Supporting Information

Adsorption and Diffusion of Hydrogen on the Surface of the Pt_{24} Subnanoparticle. A DFT Study

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I. Cartesian coordinates of the stationary points and thermodynamic parameters

Pt_{24}, Pt_{24}–H, Pt_{24}–H_2 subnanoparticle with *B3LYP/6-31G*,GRENBS* calculation

Cluster Pt_{24} (M=3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.908522	-1.94548	1.463306
2	78	0	1.378821	-0.00084	0.000468
3	78	0	0.016235	2.022137	-1.52802
4	78	0	2.885871	1.984762	1.386642
5	78	0	-0.01422	-2.02308	-1.52815
6	78	0	1.389043	-3.89683	0.057436
7	78	0	2.91149	1.944513	-1.46171
8	78	0	2.887497	-1.98664	-1.38547
9	78	0	-0.01515	2.02467	1.528448
10	78	0	0.012999	-2.02451	1.530291
11	78	0	1.44371	-0.05492	-2.81716
12	78	0	4.237587	-0.00128	0.000843
13	78	0	-1.3786	0.000004	0.000406
14	78	0	1.438521	0.054414	2.818153
15	78	0	-1.44358	-0.05446	2.817761
16	78	0	-2.91002	1.947335	1.461859
17	78	0	-2.88731	-1.98519	1.385018
18	78	0	1.391903	3.89751	-0.05739
19	78	0	-1.44203	0.053397	-2.81766
20	78	0	-1.38931	3.8984	0.05582
21	78	0	-2.88409	1.987123	-1.38786
22	78	0	-4.23597	0.001836	-0.00168
23	78	0	-2.91058	-1.94525	-1.46331
24	78	0	-1.39133	-3.89764	-0.05804

E	-658.8107449
Sigma	1
Nneg	0
E+ZPE	-658.797364

U	-658.744468
H	-658.743524
G	-658.911379

Cluster Pt_{24} (M=5) (Figure 1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.907958	1.948517	1.460097
2	78	0	-1.382805	0.002126	0.000608
3	78	0	-0.014740	-2.016837	-1.526553
4	78	0	-2.891400	-1.979334	1.384279
5	78	0	0.019247	2.016698	-1.526230
6	78	0	-1.384586	3.895775	0.049443
7	78	0	-2.914049	-1.937738	-1.464601
8	78	0	-2.881339	1.988497	-1.388810
9	78	0	0.009052	-2.020471	1.529140
10	78	0	-0.013434	2.021019	1.528665
11	78	0	-1.443502	0.050188	-2.819301
12	78	0	-4.244358	0.007778	-0.003003
13	78	0	1.382948	-0.002133	0.002226
14	78	0	-1.447440	-0.049142	2.819328
15	78	0	1.439696	0.049413	2.821292
16	78	0	2.904783	-1.947190	1.463712
17	78	0	2.886869	1.978468	1.387379
18	78	0	-1.399950	-3.890797	-0.055358
19	78	0	1.449943	-0.050965	-2.817412
20	78	0	1.384447	-3.895584	0.053078
21	78	0	2.885405	-1.989452	-1.385498
22	78	0	4.244918	-0.007818	0.001774
23	78	0	2.917308	1.937739	-1.461407
24	78	0	1.400946	3.891242	-0.052849

E	-658.8117239
Sigma	1
Nneg	0

E+ZPE	-658.798407
U	-658.745453
H	-658.744508
G	-658.913476

Cluster Pt_{24} (M=7)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.914465	-1.949690	1.472265
2	78	0	1.384178	-0.001945	0.002564
3	78	0	0.029461	2.016442	-1.502785
4	78	0	2.897911	1.994268	1.365721
5	78	0	-0.016498	-2.020925	-1.522078
6	78	0	1.384169	-3.908577	0.054097
7	78	0	2.921836	1.942781	-1.474037
8	78	0	2.894041	-2.001547	-1.368425
9	78	0	-0.012733	2.024620	1.525386
10	78	0	0.022785	-2.021613	1.506265
11	78	0	1.448135	-0.066063	-2.801013
12	78	0	4.229837	-0.005218	-0.001104
13	78	0	-1.387667	0.001849	0.001516
14	78	0	1.444202	0.064369	2.804263
15	78	0	-1.419451	-0.062536	2.862124
16	78	0	-2.913370	1.916467	1.481472
17	78	0	-2.890385	-1.969102	1.396239
18	78	0	1.395417	3.906297	-0.055748
19	78	0	-1.422941	0.063463	-2.860749
20	78	0	-1.412737	3.868243	0.057607
21	78	0	-2.884707	1.978291	-1.398603
22	78	0	-4.263716	0.006243	-0.003507
23	78	0	-2.918841	-1.910795	-1.482336
24	78	0	-1.423393	-3.865323	-0.059133

E	-658.8102782
Sigma	1
Nneg	-14

E+ZPE	-658.797096
U	-658.744966
H	-658.744022
G	--658.910615

Cluster Pt_{24} (M=9)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.930081	-1.921778	1.432716
2	78	0	1.419771	0.000420	0.004785
3	78	0	0.000763	1.977584	-1.498713
4	78	0	2.928339	1.922327	1.434443
5	78	0	0.002351	-1.974999	-1.497828
6	78	0	1.422149	-3.823949	0.010318
7	78	0	2.928042	1.935013	-1.444133
8	78	0	2.930093	-1.932368	-1.445928
9	78	0	-0.002377	1.979277	1.517265
10	78	0	-0.001132	-1.980686	1.518185
11	78	0	1.433514	0.001561	-2.860642
12	78	0	4.327664	0.001340	-0.022207
13	78	0	-1.419552	-0.000212	0.003587
14	78	0	1.430314	-0.001356	2.870202
15	78	0	-1.436411	-0.001509	2.868857
16	78	0	-2.932524	1.921897	1.431760
17	78	0	-2.931191	-1.924957	1.430028
18	78	0	1.418991	3.824873	0.012433
19	78	0	-1.428977	0.000876	-2.861886
20	78	0	-1.421489	3.824640	0.009467
21	78	0	-2.926837	1.932620	-1.446388
22	78	0	-4.326966	-0.001835	-0.025251
23	78	0	-2.925553	-1.933728	-1.448247
24	78	0	-1.419062	-3.825052	0.007179

E	-658.810552
Sigma	1
Nneg	0

E+ZPE	-658.797501
U	-658.744317
H	-658.743373
G	-658.915470

Complex Pt_{24}*H «αδδ» (M=2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.969522	-1.94946	1.537984
2	78	0	1.431075	0.000842	-0.02813
3	78	0	-0.12681	1.977177	-1.54703
4	78	0	2.889887	2.025536	1.415425
5	78	0	-0.0004	-1.99889	-1.55609
6	78	0	1.51942	-3.81296	-0.04117
7	78	0	2.777429	2.054181	-1.42695
8	78	0	2.915075	-1.94127	-1.62785
9	78	0	-0.00736	2.01444	1.490782
10	78	0	0.078169	-1.97851	1.547477
11	78	0	1.347942	0.069331	-2.84296
12	78	0	4.302483	0.138612	-0.06074
13	78	0	-1.35962	-0.04548	0.012831
14	78	0	1.465843	0.065916	2.807637
15	78	0	-1.39904	0.030191	2.881952
16	78	0	-2.90521	1.870516	1.429078
17	78	0	-2.80849	-1.98199	1.500585
18	78	0	1.301917	3.919378	-0.02323
19	78	0	-1.58157	-0.0832	-2.82953
20	78	0	-1.48663	3.838847	-0.01097
21	78	0	-2.99127	1.853731	-1.40122
22	78	0	-4.25016	-0.12591	0.05828
23	78	0	-2.88598	-2.04701	-1.36353
24	78	0	-1.2422	-3.87335	0.078057
25	1	0	3.585215	-1.61235	-0.05471

E	-659.4011419
Sigma	1

Nneg	0
E+ZPE	-659.382486
U	-659.329107
H	-659.328163
G	-659.497397

Complex Pt_{24}*H «γδε» (M=2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.75124	1.927044	1.518212
2	78	0	-1.37759	-0.00032	0.039927
3	78	0	-0.11421	-1.96148	-1.5737
4	78	0	-2.82339	-1.91858	1.524889
5	78	0	-0.13697	2.000666	-1.52643
6	78	0	-1.40292	3.881783	0.066518
7	78	0	-3.01986	-1.94627	-1.31598
8	78	0	-3.01222	1.963491	-1.34529
9	78	0	0.089014	-2.02188	1.47924
10	78	0	0.131917	1.997842	1.52255
11	78	0	-1.67485	0.000363	-2.77544
12	78	0	-4.25819	0.023108	0.158089
13	78	0	1.408563	0.0111	0.011413
14	78	0	-1.25253	-0.00558	2.883313
15	78	0	1.591095	-0.20021	2.971147
16	78	0	3.005909	-1.99147	1.283733
17	78	0	3.066708	1.988394	1.370623
18	78	0	-1.38519	-3.84982	0.030811
19	78	0	1.272828	0.032337	-2.89295
20	78	0	1.379228	-3.85617	-0.13901
21	78	0	2.784882	-1.8758	-1.56444
22	78	0	4.2817	-0.01299	-0.19721
23	78	0	2.755031	1.931412	-1.50204
24	78	0	1.420163	3.864804	-0.05839
25	1	0	1.724346	1.419722	2.372234

E	-659.4056985

Sigma	1
Nneg	0
E+ZPE	-659.386637
U	-659.333404
H	-659.332460
G	-659.501036

Complex Pt_{24}*H «δγ» (M=2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.869144	-1.88318	1.544898
2	78	0	1.398747	0.00136	0.081922
3	78	0	0.106321	1.971916	-1.52452
4	78	0	2.732127	1.960661	1.511145
5	78	0	0.130313	-1.97284	-1.55384
6	78	0	1.434282	-3.82112	0.083905
7	78	0	2.975233	1.959565	-1.3857
8	78	0	3.031314	-1.91061	-1.35137
9	78	0	-0.15838	1.998231	1.488199
10	78	0	-0.07793	-1.98647	1.552634
11	78	0	1.632934	-0.01389	-2.779
12	78	0	4.287906	0.065948	0.089315
13	78	0	-1.38561	-0.02733	-0.04373
14	78	0	1.210319	0.033378	2.997772
15	78	0	-1.66617	-0.0417	2.784711
16	78	0	-3.0345	1.909451	1.356249
17	78	0	-2.96168	-2.01441	1.316678
18	78	0	1.381205	3.867947	0.048586
19	78	0	-1.30096	0.006945	-2.90387
20	78	0	-1.45503	3.858059	-0.07656
21	78	0	-2.80576	1.902692	-1.47642
22	78	0	-4.26441	-0.06496	-0.13489
23	78	0	-2.80161	-1.94375	-1.55168
24	78	0	-1.31138	-3.84457	-0.11174
25	1	0	2.61789	-0.88404	2.909173

E	-659.4065686
Sigma	1
Nneg	0
E+ZPE	-659.386721
U	-659.333485
H	-659.332540
G	-659.500252

Complex Pt_{24}*H «ε» (M=2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.891507	-2.000295	-1.468801
2	78	0	-1.363584	-0.028442	0.015492
3	78	0	0.000007	2.078245	1.594355
4	78	0	-2.890992	2.013017	-1.449002
5	78	0	0.000028	-2.103001	1.568824
6	78	0	-1.368607	-3.927888	-0.009616
7	78	0	-2.8454	1.980606	1.394372
8	78	0	-2.912459	-2.012709	1.405603
9	78	0	-0.000032	2.072314	-1.436308
10	78	0	-0.000008	-2.03778	-1.541596
11	78	0	-1.442634	-0.043454	2.772447
12	78	0	-4.159311	-0.005618	-0.045708
13	78	0	1.363592	-0.028423	0.015475
14	78	0	-1.437692	0.029679	-2.743841
15	78	0	1.437651	0.029692	-2.743837
16	78	0	2.890947	2.013064	-1.449023
17	78	0	2.891512	-2.000276	-1.46882
18	78	0	-1.394194	3.972728	0.017365
19	78	0	1.442699	-0.043448	2.772412
20	78	0	1.394136	3.972752	0.017323
21	78	0	2.845404	1.980666	1.394358
22	78	0	4.15929	-0.005568	-0.045733
23	78	0	2.912509	-2.012707	1.405574
24	78	0	1.368645	-3.927887	-0.00966
25	1	0	0.000028	2.709228	2.991086

E	-659.3971443
Sigma	1
Nneg	0
E+ZPE	-659.377318
U	-659.323721
H	-659.322777
G	-659.490583

Complex Pt_{24}*H «αδ» (M=2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.850948	-2.114444	-1.355342
2	78	0	-1.417463	-0.058028	0.02551
3	78	0	-0.012077	2.013967	1.517921
4	78	0	-2.959877	1.904169	-1.461231
5	78	0	0.121531	-2.00868	1.524671
6	78	0	-1.225523	-3.928328	0.04527
7	78	0	-2.919541	1.878044	1.446562
8	78	0	-2.77659	-2.077463	1.545459
9	78	0	-0.127766	2.008666	-1.523274
10	78	0	0.045572	-2.007921	-1.544948
11	78	0	-1.34341	0.006868	2.853869
12	78	0	-4.293679	-0.105655	0.001439
13	78	0	1.365729	0.04436	-0.016874
14	78	0	-1.543332	-0.099562	-2.779893
15	78	0	1.389693	0.078011	-2.837163
16	78	0	2.769531	2.067763	-1.438518
17	78	0	2.9329	-1.847235	-1.49132
18	78	0	-1.547186	3.850846	0.003663
19	78	0	1.542301	-0.003854	2.810537
20	78	0	1.251146	3.940427	0.034467
21	78	0	2.865319	2.049892	1.407937
22	78	0	4.235052	0.152547	-0.076356
23	78	0	3.020126	-1.879304	1.353777
24	78	0	1.530729	-3.852045	-0.064279
25	1	0	-4.07458	-1.017034	1.413045

E	-659.4012519
Sigma	1
Nneg	0
E+ZPE	-659.381788
U	-659.328252
H	-659.327308
G	-659.496846

Complex Pt_{24}*H «βδδ» (M=2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	3.022965	1.746390	-1.431932
2	78	0	1.357264	-0.083426	0.000127
3	78	0	-0.133363	-2.013753	1.523456
4	78	0	2.733309	-2.146415	-1.425591
5	78	0	0.138662	2.01969	1.522327
6	78	0	1.71393	3.782351	0.000752
7	78	0	2.733073	-2.145852	1.425583
8	78	0	3.022506	1.745724	1.432255
9	78	0	-0.132779	-2.013611	-1.522652
10	78	0	0.139457	2.019878	-1.522003
11	78	0	1.476253	-0.076318	2.835437
12	78	0	4.220245	-0.297873	-0.000335
13	78	0	-1.399302	0.09777	-0.000116
14	78	0	1.477195	-0.076299	-2.834889
15	78	0	-1.435869	0.060977	-2.803524
16	78	0	-3.036244	-1.789745	-1.41362
17	78	0	-2.745953	2.153857	-1.471258
18	78	0	1.086158	-3.967685	0.000595
19	78	0	-1.437333	0.0609	2.803283
20	78	0	-1.677934	-3.834072	-0.000237
21	78	0	-3.036705	-1.789727	1.412673
22	78	0	-4.231923	0.278602	-0.000793
23	78	0	-2.746817	2.153879	1.470425
24	78	0	-1.073014	4.073302	0.000042
25	1	0	-2.634824	3.233568	-0.000421

E	-659.4075389
Sigma	1
Nneg	-9
E+ZPE	-659.388539
U	-659.336322
H	-659.335377
G	-659.500238

Complex Pt_{24}*H «βδε» (M=2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.853544	1.899126	1.441312
2	78	0	-1.366058	-0.035409	0.016721
3	78	0	0.008375	-1.980759	-1.557677
4	78	0	-2.866784	-2.002803	1.41889
5	78	0	-0.063029	2.021178	-1.440589
6	78	0	-1.461402	3.886781	0.048232
7	78	0	-2.893544	-1.979879	-1.438031
8	78	0	-2.94433	1.93395	-1.415641
9	78	0	0.036358	-2.077649	1.522223
10	78	0	-0.009951	2.004214	1.589522
11	78	0	-1.508364	0.006979	-2.81312
12	78	0	-4.235382	-0.048577	0.010412
13	78	0	1.391728	0.007243	0.029298
14	78	0	-1.423068	-0.054353	2.854538
15	78	0	1.469374	-0.096483	2.823315
16	78	0	2.952659	-1.988348	1.362336
17	78	0	2.888962	1.963685	1.47576
18	78	0	-1.337796	-3.893665	-0.022019
19	78	0	1.439063	0.083501	-2.778191
20	78	0	1.436264	-3.904116	-0.090128
21	78	0	2.90075	-1.932015	-1.492443
22	78	0	4.228638	0.018911	-0.074038
23	78	0	2.847891	2.045857	-1.376162
24	78	0	1.344548	4.083007	-0.111084
25	1	0	1.454216	3.090606	1.292095

E	-659.409302
Sigma	1
Nneg	0
E+ZPE	-659.390092
U	-659.336947
H	-659.336003
G	-659.503755

Complex Pt_{24}*H «ββ» (M=2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.905197	-2.008107	1.429568
2	78	0	1.356424	-0.034729	0.000775
3	78	0	-0.000027	2.067121	-1.488781
4	78	0	2.832213	1.991179	1.428157
5	78	0	0.000065	-2.087568	-1.549224
6	78	0	1.382779	-3.932566	-0.000111
7	78	0	2.832641	1.991506	-1.428154
8	78	0	2.905708	-2.008368	-1.429884
9	78	0	-0.000102	2.068137	1.489613
10	78	0	-0.000017	-2.088009	1.549217
11	78	0	1.443702	-0.022301	-2.767573
12	78	0	4.163543	0.009728	-0.001045
13	78	0	-1.356352	-0.034858	0.000751
14	78	0	1.443091	-0.022409	2.768734
15	78	0	-1.443224	-0.022378	2.768757
16	78	0	-2.832369	1.991098	1.428074
17	78	0	-2.905142	-2.008133	1.429525
18	78	0	1.435763	4.025024	-0.000572
19	78	0	-1.443494	-0.022354	-2.76761
20	78	0	-1.435968	4.02512	-0.000611
21	78	0	-2.832533	1.991365	-1.428144
22	78	0	-4.163548	0.009575	-0.001211
23	78	0	-2.905628	-2.008475	-1.429981
24	78	0	-1.382719	-3.932627	-0.000243
25	1	0	-0.000077	4.916199	-0.002075

E	-659.4107387
Sigma	1
Nneg	0
E+ZPE	-659.390368
U	-659.337279
H	-659.336335
G	-659.502943

Complex Pt_{24}*H «ββε» (M=2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.840387	1.994226	1.404550
2	78	0	-1.355535	-0.033358	0.004442
3	78	0	-0.001177	-2.083458	-1.551414
4	78	0	-2.908168	-2.015483	1.414774
5	78	0	0.001052	2.083676	-1.45563
6	78	0	-1.485796	4.065555	0.000023
7	78	0	-2.896727	-2.010335	-1.443288
8	78	0	-2.836541	1.997838	-1.428833
9	78	0	-0.000881	-2.099208	1.552953
10	78	0	0.001119	2.040114	1.554912
11	78	0	-1.441924	-0.007739	-2.756631
12	78	0	-4.159599	0.001804	-0.019951
13	78	0	1.355218	-0.034968	0.004416
14	78	0	-1.455202	-0.03671	2.771824
15	78	0	1.455723	-0.037792	2.772071
16	78	0	2.906314	-2.018256	1.414631
17	78	0	2.842461	1.991433	1.404091
18	78	0	-1.381295	-3.939519	-0.002007
19	78	0	1.441596	-0.009082	-2.757044
20	78	0	1.377079	-3.940664	-0.002115
21	78	0	2.894475	-2.012945	-1.44338
22	78	0	4.159652	-0.002319	-0.020022
23	78	0	2.838366	1.99462	-1.42899
24	78	0	1.490144	4.064135	-0.000533
25	1	0	0.00243	3.778162	0.86975

E	-659.4084613
Sigma	1
Nneg	0
E+ZPE	-659.389557
U	-659.336371
H	-659.335427
G	-659.503175

Complex Pt_{24}*H «γγε» (M=2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.846858	1.928351	1.509718
2	78	0	-1.389989	-0.009478	0.071527
3	78	0	-0.072633	-1.994356	-1.499221
4	78	0	-2.824923	-2.036094	1.405273
5	78	0	-0.090757	2.002612	-1.52479
6	78	0	-1.41922	3.894647	0.082543
7	78	0	-2.973087	-1.980444	-1.413385
8	78	0	-2.972524	1.978083	-1.36544
9	78	0	0.12033	-1.9973	1.555775
10	78	0	0.055569	2.024834	1.526873
11	78	0	-1.58688	0.023634	-2.742589
12	78	0	-4.226708	-0.012624	0.063045
13	78	0	1.375586	0.013423	0.017678
14	78	0	-1.392825	-0.079035	2.893149
15	78	0	1.68592	0.011324	2.843684
16	78	0	3.01416	-1.965936	1.30724
17	78	0	2.949379	2.002242	1.332178
18	78	0	-1.356089	-3.896551	0.004274
19	78	0	1.328241	-0.011184	-2.843467
20	78	0	1.413201	-3.873949	-0.024688
21	78	0	2.826643	-1.924053	-1.494398
22	78	0	4.237604	0.054295	-0.150281
23	78	0	2.802153	1.948193	-1.525885
24	78	0	1.342065	3.888762	-0.067494
25	1	0	0.12821	0.827202	3.017007

E	-659.4115946
Sigma	1
Nneg	0
E+ZPE	-659.392438
U	-659.339352
H	-659.338408
G	-659.505962

Complex Pt_{24}*H «γδε» (M=4) (Figure 8j)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.878769	1.916470	1.411101
2	78	0	-1.396027	-0.011194	0.021274
3	78	0	0.016163	-1.945067	-1.522022
4	78	0	-2.901824	-1.964582	1.410285
5	78	0	-0.034089	1.980378	-1.469817
6	78	0	-1.429354	3.863064	0.007638
7	78	0	-2.910734	-1.974181	-1.447929
8	78	0	-2.956833	1.948980	-1.466063
9	78	0	-0.002963	-2.031164	1.511598
10	78	0	0.002322	2.000319	1.597733
11	78	0	-1.490217	0.004934	-2.806119
12	78	0	-4.265480	-0.014387	-0.050850
13	78	0	1.402191	0.023890	0.069232
14	78	0	-1.433151	-0.002233	2.839438
15	78	0	1.407766	-0.204240	3.064994
16	78	0	2.917857	-1.903152	1.365155
17	78	0	2.940005	1.955389	1.439948
18	78	0	-1.354977	-3.862539	-0.020864
19	78	0	1.444212	0.048608	-2.825762
20	78	0	1.447165	-3.823501	-0.053682
21	78	0	2.916851	-1.878762	-1.525554
22	78	0	4.292742	0.031861	-0.146544
23	78	0	2.870897	1.980079	-1.473971
24	78	0	1.375893	3.842937	0.039279
25	1	0	1.587725	1.411150	2.457190

E	-659.408179
Sigma	1
Nneg	0
E+ZPE	-659.389146
U	-659.335916
H	-659.334971
G	-659.504545

Complex Pt_{24}*H «ε» (M=4) (Figure 8a)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.897736	-1.974223	-1.487961
2	78	0	-1.376144	-0.023996	0.014504
3	78	0	-0.000308	2.042113	1.612475
4	78	0	-2.896014	1.984645	-1.454810
5	78	0	-0.001816	-2.064822	1.597491
6	78	0	-1.378888	-3.896837	0.006217
7	78	0	-2.855630	1.946590	1.392080
8	78	0	-2.923145	-1.984196	1.364903
9	78	0	0.002553	2.051140	-1.434957
10	78	0	-0.000009	-2.016572	-1.494468
11	78	0	-1.458877	-0.050231	2.812812
12	78	0	-4.212515	0.005580	-0.061155
13	78	0	1.375759	-0.025039	0.015209
14	78	0	-1.396150	0.042863	-2.790457
15	78	0	1.399247	0.041213	-2.790107
16	78	0	2.899345	1.982341	-1.453050
17	78	0	2.897047	-1.976643	-1.486684
18	78	0	-1.397731	3.936085	0.036725
19	78	0	1.454545	-0.050801	2.814357
20	78	0	1.401938	3.934417	0.039737
21	78	0	2.856182	1.942870	1.393846
22	78	0	4.213122	0.001555	-0.059503
23	78	0	2.919073	-1.985448	1.366859
24	78	0	1.376183	-3.897588	0.007701
25	1	0	-0.002435	2.728988	2.982304

E	-659.3969718
Sigma	1
Nneg	0
E+ZPE	-659.377240
U	-659.323572
H	-659.322627
G	-659.491490

Complex Pt_{24}*H «εεωω» (M=4) (Figure 8k)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.891331	1.921464	1.417790
2	78	0	-1.381056	-0.052062	-0.000032
3	78	0	0.030076	-2.031919	-1.540559
4	78	0	-2.873768	-2.032938	1.418814
5	78	0	-0.035934	2.093009	-1.654482
6	78	0	-1.457450	3.920273	-0.001422
7	78	0	-2.873795	-2.032628	-1.419140
8	78	0	-2.893277	1.921007	-1.419218
9	78	0	0.030273	-2.033792	1.542061
10	78	0	-0.036352	2.098074	1.659716
11	78	0	-1.468237	-0.042126	-2.816011
12	78	0	-4.223726	-0.067354	0.000389
13	78	0	1.386129	-0.007140	0.000392
14	78	0	-1.467356	-0.042665	2.814950
15	78	0	1.457703	-0.008861	2.816116
16	78	0	2.948357	-1.930972	1.424078
17	78	0	2.816934	2.014023	1.423922
18	78	0	-1.291819	-3.936889	-0.000330
19	78	0	1.458842	-0.008831	-2.816024
20	78	0	1.453900	-3.882678	-0.000330
21	78	0	2.948536	-1.930964	-1.424482
22	78	0	4.223761	0.079569	0.000089
23	78	0	2.819323	2.014227	-1.424979
24	78	0	1.320654	3.960933	-0.001366

25	1	0	-0.030089	1.500622	0.004645

E	-659.4052805
Sigma	1
Nneg	0
E+ZPE	-659.387336
U	-659.333751
H	-659.332807
G	-659.502646

Complex Pt_{24}*H «αδ» (M=4) (Figure 8b)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.864639	-2.023677	-1.397745
2	78	0	-1.417245	-0.037894	0.026459
3	78	0	-0.003251	1.985813	1.539741
4	78	0	-2.897004	1.916755	-1.485495
5	78	0	0.057342	-2.012378	1.542159
6	78	0	-1.327737	-3.877357	0.029285
7	78	0	-2.890315	1.921132	1.420617
8	78	0	-2.856808	-2.010161	1.530053
9	78	0	-0.061686	1.998844	-1.519890
10	78	0	0.040434	-1.983462	-1.547168
11	78	0	-1.377106	0.005543	2.866085
12	78	0	-4.304140	-0.026652	-0.048796
13	78	0	1.367832	0.014985	-0.002314
14	78	0	-1.477868	-0.058781	-2.810418
15	78	0	1.436100	0.080015	-2.846936
16	78	0	2.828825	2.011941	-1.411383
17	78	0	2.927020	-1.870542	-1.494354
18	78	0	-1.464438	3.871108	-0.001659
19	78	0	1.498977	-0.055055	2.843357
20	78	0	1.310853	3.882972	0.059613
21	78	0	2.875881	1.959763	1.451530
22	78	0	4.253608	0.079552	-0.040721
23	78	0	2.956105	-1.921683	1.358553

24	78	0	1.441877	-3.839280	-0.078532
25	1	0	-4.104106	-0.897047	1.400848

E	-659.403982
Sigma	1
Nneg	0
E+ZPE	-659.384520
U	-659.331019
H	-659.330075
G	-659.500057

Complex Pt_{24}*H «βδδ» (M=4) (Figure 8h)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.958438	1.855218	-1.4254
2	78	0	1.351855	-0.02946	0.001704
3	78	0	-0.06259	-2.03069	1.531144
4	78	0	2.822798	-2.03469	-1.42496
5	78	0	0.066365	2.031934	1.541442
6	78	0	1.530013	3.823535	0.014638
7	78	0	2.817285	-2.04222	1.416904
8	78	0	2.951632	1.842794	1.447078
9	78	0	-0.05054	-2.02192	-1.53528
10	78	0	0.070821	2.035433	-1.54092
11	78	0	1.443602	-0.04611	2.83727
12	78	0	4.227245	-0.13411	0.002275
13	78	0	-1.39368	0.053355	-0.00113
14	78	0	1.463956	-0.0221	-2.8325
15	78	0	-1.3796	0.017849	-2.82248
16	78	0	-2.95312	-1.87147	-1.42707
17	78	0	-2.83492	2.026067	-1.49315
18	78	0	1.231742	-3.92077	-0.00671
19	78	0	-1.38755	0.019691	2.81965
20	78	0	-1.52998	-3.85713	0.000452
21	78	0	-2.96716	-1.86945	1.425556
22	78	0	-4.24799	0.112347	-0.00519

23	78	0	-2.83588	2.028035	1.481902
24	78	0	-1.25692	3.994672	-0.00515
25	1	0	-2.79434	3.057157	-0.00683

E	-659.4089005
Sigma	1
Nneg	0
E+ZPE	-659.389653
U	-659.336557
H	-659.335613
G	-659.505060

Complex Pt_{24}*H «βδε» (M=4) (Figure 8g)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.868995	1.864302	1.442690
2	78	0	-1.363400	-0.047652	0.019822
3	78	0	0.015264	-1.979014	-1.554781
4	78	0	-2.832733	-2.028677	1.421384
5	78	0	-0.090326	2.022293	-1.438873
6	78	0	-1.508290	3.866880	0.057978
7	78	0	-2.871510	-2.008306	-1.435059
8	78	0	-2.972270	1.902317	-1.411030
9	78	0	0.062375	-2.078247	1.522591
10	78	0	-0.023382	1.999675	1.591896
11	78	0	-1.522197	0.000711	-2.814276
12	78	0	-4.235263	-0.096826	0.016263
13	78	0	1.395725	0.020046	0.027547
14	78	0	-1.415047	-0.067360	2.863722
15	78	0	1.479390	-0.085599	2.815736
16	78	0	2.983762	-1.952361	1.364276
17	78	0	2.874661	1.994913	1.462288
18	78	0	-1.289966	-3.912625	-0.015944
19	78	0	1.421612	0.091583	-2.778218
20	78	0	1.491641	-3.881716	-0.090926
21	78	0	2.912586	-1.901663	-1.505142

22	78	0	4.225959	0.061619	-0.091754
23	78	0	2.814605	2.077675	-1.382968
24	78	0	1.297527	4.098202	-0.103895
25	1	0	1.425156	3.106580	1.300391

E	-659.4102437
Sigma	1
Nneg	0
E+ZPE	-659.391025
U	-659.337891
H	-659.336947
G	-659.505319

Complex Pt_{24}*H «ββ» (M=4) (Figure 8c)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.879539	-2.001682	-1.403636
2	78	0	-1.362342	-0.028355	-0.002068
3	78	0	-0.008701	2.051713	1.488765
4	78	0	-2.842331	1.975275	-1.435408
5	78	0	0.002161	-2.079345	1.490768
6	78	0	-1.389676	-3.931894	-0.004198
7	78	0	-2.850912	1.956132	1.433913
8	78	0	-2.907361	-1.996379	1.437022
9	78	0	-0.002560	2.054181	-1.503022
10	78	0	0.009712	-2.063866	-1.579662
11	78	0	-1.423187	-0.024782	2.796729
12	78	0	-4.186908	0.004853	-0.010683
13	78	0	1.361762	-0.020576	-0.000979
14	78	0	-1.452466	-0.017427	-2.788462
15	78	0	1.462745	-0.008400	-2.787496
16	78	0	2.837692	1.989776	-1.428803
17	78	0	2.896930	-1.985007	-1.399021
18	78	0	-1.447166	3.995511	0.006510
19	78	0	1.410069	-0.020134	2.799766
20	78	0	1.426098	4.000833	0.011330

21	78	0	2.835002	1.967059	1.441366
22	78	0	4.188003	0.026804	-0.000393
23	78	0	2.910641	-1.980778	1.440705
24	78	0	1.412490	-3.926191	-0.003094
25	1	0	-0.012174	4.888983	0.003832

E	-659.4099347
Sigma	1
Nneg	0
E+ZPE	-659.389645
U	-659.336500
H	-659.335556
G	-659.503317

Complex Pt_{24}*H «γγε» (M=4) (Figure 8i)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.810427	1.962928	1.486727
2	78	0	-1.400447	0.010884	0.086668
3	78	0	-0.107105	-1.970273	-1.499197
4	78	0	-2.856059	-1.943083	1.436854
5	78	0	-0.072258	1.961872	-1.504466
6	78	0	-1.361621	3.880069	0.069688
7	78	0	-3.015626	-1.932977	-1.409409
8	78	0	-2.964846	2.000740	-1.390545
9	78	0	0.083670	-1.973898	1.572088
10	78	0	0.106852	2.015911	1.530402
11	78	0	-1.603897	0.017415	-2.755777
12	78	0	-4.264527	0.049497	0.038815
13	78	0	1.391925	-0.011839	0.014915
14	78	0	-1.384697	-0.018026	2.933987
15	78	0	1.704525	-0.012516	2.841220
16	78	0	2.982805	-2.012562	1.300266
17	78	0	3.014762	1.938868	1.325190
18	78	0	-1.442287	-3.849997	0.043187
19	78	0	1.351073	-0.014545	-2.848854

20	78	0	1.323111	-3.865514	-0.030118
21	78	0	2.802829	-1.967623	-1.516571
22	78	0	4.256194	-0.032114	-0.175589
23	78	0	2.843919	1.907102	-1.523494
24	78	0	1.420116	3.849062	-0.065004
25	1	0	0.157427	0.828496	3.043372

E	-659.4139189
Sigma	1
Nneg	0
E+ZPE	-659.394836
U	-659.341739
H	-659.340795
G	-659.508895

Complex Pt_{24}*H «δγ» (M=5) (Figure 8d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.870585	-1.907120	1.518273
2	78	0	1.403624	-0.001498	0.081014
3	78	0	0.096540	1.968857	-1.524949
4	78	0	2.776627	1.929795	1.510728
5	78	0	0.105572	-1.967182	-1.539515
6	78	0	1.415117	-3.827755	0.071019
7	78	0	2.98035	1.95382	-1.398826
8	78	0	3.000892	-1.929707	-1.38255
9	78	0	-0.121756	1.988236	1.497611
10	78	0	-0.077613	-1.976183	1.544085
11	78	0	1.614233	-0.002884	-2.779653
12	78	0	4.289193	0.04058	0.047424
13	78	0	-1.395242	-0.013442	-0.046232
14	78	0	1.243889	0.019549	3.005851
15	78	0	-1.640188	-0.02472	2.774709
16	78	0	-3.004454	1.942213	1.365441
17	78	0	-2.971399	-1.992632	1.337982
18	78	0	1.398086	3.846035	0.070337

19	78	0	-1.331356	0.001864	-2.886375
20	78	0	-1.415318	3.854966	-0.08355
21	78	0	-2.824129	1.919737	-1.492322
22	78	0	-4.265859	-0.029283	-0.106835
23	78	0	-2.831817	-1.940505	-1.52308
24	78	0	-1.349478	-3.84128	-0.097478
25	1	0	2.6441	-0.893965	2.877628

E	-659.4092411
Sigma	1
Nneg	0
E+ZPE	-659.389428
U	-659.336162
H	-659.335218
G	-659.504066

Complex Pt_{24}*H «ββεε» (M=4) (Figure 8l)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.943903	1.877410	1.424258
2	78	0	-1.366371	-0.044907	0.000668
3	78	0	0.074725	-2.029745	-1.527958
4	78	0	-2.836199	-2.088908	1.404220
5	78	0	-0.042545	2.050958	-1.657145
6	78	0	-1.586776	3.939535	-0.004088
7	78	0	-2.827106	-2.082797	-1.424715
8	78	0	-2.938179	1.878332	-1.434062
9	78	0	0.062769	-2.040103	1.536092
10	78	0	-0.059158	2.054564	1.672168
11	78	0	-1.450944	-0.066839	-2.805098
12	78	0	-4.203148	-0.139844	-0.008977
13	78	0	1.353082	0.067108	0.004683
14	78	0	-1.469735	-0.078125	2.801429
15	78	0	1.452967	-0.005298	2.838323
16	78	0	2.965130	-1.859348	1.416437
17	78	0	2.785470	2.051131	1.447380

18	78	0	-1.219804	-3.965775	-0.011074
19	78	0	1.474417	-0.000353	-2.831714
20	78	0	1.530655	-3.851885	0.004742
21	78	0	2.974427	-1.859682	-1.411271
22	78	0	4.210813	0.165213	0.004455
23	78	0	2.804820	2.054049	-1.444329
24	78	0	1.262726	3.944859	0.005499
25	1	0	-0.634456	2.375040	0.005969

E	-659.4007959
Sigma	1
Nneg	0
E+ZPE	-659.382222
U	-659.328789
H	-659.327845
G	-659.498429

Complex Pt_{24}*H «ααδδ» (M=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.844427	-2.029992	1.570605
2	78	0	1.424954	-0.067265	0.01915
3	78	0	0.035724	1.964342	-1.486744
4	78	0	2.928447	1.854871	1.399821
5	78	0	-0.079346	-1.95392	-1.506688
6	78	0	1.299906	-3.840431	0.029861
7	78	0	2.965804	1.826578	-1.503652
8	78	0	2.823974	-2.073567	-1.558552
9	78	0	0.035233	2.014587	1.53588
10	78	0	-0.042088	-2.013545	1.555707
11	78	0	1.401176	-0.011425	-2.876506
12	78	0	4.375875	-0.058792	-0.028999
13	78	0	-1.387989	0.029171	0.031371
14	78	0	1.396597	0.067619	2.897492
15	78	0	-1.450846	-0.042782	2.860721
16	78	0	-2.835354	2.015867	1.445341

17	78	0	-2.944302	-1.899433	1.381084
18	78	0	1.550855	3.801833	-0.062217
19	78	0	-1.51165	0.058439	-2.808483
20	78	0	-1.260616	3.912708	0.041486
21	78	0	-2.860114	2.056479	-1.401762
22	78	0	-4.255056	0.118373	-0.010097
23	78	0	-3.004454	-1.866304	-1.466743
24	78	0	-1.496583	-3.841435	-0.057987
25	1	0	3.543176	-1.7142	-0.006989

E	-659.4033776
Sigma	1
Nneg	0
E+ZPE	-659.384595
U	-659.331190
H	-659.330246
G	-659.501428

Complex Pt_{24}*H «γδε» (M=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.754923	1.959303	1.535831
2	78	0	-1.39386	0.013481	0.057775
3	78	0	-0.136808	-1.961234	-1.529487
4	78	0	-2.806993	-1.965686	1.478997
5	78	0	-0.119093	2.018153	-1.502099
6	78	0	-1.378217	3.893126	0.090087
7	78	0	-3.049923	-1.93595	-1.351737
8	78	0	-3.044845	2.013997	-1.31501
9	78	0	0.107935	-2.031467	1.484441
10	78	0	0.142225	1.991288	1.573464
11	78	0	-1.638197	0.062789	-2.732826
12	78	0	-4.24312	0.034074	0.181585
13	78	0	1.398104	0.016575	0.015775
14	78	0	-1.248207	-0.046502	2.847227
15	78	0	1.609357	-0.181975	3.015697

16	78	0	2.995756	-1.967332	1.300911
17	78	0	3.065177	1.974904	1.346736
18	78	0	-1.422266	-3.884663	-0.023007
19	78	0	1.207925	0.039563	-2.935335
20	78	0	1.380703	-3.834597	-0.149546
21	78	0	2.762127	-1.85837	-1.565637
22	78	0	4.306821	-0.030899	-0.196281
23	78	0	2.810246	1.859472	-1.563832
24	78	0	1.427467	3.803776	-0.094627
25	1	0	1.763482	1.417678	2.410196

E	-659.4080801
Sigma	1
Nneg	0
E+ZPE	-659.389253
U	-659.335921
H	-659.334977
G	-659.504785

Complex Pt_{24}*H «δγ» (M=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.956161	-1.842651	1.524921
2	78	0	1.399433	0.026222	0.045836
3	78	0	0.019244	2.008646	-1.54977
4	78	0	2.745011	2.018619	1.506633
5	78	0	0.116781	-2.026123	-1.546888
6	78	0	1.529905	-3.791435	0.059584
7	78	0	2.886004	1.980587	-1.428189
8	78	0	3.023343	-1.831437	-1.378154
9	78	0	-0.143178	2.000705	1.467422
10	78	0	0.012026	-1.975572	1.524072
11	78	0	1.51003	-0.010767	-2.843071
12	78	0	4.287989	0.174391	0.06464
13	78	0	-1.38165	-0.049659	-0.049817
14	78	0	1.290657	0.068118	2.979425

15	78	0	-1.575997	-0.054017	2.767285
16	78	0	-3.043917	1.866754	1.411006
17	78	0	-2.888407	-2.069764	1.37153
18	78	0	1.279911	3.876697	0.009501
19	78	0	-1.317689	-0.002829	-2.8753
20	78	0	-1.546075	3.844773	-0.047254
21	78	0	-2.897199	1.848383	-1.440902
22	78	0	-4.250587	-0.138732	-0.047731
23	78	0	-2.798075	-2.017625	-1.490937
24	78	0	-1.248194	-3.892246	-0.070856
25	1	0	2.68876	-0.861054	2.887148

E	-659.4085478
Sigma	1
Nneg	0
E+ZPE	-659.388877
U	-659.335446
H	-659.334502
G	-659.505121

Complex Pt_{24}*H «ε» (M=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.988626	-1.935720	-1.460117
2	78	0	-1.386913	0.002525	0.048609
3	78	0	0.065562	2.054967	1.622145
4	78	0	-2.924127	2.025666	-1.440836
5	78	0	0.014985	-2.044103	1.597524
6	78	0	-1.480488	-3.897119	0.010373
7	78	0	-2.79148	1.991247	1.411239
8	78	0	-2.889295	-1.936744	1.397708
9	78	0	-0.013132	2.015612	-1.401576
10	78	0	-0.08209	-2.009547	-1.452525
11	78	0	-1.367715	-0.032353	2.847867
12	78	0	-4.223327	0.06283	-0.015997
13	78	0	1.405156	-0.045128	0.014267

14	78	0	-1.463777	0.047275	-2.760391
15	78	0	1.326221	0.000248	-2.815365
16	78	0	2.895493	1.935651	-1.540182
17	78	0	2.832407	-2.029129	-1.541482
18	78	0	-1.366266	3.949358	0.043567
19	78	0	1.543891	-0.006125	2.82891
20	78	0	1.470821	3.879194	0.004916
21	78	0	2.941996	1.90069	1.339572
22	78	0	4.237573	-0.06377	-0.165073
23	78	0	2.917285	-2.022484	1.344829
24	78	0	1.324511	-3.878584	0.043893
25	1	0	0.104195	2.772312	2.973581

E	-659.3956582
Sigma	1
Nneg	0
E+ZPE	-659.376010
U	-659.322254
H	-659.321310
G	-659.491013

Complex Pt_{24}*H «αδ» (M=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.922454	-2.004185	-1.357656
2	78	0	-1.427599	-0.005543	0.005234
3	78	0	0.043466	2.013887	1.506296
4	78	0	-2.842109	2.021434	-1.473019
5	78	0	0.00772	-2.010097	1.509057
6	78	0	-1.411372	-3.8843	0.051487
7	78	0	-2.853427	2.034339	1.393435
8	78	0	-2.900596	-1.973155	1.549732
9	78	0	-0.014804	2.03094	-1.520883
10	78	0	-0.004715	-2.031009	-1.528514
11	78	0	-1.396027	0.06182	2.83595
12	78	0	-4.29885	0.070872	-0.016783

13	78	0	1.365189	-0.008388	-0.013587
14	78	0	-1.473562	-0.078902	-2.811804
15	78	0	1.392769	0.043389	-2.832914
16	78	0	2.86489	1.958091	-1.399804
17	78	0	2.87214	-1.960735	-1.479506
18	78	0	-1.338565	3.934678	-0.035353
19	78	0	1.48126	-0.061105	2.810252
20	78	0	1.453772	3.89343	0.063774
21	78	0	2.940397	1.918237	1.454733
22	78	0	4.241641	-0.025696	-0.027403
23	78	0	2.899737	-2.005446	1.364243
24	78	0	1.374463	-3.921431	-0.064617
25	1	0	-4.162381	-0.86782	1.376914

E	-659.4041699
Sigma	1
Nneg	0
E+ZPE	-659.384486
U	-659.330996
H	-659.330052
G	-659.500973

Complex Pt_{24}*H «βδδ» (M=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.984306	1.827017	1.426023
2	78	0	-1.354917	-0.039353	-0.000116
3	78	0	0.074579	-2.034979	-1.515198
4	78	0	-2.794294	-2.076578	1.424209
5	78	0	-0.08422	2.039877	-1.527251
6	78	0	-1.604664	3.818526	-0.0073
7	78	0	-2.79367	-2.082689	-1.416301
8	78	0	-2.98587	1.81953	-1.440088
9	78	0	0.070126	-2.032027	1.519224
10	78	0	-0.082273	2.041174	1.530874
11	78	0	-1.437821	-0.044478	-2.821305

12	78	0	-4.222123	-0.189188	-0.000215
13	78	0	1.398307	0.067784	0.00074
14	78	0	-1.443953	-0.028812	2.821536
15	78	0	1.381236	0.013116	2.842275
16	78	0	2.981795	-1.830411	1.433067
17	78	0	2.811443	2.057563	1.494141
18	78	0	-1.196023	-3.963684	0.00638
19	78	0	1.378376	0.020165	-2.841375
20	78	0	1.588689	-3.819411	-0.004361
21	78	0	2.988904	-1.825112	-1.44093
22	78	0	4.265228	0.160726	0.001503
23	78	0	2.810885	2.059568	-1.489425
24	78	0	1.199297	4.002358	0.003843
25	1	0	2.750992	3.066776	0.003932

E	-659.4079957
Sigma	1
Nneg	-24
E+ZPE	-659.389042
U	-659.336671
H	-659.335727
G	-659.503384

Complex Pt_{24}*H «βδε» (M=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.820933	2.018989	1.391879
2	78	0	-1.378891	0.013642	0.011571
3	78	0	-0.006665	-2.006406	-1.499546
4	78	0	-2.964053	-1.910457	1.408561
5	78	0	0.046596	2.03412	-1.427746
6	78	0	-1.346002	3.909357	-0.014519
7	78	0	-2.919268	-1.908418	-1.467272
8	78	0	-2.852133	1.985753	-1.500652
9	78	0	-0.07634	-2.081201	1.532456
10	78	0	0.035896	2.030945	1.596413

11	78	0	-1.377585	0.014458	-2.852295
12	78	0	-4.241976	0.089086	-0.04153
13	78	0	1.384237	-0.031417	0.046148
14	78	0	-1.483625	0.032207	2.852943
15	78	0	1.386467	-0.144919	2.819869
16	78	0	2.828537	-2.096495	1.364255
17	78	0	2.92646	1.874617	1.522189
18	78	0	-1.487594	-3.853192	0.00178
19	78	0	1.463529	0.05931	-2.750777
20	78	0	1.31956	-3.959887	-0.101468
21	78	0	2.887553	-2.017073	-1.488188
22	78	0	4.213665	-0.114326	-0.006308
23	78	0	2.949687	1.963883	-1.329556
24	78	0	1.493204	4.058158	-0.085106
25	1	0	1.53477	3.06267	1.318108

E	-659.4094717
Sigma	1
Nneg	0
E+ZPE	-659.390287
U	-659.337064
H	-659.336120
G	-659.505453

Complex Pt_{24}*H «ββ» (M=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.910690	-1.854760	1.466830
2	78	0	1.37609	0.04256	0.023926
3	78	0	-0.037495	2.065051	-1.476069
4	78	0	2.647272	2.056383	1.55061
5	78	0	0.207975	-2.070367	-1.499795
6	78	0	1.62138	-3.843105	0.020495
7	78	0	2.799786	2.152589	-1.34666
8	78	0	3.09924	-1.836053	-1.387798
9	78	0	-0.204548	2.049682	1.493247

10	78	0	0.004182	-2.075141	1.51149
11	78	0	1.582372	0.087731	-2.772534
12	78	0	4.19886	0.23742	0.107535
13	78	0	-1.356935	-0.098832	-0.024693
14	78	0	1.260472	0.002056	2.859871
15	78	0	-1.58166	-0.067168	2.75544
16	78	0	-3.009748	1.845001	1.320976
17	78	0	-2.895003	-2.126159	1.349321
18	78	0	1.219618	4.046426	0.096821
19	78	0	-1.246001	-0.10317	-2.824249
20	78	0	-1.661437	3.959405	-0.067075
21	78	0	-2.839011	1.804372	-1.534569
22	78	0	-4.188958	-0.186824	-0.155926
23	78	0	-2.694698	-2.140809	-1.475307
24	78	0	-1.209222	-4.008866	0.007902
25	1	0	-0.25132	4.881115	0.016493

E	-659.407920
Sigma	1
Nneg	0
E+ZPE	-659.388113
U	-659.334656
H	-659.333712
G	-659.503543

Complex Pt_{24}*H «ββε» (M=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.748799	2.079920	1.381136
2	78	0	-1.377231	0.051313	0.028113
3	78	0	-0.066364	-2.00774	-1.481489
4	78	0	-3.005709	-1.836489	1.412991
5	78	0	0.106547	2.037159	-1.420869
6	78	0	-1.308971	4.008734	-0.051261
7	78	0	-2.967746	-1.846829	-1.454975
8	78	0	-2.796504	2.037199	-1.516359

9	78	0	-0.127384	-2.100459	1.54895
10	78	0	0.105351	2.02963	1.607863
11	78	0	-1.397413	0.037103	-2.840076
12	78	0	-4.239769	0.189476	-0.051701
13	78	0	1.374579	-0.075866	0.032656
14	78	0	-1.46242	0.064356	2.863461
15	78	0	1.390283	-0.164655	2.805728
16	78	0	2.777832	-2.156681	1.358901
17	78	0	2.929149	1.839195	1.447505
18	78	0	-1.587813	-3.824472	0.010602
19	78	0	1.454111	0.00386	-2.760639
20	78	0	1.226112	-3.989695	-0.091948
21	78	0	2.84307	-2.079558	-1.481075
22	78	0	4.201205	-0.181281	0.016764
23	78	0	2.99466	1.865844	-1.392013
24	78	0	1.680744	3.972465	0.016344
25	1	0	0.193418	3.702834	0.888582

E	-659.4073054
Sigma	1
Nneg	0
E+ZPE	-659.388726
U	-659.335381
H	-659.334437
G	-659.504395

Complex Pt_{24}*H «γγε» (M=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.760342	1.993771	1.492894
2	78	0	-1.408207	0.034543	0.076849
3	78	0	-0.13593	-1.966985	-1.48933
4	78	0	-2.928807	-1.848209	1.457044
5	78	0	-0.019475	1.962194	-1.489571
6	78	0	-1.294819	3.875311	0.051602
7	78	0	-3.054226	-1.87961	-1.405189

8	78	0	-2.905962	2.01347	-1.431654
9	78	0	0.023741	-1.96626	1.568501
10	78	0	0.151964	2.005057	1.523116
11	78	0	-1.568996	0.015241	-2.819914
12	78	0	-4.298138	0.153298	-0.000719
13	78	0	1.396782	-0.041989	0.016584
14	78	0	-1.385942	0.020456	2.973803
15	78	0	1.690612	-0.080044	2.842603
16	78	0	2.946075	-2.075577	1.279094
17	78	0	3.054631	1.864785	1.351268
18	78	0	-1.53095	-3.785955	0.092674
19	78	0	1.346738	-0.019229	-2.84128
20	78	0	1.24338	-3.87486	-0.046727
21	78	0	2.782358	-2.010126	-1.535612
22	78	0	4.258347	-0.105834	-0.179712
23	78	0	2.881528	1.869541	-1.501244
24	78	0	1.513414	3.836402	-0.023979
25	1	0	0.173445	0.82755	3.03424

E	-659.4111992
Sigma	1
Nneg	0
E+ZPE	-659.392259
U	-659.338976
H	-659.338032
G	-659.508931

Complex Pt_{24}*H «αδδ» (M=5) (Figure 8e)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.899390	-1.999782	1.597499
2	78	0	1.415095	-0.046619	0.004890
3	78	0	0.001055	2.009125	-1.506384
4	78	0	2.870333	1.947778	1.399402
5	78	0	-0.033155	-1.970949	-1.560744
6	78	0	1.406576	-3.831811	0.012106

7	78	0	2.903745	1.936989	-1.444791
8	78	0	2.869857	-2.010110	-1.575890
9	78	0	-0.008984	1.998518	1.533963
10	78	0	-0.000836	-2.030952	1.547282
11	78	0	1.396885	0.032662	-2.840083
12	78	0	4.305859	0.025382	-0.015870
13	78	0	-1.364629	-0.009550	0.011892
14	78	0	1.389438	0.053981	2.847478
15	78	0	-1.453698	-0.078807	2.855202
16	78	0	-2.879185	1.920471	1.463549
17	78	0	-2.901263	-1.972327	1.388225
18	78	0	1.417753	3.900876	-0.031022
19	78	0	-1.496942	0.072966	-2.830833
20	78	0	-1.355843	3.872069	0.062535
21	78	0	-2.900702	1.980255	-1.380537
22	78	0	-4.244460	0.003328	-0.001089
23	78	0	-2.918087	-1.921723	-1.469095
24	78	0	-1.363394	-3.859779	-0.067807
25	1	0	3.525123	-1.715264	0.009658

E	-659.4032511
Sigma	1
Nneg	0
E+ZPE	-659.384588
U	-659.331173
H	-659.330229
G	-659.500345

Complex Pt_{24}*H «ββε» (M=4) (Figure 8f)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.832206	1.977672	1.407952
2	78	0	-1.369365	-0.017533	0.013792
3	78	0	-0.004161	-2.025326	-1.550053
4	78	0	-2.929466	-1.987104	1.398691
5	78	0	0.017209	2.051723	-1.441676

6	78	0	-1.461084	4.035096	-0.003183
7	78	0	-2.903789	-1.965183	-1.448113
8	78	0	-2.851226	1.998308	-1.435239
9	78	0	-0.015091	-2.098897	1.528532
10	78	0	0.005538	2.023325	1.576050
11	78	0	-1.446291	0.020799	-2.782949
12	78	0	-4.201957	0.025268	-0.032562
13	78	0	1.364944	-0.029974	0.017828
14	78	0	-1.437697	-0.048503	2.813649
15	78	0	1.422744	-0.056879	2.822802
16	78	0	2.893552	-2.014765	1.405692
17	78	0	2.844864	1.941786	1.416027
18	78	0	-1.408191	-3.916138	-0.030702
19	78	0	1.467152	0.007947	-2.783529
20	78	0	1.358923	-3.931297	-0.023177
21	78	0	2.888626	-1.994435	-1.437923
22	78	0	4.204008	-0.021905	-0.018660
23	78	0	2.885168	1.964517	-1.427357
24	78	0	1.507572	4.013532	0.002651
25	1	0	0.017671	3.741277	0.893633

E	-659.4081932
Sigma	1
Nneg	0
E+ZPE	-659.389624
U	-659.336242
H	-659.335298
G	-659.505597

TS δε (see Figure 10)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.941427	-1.871905	-1.511235
2	78	0	-1.393949	0.046334	0.078053
3	78	0	0.084957	2.037154	1.646867
4	78	0	-2.900727	2.006645	-1.425421

5	78	0	0.021314	-2.041255	1.545687
6	78	0	-1.482383	-3.833464	-0.022825
7	78	0	-2.884173	1.923617	1.528061
8	78	0	-2.888667	-1.900204	1.389968
9	78	0	0.016575	1.985175	-1.459716
10	78	0	-0.061060	-1.955529	-1.503800
11	78	0	-1.346155	-0.106267	2.932557
12	78	0	-4.286350	0.031276	-0.104565
13	78	0	1.383457	-0.029354	0.009884
14	78	0	-1.483583	0.068278	-2.799421
15	78	0	1.438978	-0.005591	-2.821282
16	78	0	2.930371	1.929142	-1.504126
17	78	0	2.853695	-2.010182	-1.463343
18	78	0	-1.369571	3.847564	0.050947
19	78	0	1.521717	-0.020377	2.826197
20	78	0	1.435255	3.887839	-0.051472
21	78	0	2.909514	1.926493	1.343815
22	78	0	4.232932	-0.044630	-0.092530
23	78	0	2.915789	-2.004185	1.381590
24	78	0	1.312141	-3.895665	-0.004621
25	1	0	-1.454689	2.269062	2.396943

E	-659.40379488
Sigma	1
Nneg	-60
E+ZPE	-659.38510874
U	-659.33227197
H	-659.33132776
G	-659.49933363

TS αγδ (see Figure 10)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.879169	-1.810099	1.564213
2	78	0	1.368914	-0.027928	0.028264
3	78	0	0.076617	1.994266	-1.518677

4	78	0	2.907360	1.743346	1.483739
5	78	0	-0.024611	-1.989905	-1.535861
6	78	0	1.382805	-3.794256	0.122519
7	78	0	2.927450	1.883647	-1.491925
8	78	0	2.881632	-1.991929	-1.389718
9	78	0	-0.043716	1.982029	1.567640
10	78	0	-0.084461	-1.997145	1.582231
11	78	0	1.504268	-0.062239	-2.819577
12	78	0	4.401202	-0.025016	-0.188237
13	78	0	-1.393690	0.012679	-0.009801
14	78	0	1.234417	0.021757	2.977804
15	78	0	-1.592618	-0.046293	2.824609
16	78	0	-2.923535	1.985317	1.382029
17	78	0	-2.986209	-1.940457	1.308646
18	78	0	1.512604	3.761786	0.096984
19	78	0	-1.416040	0.067721	-2.840035
20	78	0	-1.285172	3.888995	0.031580
21	78	0	-2.817746	2.034308	-1.463751
22	78	0	-4.245546	0.071015	-0.137412
23	78	0	-2.909104	-1.912321	-1.536697
24	78	0	-1.402045	-3.844958	-0.056919
25	1	0	3.748318	-0.336838	1.431512

E	-659.384359
Sigma	1
Nneg	-135
E+ZPE	-659.384359
U	-659.331469
H	-659.330525
G	-659.498650

TS γδ (see Figure 10)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.966936	1.939605	1.426152
2	78	0	-1.401953	0.022086	0.072397
3	78	0	-0.009294	-1.950454	-1.522428

4	78	0	-2.887052	-1.903204	1.397281
5	78	0	0.017318	1.982361	-1.487070
6	78	0	-1.397186	3.828233	0.049290
7	78	0	-2.905728	-1.902371	-1.509464
8	78	0	-2.885771	1.958231	-1.486513
9	78	0	0.028015	-2.029953	1.485355
10	78	0	-0.038956	1.982906	1.595116
11	78	0	-1.450641	0.032847	-2.824491
12	78	0	-4.294521	0.000383	-0.143022
13	78	0	1.395841	0.007872	0.013304
14	78	0	-1.355940	-0.224765	3.098969
15	78	0	1.449249	0.031476	2.832049
16	78	0	2.917177	-1.938837	1.407894
17	78	0	2.871339	1.946922	1.402001
18	78	0	-1.425849	-3.836138	-0.044274
19	78	0	1.483507	0.002520	-2.809070
20	78	0	1.384195	-3.862711	-0.023705
21	78	0	2.917198	-1.957880	-1.447260
22	78	0	4.263431	0.017657	-0.056580
23	78	0	2.933712	1.972194	-1.472598
24	78	0	1.385250	3.865253	0.012568
25	1	0	-2.059585	1.229712	2.659750

E	-659.4070795
Sigma	1
Nneg	-108
E+ZPE	-659.388385
U	-659.335375
H	-659.334431
G	-659.503646

TS βδ (see Figure 10)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.951850	-1.790753	-1.529782
2	78	0	-1.397306	0.060217	0.000541

3	78	0	0.017157	2.019719	1.523365
4	78	0	-2.670863	2.144131	-1.449578
5	78	0	-0.172845	-2.067417	1.524246
6	78	0	-1.639283	-3.810700	-0.091885
7	78	0	-2.844217	2.082598	1.453506
8	78	0	-3.096849	-1.830049	1.336102
9	78	0	0.204096	2.014241	-1.483976
10	78	0	-0.044891	-1.983296	-1.550892
11	78	0	-1.527829	-0.028652	2.798868
12	78	0	-4.230033	0.235158	-0.151017
13	78	0	1.357842	-0.084447	0.035540
14	78	0	-1.346623	0.113058	-2.807655
15	78	0	1.596585	-0.067565	-2.802604
16	78	0	3.086186	1.780056	-1.390071
17	78	0	2.820184	-2.120208	-1.375391
18	78	0	-1.112354	4.110577	-0.059470
19	78	0	1.323512	-0.061447	2.877345
20	78	0	1.689974	3.797255	0.065221
21	78	0	2.897229	1.752529	1.480840
22	78	0	4.227050	-0.251667	0.085309
23	78	0	2.706193	-2.105663	1.485902
24	78	0	1.141305	-3.952858	0.017663
25	1	0	-2.525065	3.524294	0.614128

E	-659.4065444
Sigma	1
Nneg	-169
E+ZPE	-659.387664
U	-659.334716
H	-659.333771
G	-659.502076

TS ββ (see Figure 10)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.988729	-1.875529	1.426910

2	78	0	1.368307	0.025558	0.000112
3	78	0	-0.087434	2.048973	-1.487874
4	78	0	2.754136	2.083229	1.433871
5	78	0	0.079898	-2.064534	-1.540700
6	78	0	1.558762	-3.863821	-0.000212
7	78	0	2.754173	2.083559	-1.433719
8	78	0	2.988608	-1.875265	-1.427251
9	78	0	-0.087226	2.048960	1.488132
10	78	0	0.080018	-2.064827	1.540381
11	78	0	1.430550	0.026690	-2.794384
12	78	0	4.187970	0.180180	-0.000129
13	78	0	-1.359912	-0.083966	0.000004
14	78	0	1.430312	0.026265	2.794629
15	78	0	-1.440139	-0.063654	2.799173
16	78	0	-2.917445	1.858923	1.428512
17	78	0	-2.817210	-2.108297	1.421438
18	78	0	1.266868	4.049211	0.000127
19	78	0	-1.440425	-0.063489	-2.799146
20	78	0	-1.603686	3.949560	-0.000022
21	78	0	-2.917815	1.859066	-1.428529
22	78	0	-4.188048	-0.158281	-0.000017
23	78	0	-2.817122	-2.108295	-1.421280
24	78	0	-1.209327	-3.972925	-0.000033
25	1	0	-0.198126	4.891327	0.000460

E	-659.4094831
Sigma	1
Nneg	-76
E+ZPE	-659.389602
U	-659.337063
H	-659.336119
G	-659.503316

TS βε (see Figure 10)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.839038	-2.039216	-1.487384
2	78	0	-1.373177	-0.057346	0.019750
3	78	0	-0.064782	2.000065	1.641419
4	78	0	-2.921396	1.929560	-1.402917
5	78	0	0.039915	-2.091688	1.542543
6	78	0	-1.274501	-3.955713	-0.094602
7	78	0	-2.906306	1.885856	1.397931
8	78	0	-2.867821	-2.097935	1.361595
9	78	0	-0.039369	2.040709	-1.421368
10	78	0	0.065178	-1.997477	-1.536628
11	78	0	-1.486147	-0.147009	2.811462
12	78	0	-4.205763	-0.117467	-0.039722
13	78	0	1.374823	0.023406	0.023743
14	78	0	-1.436845	0.018502	-2.788447
15	78	0	1.470084	0.044433	-2.787540
16	78	0	2.845329	2.054803	-1.447905
17	78	0	2.967025	-1.882636	-1.452349
18	78	0	-1.549141	4.040207	-0.052953
19	78	0	1.422444	-0.025380	2.854534
20	78	0	1.318060	3.940198	0.043788
21	78	0	2.776899	2.009121	1.423509
22	78	0	4.234530	0.118864	-0.036912
23	78	0	2.956082	-1.887915	1.401790
24	78	0	1.504206	-3.851072	0.009337
25	1	0	-0.802648	3.520077	1.351357

E	-659.4062181
Sigma	1
Nneg	-71
E+ZPE	-659.387175
U	-659.334289
H	-659.333345
G	-659.501256

TS γε (see Figure 10)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.986371	-1.918599	-1.400724
2	78	0	-1.382578	0.012972	0.102903
3	78	0	0.107485	2.057292	1.547049
4	78	0	-2.989103	1.969767	-1.365888
5	78	0	0.108628	-2.031447	1.456491
6	78	0	-1.423707	-3.876680	-0.005543
7	78	0	-2.800369	1.947219	1.498565
8	78	0	-2.829675	-1.973399	1.453508
9	78	0	-0.087255	1.985493	-1.505352
10	78	0	-0.108195	-1.966914	-1.541948
11	78	0	-1.349207	-0.088018	2.968110
12	78	0	-4.255691	0.012919	0.078922
13	78	0	1.395783	0.000114	-0.031104
14	78	0	-1.603011	0.037019	-2.760499
15	78	0	1.358120	-0.001991	-2.847912
16	78	0	2.868562	1.925946	-1.504317
17	78	0	2.828530	-1.952136	-1.458264
18	78	0	-1.405522	3.887156	0.057123
19	78	0	1.573851	-0.012048	2.757564
20	78	0	1.404951	3.872831	-0.124724
21	78	0	2.967634	1.961394	1.362646
22	78	0	4.252651	-0.008067	-0.074764
23	78	0	2.980184	-1.970305	1.402378
24	78	0	1.383149	-3.889297	-0.102341
25	1	0	-0.689742	1.464824	2.973421

E	-659.4065671
Sigma	1
Nneg	-235
E+ZPE	-659.387778
U	-659.334886
H	-659.333942
G	-659.501912

Complex $Pt_{24}*H_2$ «L_δ» (M=5) (Figure 6d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.949555	1.903870	-1.454800
2	78	0	1.381545	-0.027752	0.003135
3	78	0	-0.022275	-2.028001	1.535563
4	78	0	2.855264	-2.027884	-1.398334
5	78	0	0.033838	2.009549	1.540191
6	78	0	1.462734	3.871204	-0.028727
7	78	0	2.878886	-1.986985	1.453394
8	78	0	2.921750	1.918982	1.387916
9	78	0	-0.043859	-2.000482	-1.533812
10	78	0	0.063286	2.015803	-1.511578
11	78	0	1.449256	0.009287	2.833744
12	78	0	4.247998	-0.070971	-0.019583
13	78	0	-1.388743	0.012193	0.016969
14	78	0	1.464108	-0.058918	-2.820446
15	78	0	-1.437739	0.081181	-2.808276
16	78	0	-2.941239	-1.880365	-1.491822
17	78	0	-2.837795	2.045815	-1.404088
18	78	0	1.325180	-3.903282	0.036250
19	78	0	-1.428550	-0.025839	2.827831
20	78	0	-1.455175	-3.857000	-0.059947
21	78	0	-2.939369	-1.911730	1.362014
22	78	0	-4.242513	0.096974	-0.061938
23	78	0	-2.874718	1.988133	1.453841
24	78	0	-1.321772	3.906429	0.073475
25	1	0	-3.606262	-3.060951	2.950317
26	1	0	-4.166679	-3.195666	2.433716

E	-659.9872631
Sigma	1
Nneg	0
E+ZPE	-659.961307
U	-659.906112
H	-659.905168

G	-660.078176

Complex $Pt_{24}*H_2$ «T_ε» (M=5) (Figure 6a)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.928633	1.941778	-1.447521
2	78	0	1.379332	-0.005474	0.007863
3	78	0	-0.005677	-2.044573	1.535536
4	78	0	2.893540	-1.985692	-1.401931
5	78	0	-0.018429	2.030826	1.539791
6	78	0	1.417256	3.898211	-0.031467
7	78	0	2.886929	-1.960287	1.447774
8	78	0	2.877743	1.965649	1.399504
9	78	0	-0.010477	-2.001234	-1.533470
10	78	0	0.032932	2.023558	-1.508716
11	78	0	1.414448	0.039689	2.822952
12	78	0	4.241943	-0.016993	0.006605
13	78	0	-1.378952	0.008127	0.000529
14	78	0	1.463631	-0.033863	-2.811122
15	78	0	-1.431090	0.065250	-2.818724
16	78	0	-2.913487	-1.919830	-1.490062
17	78	0	-2.865476	2.009444	-1.391284
18	78	0	1.372236	-3.895593	0.020102
19	78	0	-1.457605	-0.056829	2.811624
20	78	0	-1.411789	-3.885653	-0.087612
21	78	0	-2.902739	-1.973962	1.357096
22	78	0	-4.239601	0.023810	-0.025466
23	78	0	-2.904226	1.957884	1.451946
24	78	0	-1.368237	3.911344	0.055751
25	1	0	-0.027744	-3.487291	3.228156
26	1	0	-0.037751	-3.968378	3.815459

E	-659.9817983
Sigma	1
Nneg	0
E+ZPE	-659.956433

U	-659.900830
H	-659.899886
G	-660.073721

Complex $Pt_{24}*H_2$ «$B_{\beta\beta}$» (M=5) (Figure 6e)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.890404	-1.979104	-1.395938
2	78	0	-1.375776	-0.011108	-0.000868
3	78	0	0.002479	2.039800	1.518356
4	78	0	-2.879873	1.981617	-1.417782
5	78	0	-0.004622	-2.063752	1.480889
6	78	0	-1.399430	-3.925365	-0.020545
7	78	0	-2.870134	1.966981	1.430351
8	78	0	-2.905987	-1.984417	1.433992
9	78	0	0.005183	2.037224	-1.535239
10	78	0	-0.001823	-2.038912	-1.559947
11	78	0	-1.422813	-0.016015	2.796712
12	78	0	-4.215633	0.018569	0.005546
13	78	0	1.375094	-0.015807	-0.000106
14	78	0	-1.458136	0.000464	-2.790522
15	78	0	1.463480	-0.003041	-2.790245
16	78	0	2.889008	1.972293	-1.414921
17	78	0	2.885655	-1.989007	-1.393732
18	78	0	-1.448180	3.928779	-0.002092
19	78	0	1.418966	-0.019933	2.798321
20	78	0	1.462800	3.925068	0.000078
21	78	0	2.874600	1.956653	1.432549
22	78	0	4.215370	0.004081	0.009306
23	78	0	2.895637	-1.994147	1.435492
24	78	0	1.384255	-3.930649	-0.020333
25	1	0	0.427670	5.449831	0.026627
26	1	0	-0.405352	5.448848	0.026128

E	-659.9902761
Sigma	1

Nneg	0
E+ZPE	-659.964396
U	-659.909931
H	-659.908987
G	-660.080702

Complex $Pt_{24}*H_2$ «$B_{\gamma\gamma}$» (M=5) (Figure 6f)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-3.013913	-1.975337	-1.404981
2	78	0	-1.424550	0.000948	0.042112
3	78	0	0.094677	1.909090	1.582349
4	78	0	-3.029315	1.977089	-1.388163
5	78	0	0.092007	-1.937314	1.559310
6	78	0	-1.397975	-3.839378	0.055230
7	78	0	-2.858968	1.891217	1.457057
8	78	0	-2.839064	-1.911470	1.454294
9	78	0	-0.108269	1.973899	-1.484046
10	78	0	-0.095591	-1.949449	-1.496648
11	78	0	-1.364135	-0.019427	2.954905
12	78	0	-4.322358	-0.013877	0.012246
13	78	0	1.406209	0.009024	-0.024810
14	78	0	-1.615223	0.015822	-2.784638
15	78	0	1.318033	0.019722	-2.930847
16	78	0	2.842031	1.919091	-1.541885
17	78	0	2.842010	-1.889992	-1.544505
18	78	0	-1.416253	3.828640	0.107565
19	78	0	1.695819	-0.068303	2.936414
20	78	0	1.380027	3.775674	-0.011871
21	78	0	2.999140	1.881488	1.317237
22	78	0	4.376438	0.017049	-0.248256
23	78	0	3.027981	-1.856477	1.322285
24	78	0	1.401658	-3.767216	-0.050449
25	1	0	0.783191	0.437786	4.404992
26	1	0	-0.035855	0.302385	4.182333

E	-659.988960
Sigma	1
Nneg	0
E+ZPE	-659.963311
U	-659.909087
H	-659.908142
G	-660.079093

Complex Pt_{24}*H_2 «L_γ» (M=5) (Figure 6c)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	2.921736	1.960210	-1.443917
2	78	0	1.388612	0.004723	0.007436
3	78	0	0.000351	-2.030220	1.545866
4	78	0	2.933765	-1.960469	-1.371435
5	78	0	-0.059816	2.023188	1.534094
6	78	0	1.373730	3.905031	-0.034343
7	78	0	2.904707	-1.919627	1.482407
8	78	0	2.838803	1.997440	1.409711
9	78	0	0.029311	-2.006273	-1.521491
10	78	0	0.029826	2.007644	-1.508944
11	78	0	1.399159	0.052042	2.814491
12	78	0	4.249694	0.032365	0.038209
13	78	0	-1.379206	-0.009691	0.012578
14	78	0	1.489338	-0.043932	-2.814500
15	78	0	-1.391360	0.040679	-2.842610
16	78	0	-2.865966	-1.947830	-1.502766
17	78	0	-2.866120	1.955257	-1.425231
18	78	0	1.424458	-3.877366	0.064482
19	78	0	-1.530713	-0.057659	2.809080
20	78	0	-1.352771	-3.900676	-0.084812
21	78	0	-2.891869	-2.013370	1.333095
22	78	0	-4.244836	-0.028661	-0.059071
23	78	0	-2.942808	1.933973	1.410227
24	78	0	-1.415595	3.890528	0.023682
25	1	0	-1.677453	-0.667987	4.778793

26	1	0	-1.632154	0.098137	4.874659

E	-659.9868142
Sigma	1
Nneg	0
E+ZPE	-659.961083
U	-659.905751
H	-659.904807
G	-660.078393

Complex $Pt_{24}*H_2$ «L_β» (M=5) (Figure 6b)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-2.959648	-1.822269	-1.503017
2	78	0	-1.384765	0.046754	-0.009699
3	78	0	0.022597	2.014616	1.516457
4	78	0	-2.738039	2.094812	-1.427793
5	78	0	-0.125038	-2.035838	1.538925
6	78	0	-1.562677	-3.839685	-0.089772
7	78	0	-2.850616	2.064798	1.428443
8	78	0	-3.015443	-1.870804	1.338339
9	78	0	0.157549	2.000080	-1.483797
10	78	0	-0.056208	-2.019552	-1.524287
11	78	0	-1.525805	-0.011137	2.801970
12	78	0	-4.235601	0.183122	-0.064152
13	78	0	1.380062	-0.080777	0.025265
14	78	0	-1.380171	0.087661	-2.832513
15	78	0	1.520343	-0.119911	-2.789920
16	78	0	3.017488	1.813299	-1.431613
17	78	0	2.845761	-2.117408	-1.349904
18	78	0	-1.233369	3.949846	0.023144
19	78	0	1.363524	-0.014802	2.838409
20	78	0	1.570379	3.872344	-0.058866
21	78	0	2.894259	1.862298	1.405441
22	78	0	4.237953	-0.179062	0.059726
23	78	0	2.782079	-2.066646	1.495202

24	78	0	1.209447	-3.951482	0.077137
25	1	0	2.280341	5.544052	0.897977
26	1	0	2.862786	5.355848	0.418193

E	-659.988745
Sigma	1
Nneg	0
E+ZPE	-659.962538
U	-659.907557
H	-659.906612
G	-660.078760

Complex H-Pt24-H (γγε + γγε) Figure 7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-3.04168	-1.95136	-1.33786
2	78	0	-1.38871	0.000086	0.117305
3	78	0	0.119429	2.049167	1.47384
4	78	0	-3.04044	1.952905	-1.33729
5	78	0	0.117732	-2.04964	1.474679
6	78	0	-1.40999	-3.90642	-0.00228
7	78	0	-2.78477	1.992645	1.495016
8	78	0	-2.78607	-1.9919	1.494574
9	78	0	-0.13011	1.961838	-1.5159
10	78	0	-0.13063	-1.96152	-1.51594
11	78	0	-1.3085	0.000229	2.95782
12	78	0	-4.24973	0.000972	0.175473
13	78	0	1.41375	-0.00061	0.019782
14	78	0	-1.66484	0.000396	-2.72472
15	78	0	1.283949	0.000002	-2.91626
16	78	0	2.8132	1.870899	-1.52205
17	78	0	2.812801	-1.872	-1.52249
18	78	0	-1.40831	3.90724	-0.00163
19	78	0	1.671504	-0.0003	2.889588
20	78	0	1.398802	3.856181	-0.17577
21	78	0	3.004204	2.00775	1.331374

22	78	0	4.303569	-0.00101	-0.08979
23	78	0	3.002788	-2.00911	1.331369
24	78	0	1.397035	-3.85645	-0.17565
25	1	0	0.196472	-1.05735	2.994457
26	1	0	0.195961	1.057008	2.994406

E	-660.0100494
Sigma	1
Nneg	0
E+ZPE	-659.984510
U	-659.931273
H	-659.930329
G	-660.098813

Complex H-Pt24-H (γγε + γδε) Figure 7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	3.010381	2.012561	-1.36993
2	78	0	1.415761	0.035478	0.136355
3	78	0	-0.0913	-1.98009	1.488737
4	78	0	3.083485	-1.87273	-1.39374
5	78	0	-0.20627	1.970149	1.609885
6	78	0	1.328419	3.872503	0.044041
7	78	0	2.854082	-1.94023	1.446527
8	78	0	2.776782	2.037129	1.518825
9	78	0	0.168051	-1.92378	-1.50707
10	78	0	0.098972	1.952401	-1.47151
11	78	0	1.431273	-0.12697	3.095981
12	78	0	4.288081	0.076411	0.090652
13	78	0	-1.41958	-0.01928	0.006391
14	78	0	1.647094	0.042501	-2.75471
15	78	0	-1.23287	-0.0015	-2.96367
16	78	0	-2.77947	-1.86892	-1.56745
17	78	0	-2.86309	1.78404	-1.55937
18	78	0	1.473813	-3.83187	0.010686
19	78	0	-1.78224	-0.02401	2.878495

20	78	0	-1.33508	-3.81509	-0.15163
21	78	0	-2.99258	-2.0315	1.320665
22	78	0	-4.34555	-0.08315	-0.11973
23	78	0	-3.07867	1.952629	1.28454
24	78	0	-1.46303	3.772745	-0.14295
25	1	0	1.292062	1.54507	2.463287
26	1	0	-0.23687	-0.72168	2.99563

E	-660.0067598
Sigma	1
Nneg	0
E+ZPE	-659.981816
U	-659.928224
H	-659.927280
G	-660.097074

TS of molecular hydrogen dissociation from the $B_{\gamma\gamma}$ complex (M=5) (Figure 7a)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-3.0069	-1.98429	-1.38236
2	78	0	-1.40783	-0.00295	0.06784
3	78	0	0.08438	1.97354	1.55354
4	78	0	-3.05326	1.96502	-1.35728
5	78	0	0.13099	-1.9787	1.51181
6	78	0	-1.37393	-3.88031	0.01515
7	78	0	-2.8437	1.90331	1.48439
8	78	0	-2.80483	-1.97023	1.47061
9	78	0	-0.13386	1.98337	-1.4834
10	78	0	-0.09839	-1.94737	-1.51454
11	78	0	-1.36107	-0.08619	2.93195
12	78	0	-4.28649	-0.03618	0.07893
13	78	0	1.41125	0.01821	-0.02292
14	78	0	-1.64072	0.02061	-2.75097
15	78	0	1.31564	0.03782	-2.91216
16	78	0	2.81818	1.94892	-1.52667
17	78	0	2.84333	-1.87546	-1.5389

18	78	0	-1.44229	3.86042	0.09149
19	78	0	1.72082	-0.09058	2.8833
20	78	0	1.3513	3.83163	-0.05483
21	78	0	2.97986	1.95716	1.33904
22	78	0	4.3275	0.05305	-0.18189
23	78	0	3.04548	-1.92198	1.32187
24	78	0	1.41791	-3.80125	-0.11889
25	1	0	0.4816	0.60388	3.97516
26	1	0	0.03493	1.14614	3.42555

E	-659.9867702
Sigma	1
Nneg	-249
E+ZPE	-659.962857
U	-659.909024
H	-659.908080
G	-660.077982

II. DFT calculations

The unconstrained geometry optimizations were carried out for all of the considered structures with the *Gaussian 03* program package[1] using DFT with the BLYP density functional.The 6-31G(p)[2] basis set was used for the H atom. The CRENBS[3] effective core potentials (ECP) was used for the Pt atoms. The same level of theory was applied in the frequency calculations performed at all the located stationary points. The thermodynamic parameters were calculated in the rigid rotor-harmonic oscillator approximation. For all of the located transition state structures, the minimum energy reaction paths were studied using the Gonzales-Schlegel method[4].

([1]) *Gaussian 03* (Revision D.02), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, V. G.; J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain,

O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C.Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, B. B. Stefanov,G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, J. A. Pople, Gaussian, Inc., Wallingford, CT, **2007**.

([2]) M.M. Francl, W.J. Petro, W.J. Hehre, J.S. Binkley, M.S. Gordon, D.J. DeFrees and J.A. Pople. J. Chem. Phys. **1982**, 77, 3654-3665.

([3]) R.B. Ross, W.C. Ermler, P.A. Christiansen et al. J. Chem. Phys. **1990**,93, 6654

([4]) Gonzalez, C. and Schlegel, H. B. *J. Chem. Phys.***1989**, 90, 2154.