2.596796	-2.027545	0.855771
C	-1.875313	-1.826374	0.472861
O	-2.234492	-2.234774	-0.675749
N	-1.257547	5.196364	-1.345719
H	-1.046030	6.165075	-1.114621
H	-1.082654	5.062430	-2.340044
N	0.966060	5.261222	0.617847
H	0.831305	6.195221	0.236401
H	0.746878	5.288457	1.612133
N	-5.435188	-1.215453	1.582416
H	-6.403327	-0.903826	1.604895
H	-5.419724	-2.211005	1.375832
N	-5.870491	0.602431	-0.729326
H	-6.746014	0.120368	-0.540877
H	-5.993447	1.590380	-0.523432
N	-0.915408	-5.044480	1.080982
H	-0.902727	-5.993087	0.713747
H	-0.596943	-5.072297	2.047556

N	1.171151	-5.240486	-1.027615
H	0.738044	-6.155136	-0.920211
H	1.110061	-4.957947	-2.006221
N	5.923542	-0.691212	-0.921381
H	5.985230	-0.367830	-1.884757
H	6.828801	-0.546075	-0.478811
N	5.643506	1.394833	1.171079
H	5.261866	1.311276	2.114331
H	6.606158	1.066931	1.171164
H	1.949724	5.018250	0.518106
H	-2.248232	5.036740	-1.174153
H	-5.011580	-1.055799	2.496614
H	-5.630498	0.489984	-1.714967
H	-1.878612	-4.714867	1.074272
H	2.150357	-5.314031	-0.763356
H	5.732754	-1.690692	-0.934453
H	5.633989	2.371343	0.887343

**Pd-U-III d (M11L, SMD water)**

Pd	-4.495687	-0.057043	0.229863
Pd	0.011535	3.434144	0.000106
Pd	4.491666	-0.075878	-0.234565
Pd	-0.009418	-3.610513	0.006296
C	1.729995	-0.955021	2.843369
H	1.513030	-0.604778	3.846888
N	3.101895	-0.966424	0.903434
N	1.114820	-2.226974	0.926786
C	-1.411611	0.805112	3.054905
C	-2.564523	0.355300	2.479427
H	-1.107596	0.477094	4.043781
H	-3.215008	-0.356959	2.985531
N	-2.979183	0.768417	1.265457
N	-1.028136	2.088046	1.088852
C	-1.732315	-0.959730	-2.842798
C	1.408207	0.790482	-3.058473
N	1.025268	2.069988	-1.090789
N	2.976039	0.750157	-1.269197
H	1.104318	0.464196	-4.047966
H	-1.512811	-0.616823	-3.848290
C	-0.868977	-1.768889	-2.161688
N	-1.123473	-2.219618	-0.916091
N	-3.107273	-0.953538	-0.905026
H	0.066939	-2.108003	-2.606868
C	0.863440	-1.766928	2.169500
C	2.559977	0.337763	-2.483096
H	-0.072537	-2.100284	2.618808
H	3.209191	-0.375422	-2.989438
C	-0.594942	1.724154	2.336164
O	0.479495	2.227553	2.797520
C	0.592979	1.711277	-2.339905
O	-0.478101	2.219158	-2.803541
C	2.923678	-0.540140	2.191803
O	3.821980	0.182229	2.734359
C	-2.925102	-0.535480	-2.195372
O	-3.819346	0.187645	-2.743666
C	-2.211878	1.663186	0.574042
O	-2.622289	2.112055	-0.538643
C	-2.266255	-1.820973	-0.285364
O	-2.547655	-2.282634	0.864872
C	2.256287	-1.833707	0.290324

O	2.531865	-2.300524	-0.859309
C	2.211091	1.647472	-0.578799
O	2.624878	2.100918	0.531031
N	-5.867376	0.884700	1.419709
H	-6.779614	0.434261	1.394245
H	-5.540092	0.893129	2.383519
N	-5.940348	-0.872500	-0.953885
H	-6.845937	-0.416970	-0.868005
H	-5.581946	-0.736676	-1.900492
N	-0.977431	4.852757	1.089741
H	-0.576782	5.784416	1.003641
H	-1.948322	4.891420	0.786132
N	1.048856	4.817856	-1.089997
H	0.815331	5.784427	-0.872185
H	2.043571	4.682086	-0.921117
N	1.091104	-5.061468	0.928534
H	0.490751	-5.676211	1.475063
H	1.587437	-5.626215	0.242491
N	-1.124596	-5.044342	-0.924240
H	-0.562514	-5.540678	-1.612435
H	-1.488815	-5.723271	-0.258807
N	5.938590	-0.892429	0.946338
H	6.846830	-0.443979	0.852126
H	5.586600	-0.748673	1.894111
N	5.876313	0.863317	-1.408503
H	6.601208	0.220408	-1.719389
H	5.427050	1.264029	-2.229235
H	-1.911468	-4.612769	-1.405046
H	1.776154	-4.643003	1.554845
H	-5.979470	1.849546	1.116121
H	-6.057291	-1.865981	-0.773808
H	0.869226	4.659788	-2.079451
H	-0.961458	4.588463	2.072783
H	6.321913	1.618432	-0.890645
H	6.047289	-1.887779	0.771766

**Pd-U-IV d (M11L, SMD water)**

Pd	-0.099411	-3.321173	0.063759
Pd	4.679865	-0.035262	0.102019
Pd	-4.697994	0.044888	0.092428
Pd	0.004531	3.318794	-0.280910
C	1.830476	1.269639	2.951904
C	0.937107	1.915091	2.146234
H	1.636909	1.119789	4.008718
H	-0.006493	2.303271	2.531759
N	1.163480	2.122728	0.834539
N	3.206318	0.969381	1.030732
C	-1.543694	-0.435627	2.845485
C	-0.709164	-1.217562	2.098585
H	-1.209879	0.022581	3.770943
H	0.320973	-1.407236	2.400889
N	-1.102664	-1.817131	0.955072
N	-3.196923	-0.752266	1.167497
C	2.028549	-1.249776	-2.960526
C	-1.694740	0.383977	-2.828832
N	-3.242515	0.805831	-1.072732
N	-1.113571	1.817027	-1.017829
H	-1.427341	-0.112279	-3.755982
H	1.912238	-1.077869	-4.025293
N	3.273393	-1.018938	-0.945415

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N	1.201721	-2.139970	-0.911901
C	1.074696	-1.900806	-2.233430
C	-0.797737	1.162747	-2.154905
H	0.161889	-2.275236	-2.697942
H	0.222797	1.303425	-2.513918
C	-3.002491	0.224645	-2.289052
O	-3.937422	-0.424756	-2.858240
C	-2.866630	-0.200759	2.375540
O	-3.738220	0.485638	3.000150
C	3.191223	-0.782288	-2.290529
O	4.148144	-0.172299	-2.872201
C	3.026889	0.768098	2.373369
O	3.930255	0.154608	3.033205
C	-2.372185	-1.600965	0.499063
O	-2.773327	-2.206804	-0.542997
C	2.328557	-1.718246	-0.262759
O	2.492972	-2.010610	0.961541
C	2.320495	1.664655	0.269880
O	2.561811	1.923130	-0.949783
C	-2.350571	1.634566	-0.468220
O	-2.658390	2.256518	0.596098
H	0.564017	-5.795790	-0.491457
H	0.735315	-4.842199	-1.826072
H	1.874346	-4.803487	-0.634741
H	-1.188313	-5.529896	0.977207
H	-1.563772	-4.255773	1.955503
H	-2.339037	-4.437162	0.509436
H	5.814411	-0.999287	-1.888219
H	7.050075	-0.642827	-0.830427
H	6.173251	-2.027498	-0.628202
H	5.662175	0.928399	2.170930
H	6.977120	0.575486	1.211308
H	6.112402	1.955326	0.939269
H	2.124660	4.610210	0.359254
H	0.992351	5.735654	-0.054765
H	0.927526	5.001464	1.421734
H	-2.153147	4.385786	-1.179611
H	-0.992038	5.554197	-1.219716
H	-1.022310	4.381750	-2.379459
H	-5.748248	0.694562	-2.077339
H	-7.021650	0.386750	-1.055134
H	-6.237314	1.839157	-0.975054
H	-5.643782	-0.602676	2.314646
H	-6.962375	-0.264404	1.362388
H	-6.207102	-1.728155	1.229773
N	-1.445525	-4.545104	0.986930
N	0.876300	-4.883548	-0.818408
N	6.123908	-1.054001	-0.916565
N	6.045436	0.982381	1.225746
N	-1.173251	4.566999	-1.389822
N	1.139726	4.856532	0.436288
N	-6.116191	0.842955	-1.137317
N	-6.061431	-0.735322	1.393318

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