$TpPtMeH_2$ - Why is There H/D Scrambling of the Methyl Group But Not Methane Loss

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Table 1: Crystal data and structure refinement for ptar.

Identification code	ptar
Empirical formula	C10 H15 B N6 Pt
Formula weight	425.18
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 7.790(2) Å alpha = 90 deg. b = 13.342(3) Å beta = 90.20(3) deg. c = 26.078(5) Å gamma = 90 deg.
Volume	2710.2(11) $Å^3$
Z, Calculated density	8, 2.084 Mg/m^3
Absorption coefficient	10.346 mm^{-1}
F(000)	1600
Crystal size	0.02 x 0.24 x 0.24 mm
Theta range for data collection	1.56 to 22.99 deg.
Limiting indices	0<=h<=8, 0<=k<=14, -26<=l<=28
Reflections collected / unique	3120 / 3120 [R(int) = 0.0000]
Completeness to theta = 22.99	82.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3120 / 0 / 157
Goodness-of-fit on F2	1.077
Final R indices [I>2sigma(I)]	R1 = 0.0735, wR2 = 0.2046
R indices (all data)	R1 = 0.0937, wR2 = 0.2101
Largest diff. peak and hole	3.778 and -1.664 e. $Å^{-3}$

Table 2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x10^3) for ptar. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pt(1)	6989(2)	5763(1)	-1575(1)	69(1)
B(1)	7250(40)	8020(30)	-2061(12)	52(9)
N(1)	6020(30)	7100(18)	-1264(8)	51(6)
N(2)	6390(30)	7992(19)	-1527(9)	52(6)
N(3)	9150(30)	7569(18)	-1953(8)	48(6)
N(4)	9290(40)	6560(20)	-1715(11)	82(9)
N(5)	5940(40)	6310(20)	-2320(10)	76(8)
N(6)	6310(30)	7254(19)	-2406(9)	55(7)
C(1)	7850(60)	4400(30)	-1882(16)	113(13)
C(2)	5100(30)	7360(20)	-850(10)	40(7)
C(3)	4780(40)	8300(20)	-857(11)	48(8)
C(4)	5570(40)	8690(20)	-1263(11)	53(8)
C(5)	10970(40)	6440(20)	-1729(11)	63(9)
C(6)	11810(50)	7320(30)	-1899(12)	75(9)
C(7)	10780(40)	7920(30)	-2036(11)	60(9)
C(8)	5650(40)	7520(30)	-2884(12)	62(9)
C(9)	4910(50)	6610(30)	-3016(15)	82(11)
C(10)	5050(40)	5940(30)	-2684(13)	66(9)
Pt(2)	8001(2)	6547(1)	756(1)	66(1)
C(11)	7300(90)	5360(60)	330(20)	220(30)
B(2)	7490(30)	8960(30)	490(12)	47(9)
N(7)	8900(30)	7824(18)	1219(8)	48(6)
N(8)	8470(30)	8679(17)	1036(8)	45(6)
N(9)	8800(30)	7372(19)	71(9)	51(6)
N(10)	8510(20)	8394(16)	79(8)	41(6)
N(11)	5590(30)	7382(18)	659(8)	46(6)
N(12)	5750(30)	8357(17)	537(8)	46(6)
C(12)	9100(40)	9410(20)	1379(10)	47(7)
C(13)	9840(50)	8920(30)	1792(16)	97(13)
C(14)	9580(40)	7930(30)	1658(13)	73(10)
C(15)	9190(40)	8840(20)	-345(11)	58(8)
C(16)	9850(50)	7980(30)	-577(15)	86(11)
C(17)	9710(40)	7210(30)	-331(12)	62(9)
C(18)	4120(40)	8750(20)	520(11)	52(8)
C(19)	3030(50)	7970(30)	572(13)	86(10)
C(20)	3840(40)	7120(30)	637(11)	63(9)

Table 3: Bond lengths (Å) and angles (deg) for ptar.

Pt(1)-C(1)	2.10(5)
Pt(1)-N(1)	2.10(2)
Pt(1)-N(4)	2.12(3)
Pt(1)-N(5)	2.22(3)
B(1)-N(6)	1.54(4)
B(1)-N(2)	1.55(4)
B(1)-N(3)	1.62(4)
N(1)-C(2)	1.34(3)
N(1)-N(2)	1.40(3)
N(2)-C(4)	1.32(3)
N(3)-C(7)	1.37(4)
N(3)-N(4)	1.48(4)
N(4)-C(5)	1.32(4)
N(5)-C(10)	1.27(4)
N(5)-N(6)	1.32(3)
N(6)-C(8)	1.39(4)
C(2)-C(3)	1.27(4)
C(3)-C(4)	1.33(4)
C(5)-C(6)	1.41(4)
C(6)-C(7)	1.19(4)
C(8)-C(9)	1.38(5)
C(9)-C(10)	1.25(4)
Pt(2)-C(11)	2.01(8)
Pt(2)-N(9)	2.19(2)
Pt(2)-N(11)	2.20(2)
Pt(2)-N(7)	2.20(2)
B(2)-N(10)	1.53(4)
B(2)-N(12)	1.58(4)
B(2)-N(8)	1.66(4)
N(7)-C(14)	1.27(4)
N(7)-N(8)	1.28(3)
N(8)-C(12)	1.40(3)
N(9)-C(17)	1.29(3)
N(9)-N(10)	1.38(3)
N(10)-C(15)	1.37(3)
N(11)-N(12)	1.34(3)
N(11)-C(20)	1.41(4)
N(12)≠C(18)	1.37(4)
C(12)-C(13)	1.38(5)
C(13)-C(14)	1.38(5)
C(15)-C(16)	1.40(5)
C(16)-C(17)	1.22(5)
C(18)-C(19)	1.34(5)
C(19)-C(20)	1.31(4)
C(1)-Pt(1)-N(1)	177.6(14)
C(1)-Pt(1)-N(4)	95.6(14)
N(1)-Pt(1)-N(4)	86.8(10)
C(1)-Pt(1)-N(5)	93.8(14)
N(1)-Pt(1)-N(5)	86.0(10)
N(4)-Pt(1)-N(5)	89.6(11)
N(6)-B(1)-N(2)	107(2)
N(6)-B(1)-N(3)	107(2)
N(2)-B(1)-N(3)	104(2)

C(2)-N(1)-N(2)	107(2)
C(2)-N(1)-Pt(1)	136(2)
N(2)-N(1)-Pt(1)	117.2(16)
C(4)-N(2)-N(1)	104(2)
C(4)-N(2)-B(1)	131(3)
N(1)-N(2)-B(1)	123(2)
C(7)-N(3)-N(4)	108(2)
C(7)-N(3)-B(1)	134(2)
N(4)-N(3)-B(1)	118(2)
C(5)-N(4)-N(3)	100(3)
C(5)-N(4)-Pt(1)	141(3)
N(3)-N(4)-Pt(1)	118(2)
C(10)-N(5)-N(6)	111(3)
C(10)-N(5)-Pt(1)	136(3)
N(6)-N(5)-Pt(1)	112(2)
N(5)-N(6)-C(8)	109(2)
N(5)-N(6)-B(1)	130(3)
C(8)-N(6)-B(1)	122(3)
C(3)-C(2)-N(1)	110(2)
C(2)-C(3)-C(4)	108(3)
N(2)-C(4)-C(3)	111(3)
N(4)-C(5)-C(6)	111(3)
C(7)-C(6)-C(5)	110(3)
C(6)-C(7)-N(3)	110(3)
C(9)-C(8)-N(6)	99(3)
C(10)-C(9)-C(8)	115(4)
C(9)-C(10)-N(5)	107(3)
C(11)-Pt(2)-N(9)	91(2)
C(11)-Pt(2)-N(11)	96(2)
N(9)-Pt(2)-N(11)	84.0(8)
C(11)-Pt(2)-N(7)	177(2)
N(9)-Pt(2)-N(7)	88.1(9)
N(11)-Pt(2)-N(7)	86.7(9)
N(10)-B(2)-N(12)	105(2)
N(10)-B(2)-N(8)	104(2)
N(12)-B(2)-N(8)	102(2)
C(14)-N(7)-N(8)	110(3)
C(14)-N(7)-Pt(2)	136(2)
N(8)-N(7)-Pt(2)	113.8(17)
N(7)-N(8)-C(12)	107(2)
N(7)-N(8)-B(2)	130(2)
C(12)-N(8)-B(2)	123(2)
C(17)-N(9)-N(10)	105(2)
C(17)-N(9)-Pt(2)	138(2)
N(10)-N(9)-Pt(2)	116.0(16)
C(15)-N(10)-N(9)	111(2)
C(15)-N(10)-B(2)	124(2)
N(9)-N(10)-B(2)	125(2)
N(12)-N(11)-C(20)	108(2)
N(12)-N(11)-Pt(2)	116.0(16)
C(20)-N(11)-Pt(2)	135(2)
N(11)-N(12)-C(18)	107(2)
N(11)-N(12)-B(2)	126(2)
C(18)-N(12)-B(2)	127(2)
C(13)-C(12)-N(8)	108(3)
C(14)-C(13)-C(12)	101(3)
N(7)-C(14)-C(13)	113(3)

N(10)-C(15)-C(16)	98(3)
C(17)-C(16)-C(15)	116(4)
C(16)-C(17)-N(9)	110(3)
C(19)-C(18)-N(12)	107(3)
C(20)-C(19)-C(18)	112(3)
C(19)-C(20)-N(11)	105(3)

Table 4: Anisotropic displacement parameters ($Å^2x10^3$) for ptar.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Pt(1)	75(1)	62(1)	69(1)	-8(1)	-9(1)	10(1)
Pt(2)	62(1)	54(1)	81(1)	11(1)	1(1)	0(1)

Numbering Schemes for Wiberg Bond Indices (top:1, bottom: 2)

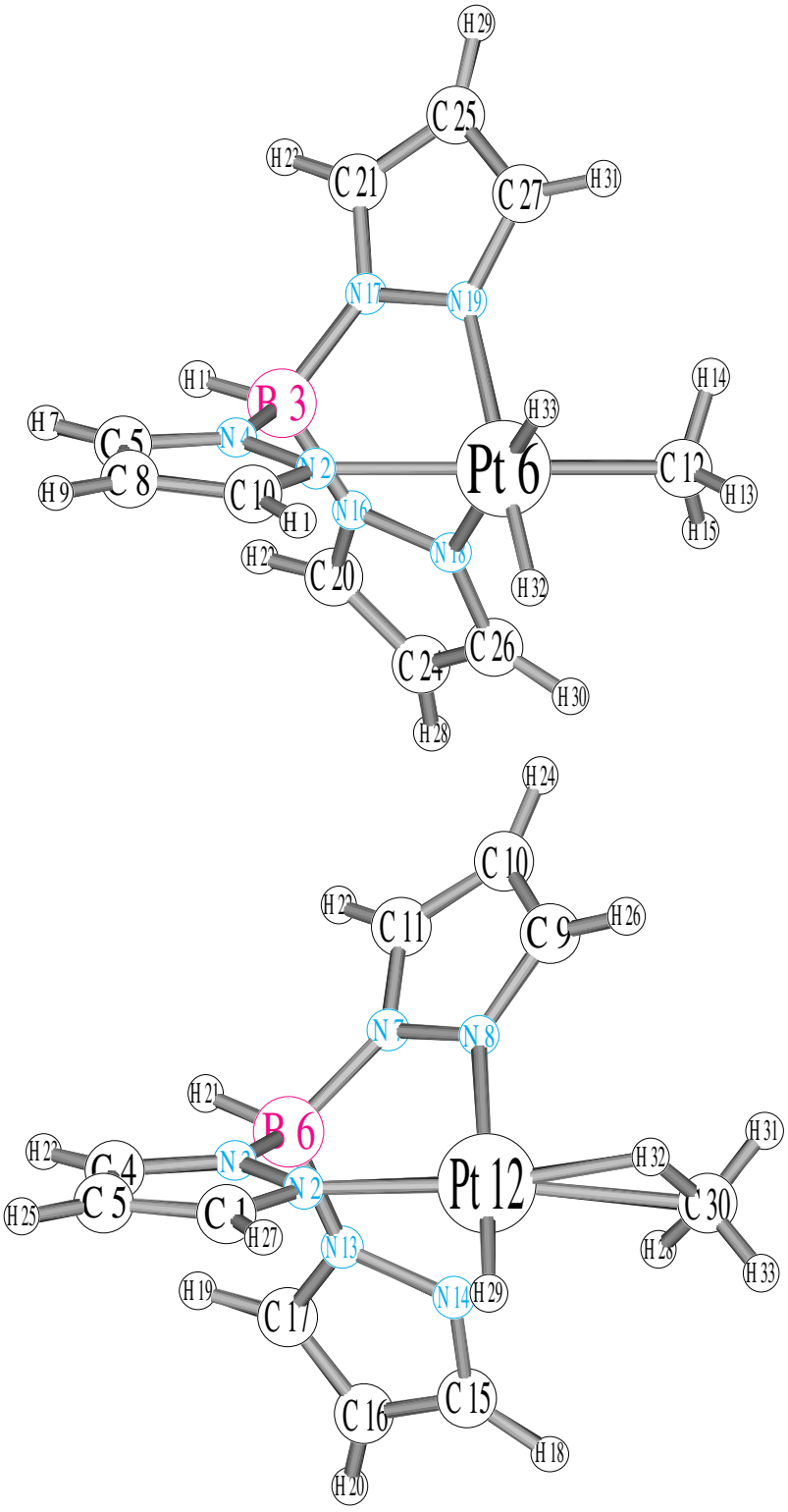

Table 5 Wiberg bond indices for **1**.

Atom	1	2	3	4	5	6	7	8	9
1 H	0.0000	0.0053	0.0003	0.0130	0.0100	0.0005	0.0001	0.0024	0.00090
2 N	0.0053	0.0000	0.0104	1.1660	0.1614	0.2177	0.0118	0.0462	0.00770
3 B	0.0003	0.0104	0.0000	0.6821	0.0113	0.0039	0.0008	0.0125	0.00010
4 N	0.0130	1.1660	0.6821	0.0000	1.2690	0.0126	0.0034	0.0576	0.00850
5 C	0.0100	0.1614	0.0113	1.2690	0.0000	0.0073	0.9161	1.4942	0.00310
6 Pt	0.0005	0.2177	0.0039	0.0126	0.0073	0.0000	0.0003	0.0053	0.00020
7 H	0.0001	0.0118	0.0008	0.0034	0.9161	0.0003	0.0000	0.0031	0.00100
8 C	0.0024	0.0462	0.0125	0.0576	1.4942	0.0053	0.0031	0.0000	0.91960
9 H	0.0009	0.0077	0.0001	0.0085	0.0031	0.0002	0.0010	0.9196	0.00000
10 C	0.9136	1.4145	0.0138	0.1224	0.0110	0.0192	0.0111	1.3923	0.00290
11 H	0.0003	0.0070	0.9538	0.0048	0.0011	0.0018	0.0001	0.0006	0.00000
12 C	0.0004	0.1470	0.0007	0.0013	0.0046	0.6467	0.0003	0.0041	0.00020
13 H	0.0000	0.0002	0.0001	0.0000	0.0000	0.0072	0.0000	0.0000	0.00000
14 H	0.0000	0.0003	0.0000	0.0001	0.0001	0.0091	0.0000	0.0000	0.00000
15 H	0.0000	0.0003	0.0000	0.0001	0.0001	0.0091	0.0000	0.0000	0.00000
16 N	0.0000	0.0036	0.6837	0.0115	0.0064	0.0114	0.0002	0.0012	0.00010
17 N	0.0000	0.0036	0.6837	0.0115	0.0064	0.0114	0.0002	0.0012	0.00010
18 N	0.0001	0.0045	0.0106	0.0036	0.0012	0.1622	0.0000	0.0004	0.00000
19 N	0.0001	0.0045	0.0106	0.0036	0.0012	0.1622	0.0000	0.0004	0.00000
20 C	0.0000	0.0011	0.0114	0.0064	0.0005	0.0057	0.0000	0.0003	0.00000
21 C	0.0000	0.0011	0.0114	0.0064	0.0005	0.0057	0.0000	0.0003	0.00000
22 H	0.0000	0.0000	0.0008	0.0002	0.0000	0.0002	0.0000	0.0000	0.00000
23 H	0.0000	0.0000	0.0008	0.0002	0.0000	0.0002	0.0000	0.0000	0.00000
24 C	0.0000	0.0004	0.0125	0.0012	0.0003	0.0039	0.0000	0.0003	0.00000
25 C	0.0000	0.0004	0.0125	0.0012	0.0003	0.0039	0.0000	0.0003	0.00000
26 C	0.0000	0.0016	0.0139	0.0021	0.0007	0.0175	0.0000	0.0001	0.00000
27 C	0.0000	0.0016	0.0139	0.0021	0.0007	0.0175	0.0000	0.0001	0.00000
28 H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.00000
29 H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0002	0.0000	0.0000	0.00000
30 H	0.0000	0.0000	0.0003	0.0000	0.0000	0.0005	0.0000	0.0000	0.00000
31 H	0.0000	0.0000	0.0003	0.0000	0.0000	0.0005	0.0000	0.0000	0.00000
32 H	0.0001	0.0132	0.0005	0.0006	0.0001	0.6577	0.0000	0.0007	0.00000
33 H	0.0001	0.0132	0.0005	0.0006	0.0001	0.6577	0.0000	0.0007	0.00000

Atom	10	11	12	13	14	15	16	17	18
1 H	0.9136	0.0003	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.00010
2 N	1.4145	0.0070	0.1470	0.0002	0.0003	0.0003	0.0036	0.0036	0.00450
3 B	0.0138	0.9538	0.0007	0.0001	0.0000	0.0000	0.6837	0.6837	0.01060
4 N	0.1224	0.0048	0.0013	0.0000	0.0001	0.0001	0.0115	0.0115	0.00360
5 C	0.0110	0.0011	0.0046	0.0000	0.0001	0.0001	0.0064	0.0064	0.00120
6 Pt	0.0192	0.0018	0.6467	0.0072	0.0091	0.0091	0.0114	0.0114	0.16220
7 H	0.0111	0.0001	0.0003	0.0000	0.0000	0.0000	0.0002	0.0002	0.00000
8 C	1.3923	0.0006	0.0041	0.0000	0.0000	0.0000	0.0012	0.0012	0.00040
9 H	0.0029	0.0000	0.0002	0.0000	0.0000	0.0000	0.0001	0.0001	0.00000
10 C	0.0000	0.0002	0.0029	0.0001	0.0002	0.0002	0.0021	0.0021	0.00160
11 H	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0048	0.0048	0.00710
12 C	0.0029	0.0001	0.0000	0.9423	0.9454	0.9454	0.0007	0.0007	0.01560
13 H	0.0001	0.0000	0.9423	0.0000	0.0002	0.0002	0.0000	0.0000	0.00070
14 H	0.0002	0.0000	0.9454	0.0002	0.0000	0.0003	0.0000	0.0001	0.00010
15 H	0.0002	0.0000	0.9454	0.0002	0.0003	0.0000	0.0001	0.0000	0.00250
16 N	0.0021	0.0048	0.0007	0.0000	0.0000	0.0001	0.0000	0.0116	1.16840
17 N	0.0021	0.0048	0.0007	0.0000	0.0001	0.0000	0.0116	0.0000	0.00340
18 N	0.0016	0.0071	0.0156	0.0007	0.0001	0.0025	1.1684	0.0034	0.00000
19 N	0.0016	0.0071	0.0156	0.0007	0.0025	0.0001	0.0034	1.1684	0.00400
20 C	0.0007	0.0011	0.0002	0.0000	0.0000	0.0001	1.2684	0.0064	0.16250
21 C	0.0007	0.0011	0.0002	0.0000	0.0001	0.0000	0.0064	1.2684	0.00120
22 H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0034	0.0002	0.01190
23 H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0034	0.00000
24 C	0.0001	0.0006	0.0008	0.0000	0.0000	0.0001	0.0575	0.0011	0.04710
25 C	0.0001	0.0006	0.0008	0.0000	0.0001	0.0000	0.0011	0.0575	0.00040
26 C	0.0004	0.0002	0.0014	0.0001	0.0001	0.0008	0.1219	0.0020	1.41790
27 C	0.0004	0.0002	0.0014	0.0001	0.0008	0.0001	0.0020	0.1219	0.00160
28 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0085	0.0001	0.00770
29 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0085	0.00000
30 H	0.0000	0.0004	0.0002	0.0000	0.0000	0.0001	0.0130	0.0000	0.00550
31 H	0.0000	0.0004	0.0002	0.0000	0.0001	0.0000	0.0000	0.0130	0.00000
32 H	0.0003	0.0000	0.0736	0.0009	0.0005	0.0001	0.0005	0.0012	0.01060
33 H	0.0003	0.0000	0.0736	0.0009	0.0001	0.0005	0.0012	0.0005	0.16530

Atom	19	20	21	22	23	24	25	26	27
1 H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
2 N	0.0045	0.0011	0.0011	0.0000	0.0000	0.0004	0.0004	0.0016	0.00160
3 B	0.0106	0.0114	0.0114	0.0008	0.0008	0.0125	0.0125	0.0139	0.01390
4 N	0.0036	0.0064	0.0064	0.0002	0.0002	0.0012	0.0012	0.0021	0.00210
5 C	0.0012	0.0005	0.0005	0.0000	0.0000	0.0003	0.0003	0.0007	0.00070
6 Pt	0.1622	0.0057	0.0057	0.0002	0.0002	0.0039	0.0039	0.0175	0.01750
7 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
8 C	0.0004	0.0003	0.0003	0.0000	0.0000	0.0003	0.0003	0.0001	0.00010
9 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
10 C	0.0016	0.0007	0.0007	0.0000	0.0000	0.0001	0.0001	0.0004	0.00040
11 H	0.0071	0.0011	0.0011	0.0001	0.0001	0.0006	0.0006	0.0002	0.00020
12 C	0.0156	0.0002	0.0002	0.0000	0.0000	0.0008	0.0008	0.0014	0.00140
13 H	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.00010
14 H	0.0025	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0001	0.00080
15 H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0008	0.00010
16 N	0.0034	1.2684	0.0064	0.0034	0.0002	0.0575	0.0011	0.1219	0.00200
17 N	1.1684	0.0064	1.2684	0.0002	0.0034	0.0011	0.0575	0.0020	0.12190
18 N	0.0040	0.1625	0.0012	0.0119	0.0000	0.0471	0.0004	1.4179	0.00160
19 N	0.0000	0.0012	0.1625	0.0000	0.0119	0.0004	0.0471	0.0016	1.41790
20 C	0.0012	0.0000	0.0005	0.9161	0.0000	1.4950	0.0003	0.0112	0.00070
21 C	0.1625	0.0005	0.0000	0.0000	0.9161	0.0003	1.4950	0.0007	0.01120
22 H	0.0000	0.9161	0.0000	0.0000	0.0000	0.0031	0.0000	0.0111	0.00000
23 H	0.0119	0.0000	0.9161	0.0000	0.0000	0.0000	0.0031	0.0000	0.01110
24 C	0.0004	1.4950	0.0003	0.0031	0.0000	0.0000	0.0003	1.3916	0.00010
25 C	0.0471	0.0003	1.4950	0.0000	0.0031	0.0003	0.0000	0.0001	1.39160
26 C	0.0016	0.0112	0.0007	0.0111	0.0000	1.3916	0.0001	0.0000	0.00030
27 C	1.4179	0.0007	0.0112	0.0000	0.0111	0.0001	1.3916	0.0003	0.00000
28 H	0.0000	0.0031	0.0000	0.0010	0.0000	0.9196	0.0000	0.0029	0.00000
29 H	0.0077	0.0000	0.0031	0.0000	0.0010	0.0000	0.9196	0.0000	0.00290
30 H	0.0000	0.0100	0.0000	0.0001	0.0000	0.0024	0.0000	0.9139	0.00000
31 H	0.0055	0.0000	0.0100	0.0000	0.0001	0.0000	0.0024	0.0000	0.91390
32 H	0.1653	0.0001	0.0049	0.0000	0.0003	0.0006	0.0045	0.0002	0.00270
33 H	0.0106	0.0049	0.0001	0.0003	0.0000	0.0045	0.0006	0.0027	0.00020

Atom		28	29	30	31	32	33
1	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
2	N	0.0000	0.0000	0.0000	0.0000	0.0132	0.0132
3	B	0.0001	0.0001	0.0003	0.0003	0.0005	0.0005
4	N	0.0001	0.0001	0.0000	0.0000	0.0006	0.0006
5	C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
6	Pt	0.0002	0.0002	0.0005	0.0005	0.6577	0.6577
7	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	C	0.0000	0.0000	0.0000	0.0000	0.0007	0.0007
9	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	C	0.0000	0.0000	0.0000	0.0000	0.0003	0.0003
11	H	0.0000	0.0000	0.0004	0.0004	0.0000	0.0000
12	C	0.0000	0.0000	0.0002	0.0002	0.0736	0.0736
13	H	0.0000	0.0000	0.0000	0.0000	0.0009	0.0009
14	H	0.0000	0.0000	0.0000	0.0001	0.0005	0.0001
15	H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0005
16	N	0.0085	0.0001	0.0130	0.0000	0.0005	0.0012
17	N	0.0001	0.0085	0.0000	0.0130	0.0012	0.0005
18	N	0.0077	0.0000	0.0055	0.0000	0.0106	0.1653
19	N	0.0000	0.0077	0.0000	0.0055	0.1653	0.0106
20	C	0.0031	0.0000	0.0100	0.0000	0.0001	0.0049
21	C	0.0000	0.0031	0.0000	0.0100	0.0049	0.0001
22	H	0.0010	0.0000	0.0001	0.0000	0.0000	0.0003
23	H	0.0000	0.0010	0.0000	0.0001	0.0003	0.0000
24	C	0.9196	0.0000	0.0024	0.0000	0.0006	0.0045
25	C	0.0000	0.9196	0.0000	0.0024	0.0045	0.0006
26	C	0.0029	0.0000	0.9139	0.0000	0.0002	0.0027
27	C	0.0000	0.0029	0.0000	0.9139	0.0027	0.0002
28	H	0.0000	0.0000	0.0009	0.0000	0.0000	0.0002
29	H	0.0000	0.0000	0.0000	0.0009	0.0002	0.0000
30	H	0.0009	0.0000	0.0000	0.0000	0.0001	0.0004
31	H	0.0000	0.0009	0.0000	0.0000	0.0004	0.0001
32	H	0.0000	0.0002	0.0001	0.0004	0.0000	0.0639
33	H	0.0002	0.0000	0.0004	0.0001	0.0639	0.0000

Table 6 Wiberg bond indices for **2**.

Atom	1	2	3	4	5	6	7	8	9
1 C	0.0000	1.3702	0.1289	0.0109	1.4098	0.0133	0.0016	0.0016	0.00020
2 N	1.3702	0.0000	1.1533	0.1497	0.0455	0.0107	0.0029	0.0125	0.00080
3 N	0.1289	1.1533	0.0000	1.2878	0.0538	0.6617	0.0101	0.0035	0.00130
4 C	0.0109	0.1497	1.2878	0.0000	1.4761	0.0119	0.0060	0.0014	0.00050
5 C	1.4098	0.0455	0.0538	1.4761	0.0000	0.0121	0.0007	0.0003	0.00010
6 B	0.0133	0.0107	0.6617	0.0119	0.0121	0.0000	0.6820	0.0111	0.01370
7 N	0.0016	0.0029	0.0101	0.0060	0.0007	0.6820	0.0000	1.1737	0.12430
8 N	0.0016	0.0125	0.0035	0.0014	0.0003	0.0111	1.1737	0.0000	1.40730
9 C	0.0002	0.0008	0.0013	0.0005	0.0001	0.0137	0.1243	1.4073	0.00000
10 C	0.0001	0.0004	0.0008	0.0003	0.0002	0.0124	0.0541	0.0515	1.39870
11 C	0.0006	0.0008	0.0062	0.0005	0.0003	0.0120	1.2769	0.1604	0.01170
12 Pt	0.0355	0.4976	0.0248	0.0179	0.0125	0.0048	0.0151	0.1903	0.02120
13 N	0.0026	0.0028	0.0130	0.0064	0.0011	0.7088	0.0119	0.0031	0.00280
14 N	0.0004	0.0020	0.0030	0.0007	0.0004	0.0137	0.0028	0.0024	0.00100
15 C	0.0005	0.0004	0.0025	0.0008	0.0001	0.0152	0.0013	0.0005	0.00020
16 C	0.0001	0.0004	0.0017	0.0003	0.0002	0.0136	0.0009	0.0003	0.00030
17 C	0.0006	0.0006	0.0055	0.0004	0.0002	0.0124	0.0062	0.0005	0.00060
18 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.00000
19 H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0010	0.0003	0.0000	0.00000
20 H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0002	0.0000	0.00000
21 H	0.0003	0.0079	0.0062	0.0015	0.0009	0.9459	0.0055	0.0075	0.00050
22 H	0.0000	0.0000	0.0004	0.0000	0.0000	0.0010	0.0036	0.0117	0.01120
23 H	0.0110	0.0115	0.0038	0.9138	0.0032	0.0010	0.0004	0.0001	0.00000
24 H	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0085	0.0078	0.00290
25 H	0.0031	0.0078	0.0084	0.0032	0.9181	0.0001	0.0001	0.0000	0.00000
26 H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0003	0.0128	0.0052	0.91830
27 H	0.9127	0.0041	0.0122	0.0101	0.0027	0.0003	0.0000	0.0001	0.00000
28 H	0.0002	0.0032	0.0001	0.0001	0.0001	0.0000	0.0001	0.0003	0.00020
29 H	0.0009	0.0573	0.0014	0.0010	0.0033	0.0008	0.0011	0.1448	0.00320
30 C	0.0013	0.0350	0.0008	0.0018	0.0009	0.0002	0.0005	0.0056	0.00220
31 H	0.0001	0.0014	0.0001	0.0001	0.0001	0.0000	0.0000	0.0011	0.00060
32 H	0.0004	0.0121	0.0001	0.0005	0.0004	0.0001	0.0001	0.0012	0.00040
33 H	0.0001	0.0009	0.0000	0.0000	0.0000	0.0000	0.0001	0.0008	0.00030

Atom	10	11	12	13	14	15	16	17	18
1 C	0.0001	0.0006	0.0355	0.0026	0.0004	0.0005	0.0001	0.0006	0.00000
2 N	0.0004	0.0008	0.4976	0.0028	0.0020	0.0004	0.0004	0.0006	0.00000
3 N	0.0008	0.0062	0.0248	0.0130	0.0030	0.0025	0.0017	0.0055	0.00000
4 C	0.0003	0.0005	0.0179	0.0064	0.0007	0.0008	0.0003	0.0004	0.00000
5 C	0.0002	0.0003	0.0125	0.0011	0.0004	0.0001	0.0002	0.0002	0.00000
6 B	0.0124	0.0120	0.0048	0.7088	0.0137	0.0152	0.0136	0.0124	0.00030
7 N	0.0541	1.2769	0.0151	0.0119	0.0028	0.0013	0.0009	0.0062	0.00000
8 N	0.0515	0.1604	0.1903	0.0031	0.0024	0.0005	0.0003	0.0005	0.00000
9 C	1.3987	0.0117	0.0212	0.0028	0.0010	0.0002	0.0003	0.0006	0.00000
10 C	0.0000	1.4879	0.0049	0.0012	0.0003	0.0001	0.0001	0.0002	0.00000
11 C	1.4879	0.0000	0.0075	0.0061	0.0007	0.0004	0.0004	0.0005	0.00000
12 Pt	0.0049	0.0075	0.0000	0.0017	0.0189	0.0022	0.0008	0.0008	0.00000
13 N	0.0012	0.0061	0.0017	0.0000	1.1913	0.1000	0.0666	1.2322	0.01390
14 N	0.0003	0.0007	0.0189	1.1913	0.0000	1.5082	0.0513	0.1808	0.00730
15 C	0.0001	0.0004	0.0022	0.1000	1.5082	0.0000	1.3528	0.0152	0.92040
16 C	0.0001	0.0004	0.0008	0.0666	0.0513	1.3528	0.0000	1.5261	0.00220
17 C	0.0002	0.0005	0.0008	1.2322	0.1808	0.0152	1.5261	0.0000	0.01000
18 H	0.0000	0.0000	0.0000	0.0139	0.0073	0.9204	0.0022	0.0100	0.00000
19 H	0.0000	0.0000	0.0000	0.0032	0.0123	0.0119	0.0032	0.9199	0.00010
20 H	0.0000	0.0000	0.0001	0.0091	0.0080	0.0027	0.9229	0.0032	0.00090
21 H	0.0009	0.0017	0.0019	0.0045	0.0079	0.0005	0.0010	0.0015	0.00040
22 H	0.0030	0.9151	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.00000
23 H	0.0000	0.0000	0.0008	0.0002	0.0000	0.0000	0.0000	0.0000	0.00000
24 H	0.9196	0.0032	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
25 H	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.00000
26 H	0.0026	0.0101	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
27 H	0.0000	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
28 H	0.0000	0.0000	0.0155	0.0003	0.0024	0.0002	0.0003	0.0001	0.00000
29 H	0.0042	0.0044	0.7350	0.0000	0.0013	0.0001	0.0000	0.0001	0.00000
30 C	0.0005	0.0001	0.1524	0.0001	0.0023	0.0003	0.0001	0.0001	0.00000
31 H	0.0001	0.0001	0.0070	0.0000	0.0001	0.0000	0.0000	0.0000	0.00000
32 H	0.0001	0.0001	0.0968	0.0000	0.0011	0.0000	0.0001	0.0001	0.00000
33 H	0.0000	0.0001	0.0045	0.0000	0.0001	0.0000	0.0000	0.0000	0.00000

Atom	19	20	21	22	23	24	25	26	27
1 C	0.0000	0.0000	0.0003	0.0000	0.0110	0.0000	0.0031	0.0000	0.91270
2 N	0.0000	0.0000	0.0079	0.0000	0.0115	0.0000	0.0078	0.0001	0.00410
3 N	0.0001	0.0001	0.0062	0.0004	0.0038	0.0002	0.0084	0.0000	0.01220
4 C	0.0000	0.0000	0.0015	0.0000	0.9138	0.0000	0.0032	0.0000	0.01010
5 C	0.0000	0.0000	0.0009	0.0000	0.0032	0.0000	0.9181	0.0000	0.00270
6 B	0.0010	0.0001	0.9459	0.0010	0.0010	0.0001	0.0001	0.0003	0.00030
7 N	0.0003	0.0002	0.0055	0.0036	0.0004	0.0085	0.0001	0.0128	0.00000
8 N	0.0000	0.0000	0.0075	0.0117	0.0001	0.0078	0.0000	0.0052	0.00010
9 C	0.0000	0.0000	0.0005	0.0112	0.0000	0.0029	0.0000	0.9183	0.00000
10 C	0.0000	0.0000	0.0009	0.0030	0.0000	0.9196	0.0000	0.0026	0.00000
11 C	0.0000	0.0000	0.0017	0.9151	0.0000	0.0032	0.0000	0.0101	0.00000
12 Pt	0.0000	0.0001	0.0019	0.0003	0.0008	0.0002	0.0004	0.0003	0.00050
13 N	0.0032	0.0091	0.0045	0.0001	0.0002	0.0000	0.0001	0.0000	0.00000
14 N	0.0123	0.0080	0.0079	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
15 C	0.0119	0.0027	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
16 C	0.0032	0.9229	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
17 C	0.9199	0.0032	0.0015	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
18 H	0.0001	0.0009	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
19 H	0.0000	0.0010	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
20 H	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
21 H	0.0001	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0004	0.00040
22 H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0010	0.0000	0.0001	0.00000
23 H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0011	0.0000	0.00010
24 H	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0009	0.00000
25 H	0.0000	0.0000	0.0000	0.0000	0.0011	0.0000	0.0000	0.0000	0.00100
26 H	0.0000	0.0000	0.0004	0.0001	0.0000	0.0009	0.0000	0.0000	0.00000
27 H	0.0000	0.0000	0.0004	0.0000	0.0001	0.0000	0.0010	0.0000	0.00000
28 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000
29 H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0001	0.0004	0.00010
30 C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0003	0.00010
31 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.00000
32 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.00000
33 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00000

Atom	28	29	30	31	32	33
1 C	0.0002	0.0009	0.0013	0.0001	0.0004	0.0001
2 N	0.0032	0.0573	0.0350	0.0014	0.0121	0.0009
3 N	0.0001	0.0014	0.0008	0.0001	0.0001	0.0000
4 C	0.0001	0.0010	0.0018	0.0001	0.0005	0.0000
5 C	0.0001	0.0033	0.0009	0.0001	0.0004	0.0000
6 B	0.0000	0.0008	0.0002	0.0000	0.0001	0.0000
7 N	0.0001	0.0011	0.0005	0.0000	0.0001	0.0001
8 N	0.0003	0.1448	0.0056	0.0011	0.0012	0.0008
9 C	0.0002	0.0032	0.0022	0.0006	0.0004	0.0003
10 C	0.0000	0.0042	0.0005	0.0001	0.0001	0.0000
11 C	0.0000	0.0044	0.0001	0.0001	0.0001	0.0001
12 Pt	0.0155	0.7350	0.1524	0.0070	0.0968	0.0045
13 N	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000
14 N	0.0024	0.0013	0.0023	0.0001	0.0011	0.0001
15 C	0.0002	0.0001	0.0003	0.0000	0.0000	0.0000
16 C	0.0003	0.0000	0.0001	0.0000	0.0001	0.0000
17 C	0.0001	0.0001	0.0001	0.0000	0.0001	0.0000
18 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22 H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
23 H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
24 H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
25 H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
26 H	0.0000	0.0004	0.0003	0.0001	0.0001	0.0000
27 H	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000
28 H	0.0000	0.0008	0.8928	0.0014	0.0003	0.0015
29 H	0.0008	0.0000	0.0112	0.0003	0.0119	0.0015
30 C	0.8928	0.0112	0.0000	0.9241	0.8361	0.9212
31 H	0.0014	0.0003	0.9241	0.0000	0.0009	0.0002
32 H	0.0003	0.0119	0.8361	0.0009	0.0000	0.0011
33 H	0.0015	0.0015	0.9212	0.0002	0.0011	0.0000

Computed Structures of Complexes 1-25 and the transition states (in .xyz format)

```
1.xyz
   33
 SCF Done:  E(RmPW+HF-PW91) =  -862.314541145     A.U. after    1 cycles
   H     3.402445    1.218923    0.000000
   N     1.736939   -0.050110    0.000000
   B     0.172059   -2.021765    0.000000
   N     1.580739   -1.402486    0.000000
   C     2.798332   -1.993209    0.000000
   Pt    0.000000    1.180283    0.000000
   H     2.896682   -3.060349    0.000000
   C     3.767981   -0.998946    0.000000
   H     4.831284   -1.125527    0.000000
   C     3.047463    0.208278    0.000000
   H     0.242685   -3.213261    0.000000
   C    -1.670071    2.364730    0.000000
   H    -1.415066    3.420792    0.000000
   H    -2.265530    2.140963    0.885295
   H    -2.265530    2.140963   -0.885295
   N    -0.574345   -1.529568   -1.249994
   N    -0.574345   -1.529568    1.249994
   N    -0.760636   -0.197290   -1.458617
   N    -0.760636   -0.197290    1.458617
   C    -1.105080   -2.223891   -2.283397
   C    -1.105080   -2.223891    2.283397
   H    -1.062508   -3.294316   -2.312397
   H    -1.062508   -3.294316    2.312397
   C    -1.648913   -1.319002   -3.185461
   C    -1.648913   -1.319002    3.185461
   C    -1.404207   -0.054944   -2.620187
   C    -1.404207   -0.054944    2.620187
   H    -2.143197   -1.537229   -4.109967
   H    -2.143197   -1.537229    4.109967
   H    -1.651267    0.918734   -2.992438
   H    -1.651267    0.918734    2.992438
   H     0.564421    2.191474   -1.036181
   H     0.564421    2.191474    1.036181


10a.xyz
   15
 SCF Done:  E(RmPW+HF-PW91) =  -273.114983274     A.U. after    1 cycles
   C    -2.030714   -0.410810   -0.076559
   Pt   -0.006438   -0.184158   -0.002386
   N     2.206939   -0.067186   -0.054058
   N    -0.294952    2.017798    0.012655
   H     0.100281   -1.727319   -0.085811
   H     2.558949   -0.196230   -0.997870
   H    -0.203686   -0.628346    1.433129
   H    -2.343951   -1.416864    0.176421
   H    -2.305699   -0.200831   -1.114371
   H    -2.528380    0.293403    0.588580
   H     0.293663    2.528723   -0.637215
   H    -0.119777    2.359259    0.952251
   H    -1.267593    2.197364   -0.217006
   H     2.574172    0.800504    0.319931
```

```
   H     2.544557   -0.834757    0.517209


10b.xyz
   15
 SCF Done:  E(RmPW+HF-PW91) =  -273.112677603     A.U. after   12 cycles
   C    -1.829295   -0.628376    0.000000
   Pt    0.000000    0.290716    0.000000
   H     0.125092   -1.212205    2.238928
   N     0.894039   -0.899940   -1.654885
   H    -0.648458    1.235155    1.041284
   N     0.894039   -0.899940    1.654885
   H    -0.648458    1.235155   -1.041284
   H    -2.368515   -0.330436    0.890690
   H    -1.599016   -1.691776    0.000000
   H    -2.368515   -0.330436   -0.890690
   H     1.434161   -1.707304   -1.364776
   H     1.486836   -0.292531   -2.212790
   H     0.125092   -1.212205   -2.238928
   H     1.486836   -0.292531    2.212790
   H     1.434161   -1.707304    1.364776


11.xyz
   15
 SCF Done:  E(RmPW+HF-PW91) =  -273.133502234     A.U. after    1 cycles
   H    -3.001590    0.493938   -0.025144
   Pt    0.038808   -0.172011   -0.024562
   C    -2.356780   -0.368059    0.101383
   N    -0.115500    2.039333    0.006724
   H     0.125512   -1.723645   -0.055758
   N     2.072842   -0.244268    0.097764
   H    -1.970097   -0.386036    1.123809
   H    -2.897198   -1.294637   -0.050202
   H     2.519750    0.666444    0.095403
   H    -1.656050   -0.354964   -0.798059
   H     0.370901    2.434544    0.804389
   H    -1.092363    2.306198    0.072235
   H     0.264058    2.431394   -0.848728
   H     2.420553   -0.779749   -0.693150
   H     2.328823   -0.733724    0.951300


12.xyz
   10
 SCF Done:  E(RmPW+HF-PW91) =  -232.601587783     A.U. after    1 cycles
   H     2.051362    1.049570   -0.825995
   Pt    0.044286   -0.249589   -0.000004
   N     1.469561    1.168287   -0.000001
   N    -1.925769    0.777353    0.000001
   H     1.295512   -1.160378    0.000094
   H    -2.030160    1.354503    0.827987
   H    -2.678458    0.093479   -0.000830
   H     2.051271    1.049526    0.826050
   H     1.079474    2.105757   -0.000017
   H    -2.029821    1.355995   -0.826982
```

13.xyz

14

SCF Done: E(RmPW+HF-PW91) = -289.233696268 A.U. after 9 cycles

H	2.339202	-0.780938	-0.861441
Pt	-0.002930	-0.171331	-0.000263
N	2.056998	-0.323164	0.000369
N	0.030219	2.049615	0.000711
H	-0.018400	-1.732960	0.002596
N	-2.064356	-0.288949	0.000353
H	-2.337143	-0.882268	0.778343
H	2.320646	-0.919157	0.779440
H	2.556133	0.555412	0.083321
H	-2.353644	-0.740319	-0.862504
H	0.757965	2.391901	-0.617106
H	0.205058	2.378831	0.944336
H	-0.850535	2.434308	-0.321783
H	-2.550783	0.596470	0.085307

14.xyz

16

SCF Done: E(RmPW+HF-PW91) = -348.347993787 A.U. after 1 cycles

H	0.907671	2.470384	-0.568489
Pt	0.212722	-0.149619	-0.060046
H	0.585974	2.347795	1.052310
N	0.302216	2.048142	0.126385
H	0.065007	-1.697795	-0.210794
N	2.186350	-0.520507	0.279175
H	2.562859	-1.006626	-0.529844
H	2.740111	0.312317	0.447706
O	-1.806014	0.123925	-0.430130
H	2.264298	-1.134868	1.084752
H	-0.651886	2.352159	-0.040485
C	-2.810618	-0.367561	0.523478
H	-2.060067	-0.040941	-1.347420
H	-2.540047	0.034295	1.490099
H	-2.791235	-1.451996	0.546327
H	-3.783114	0.006058	0.220657

15.xyz

15

SCF Done: E(RmPW+HF-PW91) = -273.119013851 A.U. after 8 cycles

C	2.046730	-0.324140	0.000294
Pt	0.011620	-0.162626	-0.000085
N	-2.208325	-0.051087	0.000275
H	-2.547715	0.420147	0.832289
H	-0.033158	-1.819661	0.428266
N	0.255293	1.881291	0.000070
H	-0.034566	-1.819643	-0.428233
H	2.365874	-0.855110	0.896358
H	2.534441	0.650119	-0.016488
H	2.365295	-0.884143	-0.877981
H	-2.592829	-0.990011	-0.005681
H	-2.547955	0.430564	-0.825638
H	0.803289	2.137181	0.817612
H	-0.611123	2.408747	0.011826
H	0.782925	2.140047	-0.829888

16.xyz
13
SCF Done: E(RmPW+HF-PW91) = -271.907743587 A.U. after 1 cycles

C	1.962191	-0.584800	-0.000784
Pt	-0.011292	-0.163100	0.000179
N	-2.233311	-0.045921	-0.000729
N	0.524912	1.778053	-0.000333
H	-2.569245	0.479809	0.798840
H	-2.628685	-0.980606	0.052445
H	-2.570956	0.388310	-0.852923
H	2.021653	-1.678292	0.019591
H	2.473308	-0.197781	0.881323
H	2.460877	-0.231826	-0.904289
H	0.248776	2.215491	0.874575
H	0.094722	2.268046	-0.779522
H	1.535968	1.842549	-0.091877

17.xyz
17
SCF Done: E(RmPW+HF-PW91) = -328.533556157 A.U. after 1 cycles

C	0.169041	2.043201	0.000000
Pt	0.000000	0.013675	0.000000
N	-0.163410	-2.201706	0.000000
N	0.004468	0.108540	2.065504
H	0.766209	-2.607738	0.000000
N	0.004468	0.108540	-2.065504
H	-0.668370	-2.524555	0.817716
H	-0.305915	2.493176	-0.874381
H	1.225575	2.323683	0.000000
H	-0.305915	2.493176	0.874381
H	0.355323	-0.727388	2.519973
H	-0.939612	0.294867	2.390813
H	0.596220	0.889175	2.334279
H	-0.939612	0.294867	-2.390813
H	0.355323	-0.727388	-2.519973
H	0.596220	0.889175	-2.334279
H	-0.668370	-2.524555	-0.817716

18.xyz
19
SCF Done: E(RmPW+HF-PW91) = -387.648899338 A.U. after 1 cycles

H	0.889566	2.588151	-0.681534
Pt	0.215144	-0.005392	-0.043311
H	0.511491	2.556830	0.931511
N	0.265956	2.198151	0.015849
C	0.039353	-2.030453	-0.114052
N	2.200014	-0.291373	0.320706
H	2.666946	0.526152	0.697891
H	2.297673	-1.055985	0.982637
O	-1.810432	0.219107	-0.437226
H	2.653846	-0.559346	-0.548164
H	-0.685446	2.476280	-0.202527
C	-2.817799	-0.168219	0.558288
H	-2.067294	-0.019997	-1.337066

```
   H    -2.569152    0.358768    1.469243
   H    -2.779685   -1.240335    0.719644
   H    -3.794245    0.141780    0.200996
   H     0.926707   -2.518299   -0.523124
   H    -0.802431   -2.320287   -0.746145
   H    -0.136851   -2.421420    0.891380
```

```
19a.xyz
   34
 SCF Done:  E(RmPW+HF-PW91) =  -862.913038644     A.U. after   15 cycles
   C    -0.137516    2.909144    0.757143
   N     0.047629    1.603568    0.491005
   N     1.156690    1.203455    1.194562
   C     1.646502    2.258538    1.891539
   C     0.850589    3.365588    1.638852
   B     1.701904   -0.211445    1.131560
   N     0.621197   -1.260604    1.366817
   N    -0.569218   -1.304298    0.688882
   C    -1.213979   -2.418167    1.086274
   C    -0.446780   -3.102856    2.030954
   C     0.704193   -2.339934    2.178183
   Pt   -1.302951    0.261984   -0.473542
   H    -2.266195    1.442841   -0.808435
   N     2.342656   -0.427402   -0.299284
   N     2.121175    0.377761   -1.367111
   C     2.819185   -0.054405   -2.435061
   C     3.522923   -1.187369   -2.044582
   C     3.196433   -1.383081   -0.699195
   H     2.780519    0.452102   -3.378587
   H     3.533721   -2.139564   -0.019379
   H     4.181328   -1.779543   -2.645107
   H     2.565571   -0.361025    1.937187
   H     1.559189   -2.497148    2.805682
   H     2.514251    2.157686    2.512897
   H    -0.694771   -4.012253    2.538068
   H     0.963115    4.352481    2.037967
   H    -2.179993   -2.664590    0.695437
   H    -0.957963    3.446585    0.324384
   C    -2.670579   -0.980311   -1.344523
   H    -1.273140    0.952074   -1.859512
   H     1.490551    1.158172   -1.282545
   H    -3.128714   -0.549002   -2.228842
   H    -2.177256   -1.911266   -1.619849
   H    -3.456284   -1.175339   -0.612499
```

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19b.xyz
   34
 SCF Done:  E(RmPW+HF-PW91) =  -862.913107000     A.U. after   14 cycles
   C     0.534240   -2.777951    0.736518
   N     0.182342   -1.510926    0.474586
   N    -0.818568   -1.177981    1.348354
   C    -1.074010   -2.239696    2.159039
   C    -0.234858   -3.282260    1.797462
   B    -1.522929    0.169296    1.310122
   N    -0.589232    1.359277    1.333697
```

```
   N     0.467890    1.486534    0.471348
   C     1.028769    2.681892    0.705307
   C     0.339682    3.344671    1.732804
   C    -0.674234    2.475337    2.102912
   Pt    1.174317   -0.090778   -0.770775
   C     3.050574   -0.272379    0.017182
   N    -2.305749    0.232258   -0.073646
   N    -2.939193   -0.847286   -0.593249
   C    -3.639006   -0.499439   -1.693074
   C    -3.454971    0.862883   -1.889710
   C    -2.615461    1.281931   -0.850829
   H    -4.202504   -1.216655   -2.255736
   H    -2.232818    2.259052   -0.633953
   H    -3.867193    1.465042   -2.672186
   H    -2.305553    0.235880    2.206926
   H     3.780195   -0.334766   -0.778632
   H     3.030283   -1.176756    0.617148
   H     3.195174    0.612204    0.629439
   H    -1.435504    2.577513    2.850891
   H    -1.814930   -2.182729    2.932410
   H     0.552290    4.309656    2.144699
   H    -0.178646   -4.255752    2.239450
   H     1.881543    3.005562    0.142104
   H     1.306759   -3.259305    0.170172
   H     1.895244    0.889673   -1.739246
   H     1.694840   -1.186024   -1.747321
   H    -2.828023   -1.751495   -0.169588


2.xyz
   33
 SCF Done:  E(RmPW+HF-PW91) =  -862.278334980     A.U. after    1 cycles
   C    -0.281992    3.007547    0.216998
   N    -0.094510    1.680413    0.223024
   N     1.071688    1.414421    0.874143
   C     1.612411    2.585502    1.277647
   C     0.783116    3.627561    0.880738
   B     1.691106   -0.001946    1.042496
   N     0.618762   -0.937479    1.615724
   N    -0.638314   -1.008216    1.106665
   C    -1.310363   -1.923446    1.817445
   C    -0.474672   -2.467578    2.805410
   C     0.738004   -1.811282    2.641237
   Pt   -1.211707    0.230117   -0.509935
   N     2.260531   -0.539518   -0.262855
   N     1.475016   -1.044534   -1.262218
   C     2.311831   -1.387969   -2.247173
   C     3.653741   -1.111225   -1.898281
   C     3.574027   -0.572941   -0.626351
   H     1.930083   -1.815148   -3.154256
   H     4.345781   -0.225131    0.031730
   H     4.535668   -1.283333   -2.482133
   H     2.578917    0.106493    1.840284
   H     1.659201   -1.907347    3.179741
   H     2.540574    2.602903    1.812004
   H    -0.718673   -3.216666    3.530579
   H     0.926935    4.675440    1.045472
```

```
   H    -2.339461   -2.136010    1.607045
   H    -1.146857    3.430724   -0.250254
   H    -1.217283   -1.652808   -1.795143
   H    -1.633791    1.193291   -1.674778
   C    -2.294785   -1.600333   -1.620834
   H    -2.601257   -2.503896   -1.105428
   H    -2.727232   -0.752953   -0.990427
   H    -2.795136   -1.485561   -2.574351


20.xyz
   34
 SCF Done:  E(RmPW+HF-PW91) =  -862.635278833     A.U. after    1 cycles
   Pt    0.635801   -0.392310   -0.831410
   B    -1.304925    0.649343    1.413310
   N    -1.492173   -0.439837   -0.836572
   N    -2.128038    0.075865    0.253964
   N    -0.333590   -0.465738    1.883501
   N     0.577624   -1.021515    1.034735
   N     0.482573    1.585972   -0.077074
   N    -0.444728    1.809492    0.896865
   C     2.704041   -0.340804   -0.757064
   C    -2.429470   -0.910845   -1.673074
   C    -3.698731   -0.692068   -1.122764
   C    -3.462352   -0.069267    0.097033
   C     1.274364   -1.961676    1.696043
   C     0.807282   -2.018975    3.008657
   C    -0.202965   -1.062596    3.084021
   C    -0.393037    3.107895    1.265471
   C     0.588429    3.743043    0.513095
   C     1.115409    2.745396   -0.315725
   H     0.750549   -1.885466   -1.287412
   H    -2.000022    0.993403    2.311113
   H    -2.167368   -1.379369   -2.601081
   H    -4.646171   -0.952984   -1.547042
   H    -4.151220    0.268745    0.845359
   H     2.042965   -2.532081    1.215352
   H     1.151120   -2.664155    3.790209
   H    -0.824840   -0.779229    3.909440
   H     1.899811    2.816127   -1.043035
   H     0.879761    4.771950    0.559896
   H    -1.040610    3.496571    2.025915
   H     3.117771   -1.330540   -0.919375
   H     2.975582    0.035682    0.223844
   H     3.065628    0.336970   -1.526519
   H     0.646083    0.445025   -2.419492
   H     0.783597   -0.337524   -2.615796


21.xyz
   32
 SCF Done:  E(RmPW+HF-PW91) =  -861.431006727     A.U. after    1 cycles
   C     0.897532    2.844765   -0.297265
   N     0.367048    1.632174   -0.069534
   N    -0.534043    1.756541    0.946916
   C    -0.572303    3.045998    1.349282
   C     0.323544    3.776369    0.576780
   Pt    0.640366   -0.321797   -0.856691
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   C     2.670290   -0.095348   -0.962068
   B    -1.283826    0.517336    1.444343
   N    -0.210127   -0.553861    1.828692
   N     0.695641   -1.038692    0.930497
   C     1.473158   -1.965124    1.518192
   C     1.062735   -2.086620    2.844433
   C     0.008019   -1.187351    2.997096
   N    -1.471650   -0.515906   -0.823682
   N    -2.109821   -0.071937    0.297700
   C    -3.437267   -0.290336    0.166721
   C    -3.666387   -0.888774   -1.066774
   C    -2.400425   -1.019386   -1.652010
   H     0.841445   -1.767973   -1.407970
   H    -1.955329    0.762060    2.390896
   H    -2.132633   -1.444841   -2.598959
   H    -4.607479   -1.190543   -1.477906
   H    -4.127044   -0.017516    0.940498
   H     2.247226   -2.474356    0.981714
   H     1.473273   -2.738397    3.587447
   H    -0.591446   -0.967993    3.857905
   H     1.643978    2.996718   -1.051836
   H     0.531460    4.824540    0.639159
   H    -1.217316    3.363780    2.144160
   H     3.198371   -1.042104   -0.979307
   H     3.014400    0.519204   -0.135982
   H     2.838948    0.427533   -1.910045


22.xyz
   34
 SCF Done:  E(RmPW+HF-PW91) =  -862.653883199     A.U. after    1 cycles
   H    -2.022280   -2.854993    0.513995
   N    -0.586221   -1.329550    0.763017
   B     1.306436    0.113569    1.555593
   N     0.334501   -1.059043    1.732750
   C     0.235558   -1.987609    2.708918
   Pt   -0.594006   -0.056156   -0.939504
   H     0.874031   -1.961490    3.569377
   C    -0.771025   -2.882950    2.366681
   H    -1.099418   -3.736300    2.923208
   C    -1.254417   -2.433440    1.131569
   H     2.092195    0.164075    2.442949
   H    -3.237151   -1.116711   -0.932123
   H    -2.329552    0.399040   -1.444183
   H    -3.929709    0.514985   -1.032757
   H    -0.496737    0.851212   -2.210171
   N     0.512431    1.418063    1.432062
   N     2.039959   -0.111060    0.203792
   N    -0.383570    1.568255    0.414990
   N     1.355044   -0.225865   -0.968912
   C     0.548220    2.554725    2.161716
   C     3.352181   -0.245860   -0.069927
   H     1.192554    2.650525    3.012838
   H     4.084245   -0.191916    0.710791
   C    -0.343814    3.464477    1.606049
   C     3.513720   -0.449483   -1.438859
   C    -0.901627    2.802631    0.504722
   C     2.225767   -0.429987   -1.972700
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   H    -0.552775    4.458828    1.942769
   H     4.431350   -0.591305   -1.970950
   H    -1.621654    3.159845   -0.204735
   H     1.895857   -0.546518   -2.985029
   H    -0.687874   -1.239995   -1.952047
   H    -2.900034    0.106897    0.343388
   C    -3.070855   -0.072420   -0.709486


23.xyz
   29
 SCF Done:  E(RmPW+HF-PW91) =  -822.125111475     A.U. after    1 cycles
   H     3.020181   -1.115439   -1.678965
   N     1.458751   -0.811456   -0.291063
   B    -0.001211   -0.750592    1.738702
   N     1.247250   -1.228108    0.991339
   C     2.281828   -2.006020    1.378337
   Pt    0.000743    0.475718   -1.114795
   H     2.319390   -2.438049    2.358602
   C     3.184824   -2.097308    0.324867
   H     4.108031   -2.638588    0.305486
   C     2.631962   -1.321856   -0.701106
   H    -0.001572   -1.105515    2.869895
   H    -1.056835    1.462189   -1.708494
   N    -1.252020   -1.223024    0.991911
   N     0.002217    0.815913    1.682844
   N    -1.462437   -0.805262   -0.290354
   N     0.003175    1.508237    0.506738
   C    -2.289673   -1.996624    1.379304
   C     0.004682    1.724637    2.676877
   H    -2.328425   -2.428893    2.359419
   H     0.004622    1.412825    3.702219
   C    -3.193493   -2.084116    0.326205
   C     0.007029    3.007956    2.130387
   C    -2.637890   -1.310865   -0.699942
   C     0.005826    2.831379    0.748381
   H    -4.118817   -2.621781    0.307108
   H     0.009172    3.938737    2.658641
   H    -3.025669   -1.102777   -1.677621
   H     0.006700    3.549544   -0.046219
   H     1.062164    1.457460   -1.709301


24.xyz
   39
 SCF Done:  E(RmPW+HF-PW91) =  -977.989159669     A.U. after    1 cycles
   C    -0.993599   -1.222379    2.645215
   N    -0.846448   -0.555164    1.497313
   N    -1.811137    0.403249    1.446847
   C    -2.565693    0.336671    2.567542
   C    -2.077964   -0.691429    3.364719
   Pt    0.522083   -0.701547   -0.131407
   C     0.395433   -2.749856   -0.194008
   B    -1.900639    1.349151    0.235531
   N    -2.108157    0.496496   -1.029147
   N    -1.190507   -0.446616   -1.375941
   C    -1.607767   -1.026754   -2.504616
   C    -2.825716   -0.452915   -2.908263
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   C    -3.104305    0.507914   -1.944296
   N     0.598749    1.422620   -0.061070
   N    -0.571509    2.103494    0.103865
   C    -0.313573    3.432124    0.116027
   C     1.053086    3.614592   -0.044572
   C     1.588206    2.318138   -0.152452
   O     4.072885    0.381041   -0.506695
   C     5.125464   -0.138518    0.319184
   H     1.515841   -0.821972   -1.325838
   H    -2.806312    2.113857    0.373424
   H     2.604967    1.996966   -0.287976
   H     1.586548    4.542424   -0.080818
   H    -1.102306    4.148079    0.234795
   H    -1.031464   -1.804123   -2.963999
   H    -3.410174   -0.698880   -3.771116
   H    -3.930606    1.184531   -1.855817
   H    -0.333737   -2.027913    2.896500
   H    -2.447280   -1.007292    4.318900
   H    -3.384181    1.010147    2.725426
   H     0.784698   -3.139287   -1.132539
   H    -0.659405   -3.009046   -0.102394
   H     0.951875   -3.203045    0.624219
   H     1.772426   -0.902893    0.776563
   H     3.314258   -0.220516   -0.551827
   H     4.791898   -0.305964    1.345028
   H     5.912602    0.607304    0.324162
   H     5.529608   -1.069896   -0.081036


25.xyz
   36
 SCF Done:  E(RmPW+HF-PW91) =  -938.708985487     A.U. after    1 cycles
   C    -1.159280   -1.124664    2.573813
   N    -0.839075   -0.488912    1.443319
   N    -1.716026    0.538974    1.282114
   C    -2.588988    0.547800    2.315154
   C    -2.270193   -0.501523    3.168079
   Pt    0.674592   -0.764483   -0.031136
   C     0.399217   -2.798738   -0.075121
   B    -1.605624    1.469980    0.060396
   N    -1.745616    0.614157   -1.211643
   N    -0.871240   -0.400174   -1.452421
   C    -1.212231   -0.966230   -2.613555
   C    -2.335146   -0.310157   -3.146820
   C    -2.638384    0.684387   -2.225355
   N     0.909276    1.348748    0.023557
   N    -0.216191    2.118765    0.062320
   C     0.140559    3.424099    0.091065
   C     1.526296    3.500097    0.070117
   C     1.968887    2.165436    0.027305
   O     4.294473    0.061356   -0.052116
   H     4.925428   -0.339452    0.554307
   H     1.771945   -0.982088   -1.116319
   H    -2.459387    2.302886    0.096462
   H     2.966799    1.766726   -0.001559
   H     2.130400    4.384233    0.082038
   H    -0.598873    4.199369    0.123077
   H    -0.651764   -1.791686   -3.003512
```

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   H    -2.844261   -0.526106   -4.063750
   H    -3.415958    1.421764   -2.228921
   H    -0.594783   -1.974049    2.901512
   H    -2.762565   -0.773582    4.079219
   H    -3.365126    1.283930    2.378446
   H     0.968872   -3.261916   -0.877563
   H    -0.664567   -2.978214   -0.231483
   H     0.704006   -3.248205    0.868648
   H     1.803024   -1.045221    1.006048
   H     3.508612   -0.493392   -0.161951


26.xyz
   33
 SCF Done:  E(RmPW+HF-PW91) =  -862.450665270     A.U. after   28 cycles
   H     1.715186    3.263355   -0.283148
   N     0.414236    1.706059    0.202976
   B    -1.557792    0.352231    1.105794
   N    -0.800903    1.645501    0.821771
   C    -1.188191    2.904450    1.167083
   H     1.602658   -1.758607   -2.654849
   H    -2.111298    3.077975    1.683256
   C    -0.209593    3.792546    0.756974
   H    -0.201560    4.856500    0.878630
   C     0.779382    2.987088    0.158512
   H    -2.429833    0.589534    1.890906
   H     1.083395   -2.622969   -1.148059
   H     2.614305    0.519519    0.149162
   H     1.908279    0.604022   -1.878771
   C     1.220848   -1.656823   -1.642629
   N    -0.653291   -0.730972    1.674050
   N    -2.323577   -0.178420   -0.171916
   N     0.551406   -1.063964    1.128313
   N    -1.784572   -0.787970   -1.254499
   C    -0.875226   -1.502651    2.771640
   C    -3.655659   -0.118983   -0.368579
   H    -1.766662   -1.390065    3.355709
   H    -4.295966    0.319032    0.369776
   C     0.204422   -2.353713    2.934316
   C    -3.970966   -0.694240   -1.599328
   C     1.076668   -2.037032    1.874372
   C    -2.746867   -1.106084   -2.128864
   H     0.348730   -3.084261    3.703870
   H    -4.940553   -0.798377   -2.040073
   H     2.036185   -2.444948    1.629208
   H    -2.512372   -1.592366   -3.054100
   H    -0.728529   -0.916729   -1.355904
   Pt    1.331218   -0.074381   -0.604108


3.xyz
   28
 SCF Done:  E(RmPW+HF-PW91) =  -821.752714943     A.U. after   18 cycles
   C    -3.398363   -0.759572    0.170720
   N    -2.149894   -0.213497    0.164386
   N    -1.792658    0.141101   -1.109221
   C    -2.825823   -0.192464   -1.888524
   C    -3.871200   -0.766657   -1.129472
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   B    -1.224199   -0.022245    1.358121
   N    -0.517630    1.337338    1.290672
   N     0.471297    1.576076    0.390610
   C     0.881103    2.839534    0.564447
   C     0.137727    3.441512    1.592702
   C    -0.734488    2.451129    2.026126
   Pt    1.027261    0.018293   -0.931268
   N    -0.129670   -1.132409    1.431800
   N     0.881208   -1.270801    0.528742
   C     1.606798   -2.348420    0.854475
   C     1.061352   -2.931764    2.004905
   C    -0.029333   -2.134316    2.332946
   H    -2.784225   -0.009906   -2.944547
   H    -3.858912   -1.091773    1.080198
   H    -4.819816   -1.122367   -1.478381
   H    -1.854114   -0.095693    2.373644
   H    -1.478684    2.468933    2.796710
   H    -0.731275   -2.217417    3.137739
   H     0.226809    4.441180    1.965801
   H     1.409794   -3.803770    2.518704
   H     1.673160    3.248819   -0.030653
   H     2.451085   -2.635194    0.262977
   H     1.455614   -1.156944   -1.882745


4.xyz
   28
 SCF Done:  E(RmPW+HF-PW91) =  -821.757499029     A.U. after   15 cycles
   C    -0.000372    2.880686   -0.906934
   N    -0.000231    1.628421   -0.442109
   N    -0.000249    1.690751    0.915170
   C    -0.000398    2.984079    1.311244
   C    -0.000482    3.782907    0.174078
   B    -0.000060    0.358890    1.679059
   N    -1.323810   -0.387305    1.312500
   N    -1.741363   -0.596689    0.014616
   C    -2.938784   -1.183766    0.064934
   C    -3.331997   -1.354572    1.405522
   C    -2.285159   -0.837625    2.155036
   Pt    0.000085   -0.390695   -1.120653
   N     1.323885   -0.386950    1.312537
   N     1.741591   -0.596156    0.014668
   C     2.939077   -1.183100    0.065057
   C     3.332178   -1.353987    1.405666
   C     2.285205   -0.837237    2.155125
   H     3.450211   -1.453505   -0.836452
   H     2.169333   -0.757891    3.217484
   H     4.242250   -1.785822    1.769154
   H    -0.000108    0.545625    2.859655
   H    -2.169401   -0.758167    3.217400
   H    -0.000425    3.251226    2.348952
   H    -4.242055   -1.786474    1.768962
   H    -0.000596    4.852974    0.130900
   H    -3.449796   -1.454308   -0.836603
   H    -0.000391    3.077414   -1.960055
   H     0.000291   -1.900104   -1.533774
```

5.xyz

34

SCF Done: E(RmPW+HF-PW91) = -937.483334350 A.U. after 1 cycles

C	-0.163311	3.325237	-0.828739
N	0.009149	2.168727	-0.136328
N	1.332004	1.799067	-0.184948
C	1.957440	2.737145	-0.911201
C	1.055878	3.725163	-1.348008
B	-1.125328	1.483120	0.670859
N	-0.539597	0.697796	1.836037
N	0.124609	-0.459040	1.587015
C	0.570545	-0.932545	2.753961
C	0.184979	-0.064259	3.792112
C	-0.517251	0.956151	3.163611
H	0.404257	-1.507879	-1.937323
N	-2.032849	0.525294	-0.166454
N	-1.636833	-0.693916	-0.644871
C	-2.678784	-1.268349	-1.250458
C	-3.792818	-0.417207	-1.165213
C	-3.341152	0.698174	-0.473556
H	3.013946	2.669521	-1.087489
H	-1.126250	3.791814	-0.892910
H	1.263453	4.594102	-1.938838
H	-1.853335	2.341837	1.083091
H	-0.988964	1.829080	3.568134
H	-3.861331	1.586679	-0.177520
H	0.385939	-0.167016	4.838974
H	-4.776889	-0.592032	-1.548940
H	1.130784	-1.844492	2.794990
H	-2.577578	-2.230658	-1.708524
Pt	0.286545	-1.065514	-0.429304
O	2.318054	-0.716790	-0.142512
C	3.369578	-1.091317	-1.052618
H	2.167757	0.276851	-0.025516
H	4.317039	-0.705750	-0.681841
H	3.165835	-0.714337	-2.052889
H	3.400994	-2.173569	-1.074353

6.xyz

31

SCF Done: E(RmPW+HF-PW91) = -861.055812274 A.U. after 1 cycles

C	-0.218933	-1.532080	2.785057
N	-0.319334	-0.778726	1.667981
N	0.882823	-0.805056	1.028147
C	1.729385	-1.567961	1.732889
C	1.066951	-2.054214	2.866322
B	-1.580238	-0.024886	1.143790
N	-1.176515	1.427378	0.861168
N	-0.066327	1.732714	0.140823
C	0.009728	3.067802	0.060830
C	-1.077618	3.646341	0.735184
C	-1.801095	2.568954	1.229811
Pt	1.120807	0.179522	-0.641511
N	-2.172471	-0.685992	-0.091536
C	-3.264220	-1.501022	-0.141214
C	-3.445373	-1.896067	-1.454500
C	-2.397805	-1.261125	-2.161231

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   N    -1.634225   -0.533008   -1.340664
   H    -2.175598   -1.299726   -3.209888
   H    -3.829767   -1.733089    0.739688
   H    -4.212529   -2.533716   -1.845863
   H    -2.383437   -0.048561    2.032296
   H    -2.700933    2.543694    1.810855
   H    -1.056942   -1.647830    3.441986
   H    -1.297986    4.687934    0.849452
   H     1.466418   -2.688528    3.630456
   H     0.821465    3.543143   -0.453250
   H     2.734868   -1.719291    1.399836
   C     2.253483   -1.278895   -1.477430
   H     2.345315   -1.046870   -2.547928
   H     3.259179   -1.327914   -1.053060
   H     1.783523   -2.259080   -1.391379


7.xyz
   31
 SCF Done:  E(RmPW+HF-PW91) =  -861.058478379     A.U. after    1 cycles
   B     0.030124   -1.818116    0.000000
   C     1.690964    2.214173    0.000000
   C     1.303469   -1.960791    2.288012
   C     1.064785    0.142468    2.946579
   C     1.589315   -1.103057    3.340383
   C    -3.079519    0.015525    0.000000
   C    -2.600564   -2.152766    0.000000
   C    -3.668485   -1.263530    0.000000
   C     1.303469   -1.960791   -2.288012
   C     1.064785    0.142468   -2.946579
   C     1.589315   -1.103057   -3.340383
   H     1.380154    3.266309    0.000000
   H     2.303965    2.032453    0.884241
   H     1.513848   -3.004993    2.170836
   H     1.073106    1.080289    3.464265
   H     2.093529   -1.339731    4.255105
   H     0.162282   -3.006227    0.000000
   H    -3.543615    0.981153    0.000000
   H    -2.587376   -3.224253    0.000000
   H    -4.712777   -1.501153    0.000000
   H     2.303965    2.032453   -0.884241
   H     1.513848   -3.004993   -2.170836
   H     1.073106    1.080289   -3.464265
   H     2.093529   -1.339731   -4.255105
   N     0.650779   -1.267478    1.323473
   N     0.497197    0.036553    1.743081
   N    -1.749472   -0.106440    0.000000
   N    -1.455536   -1.432616    0.000000
   N     0.650779   -1.267478   -1.323473
   N     0.497197    0.036553   -1.743081
   Pt    0.000000    1.092580    0.000000


8.xyz
   37
 SCF Done:  E(RmPW+HF-PW91) =  -976.781508497     A.U. after    1 cycles
   C    -0.963112    3.211453   -1.061411
   N    -0.425135    2.186800   -0.348775
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   N     0.884573    2.012864   -0.723293
   C     1.135701    2.930963   -1.667037
   C    -0.003243    3.715683   -1.921947
   B    -1.197136    1.443469    0.771135
   N    -0.245023    0.925172    1.844936
   N     0.519101   -0.169188    1.596092
   C     1.195733   -0.450504    2.715170
   C     0.872077    0.486090    3.714112
   C    -0.048968    1.337954    3.118610
   C     0.230698   -1.760051   -2.225518
   N    -2.083147    0.249000    0.287933
   N    -1.592268   -0.960894   -0.124210
   C    -2.623172   -1.766692   -0.387476
   C    -3.824296   -1.082567   -0.136118
   C    -3.436726    0.180478    0.288891
   H     2.105242    2.985177   -2.123167
   H    -1.976878    3.521231   -0.902413
   H    -0.106298    4.523202   -2.617918
   H    -1.959065    2.228871    1.262172
   H    -0.567846    2.188457    3.512878
   H    -4.028756    1.019233    0.595013
   H     1.244613    0.528133    4.717332
   H    -4.821885   -1.455496   -0.245909
   H     1.851228   -1.297032    2.761017
   H    -2.457716   -2.764433   -0.739131
   Pt    0.366080   -0.993444   -0.352255
   O     2.269310   -0.217023   -0.725412
   C     3.537941   -0.528863   -0.131321
   H     1.926172    0.743417   -0.654023
   H     3.520899   -0.370508    0.945985
   H     4.307986    0.094443   -0.581559
   H     3.751369   -1.569610   -0.347188
   H     0.180114   -2.853126   -2.181340
   H     1.118444   -1.471845   -2.791631
   H    -0.653199   -1.392527   -2.751146


9.xyz
   19
 SCF Done:  E(RmPW+HF-PW91) =  -329.701511096     A.U. after    1 cycles
   C     2.028657    0.006356   -0.483829
   Pt   -0.006565    0.000108   -0.229721
   N    -2.227778   -0.028575   -0.140579
   N     0.186405    1.646926    1.259447
   H    -0.048311   -1.040160   -1.378416
   N     0.234171   -1.623834    1.279158
   H    -0.067229    1.036035   -1.380248
   H     2.361802   -0.947634   -0.884999
   H     2.506761    0.174640    0.484964
   H     2.331662    0.789907   -1.171874
   H     0.052527    1.372711    2.225544
   H    -0.461311    2.390797    1.027185
   H     1.132248    1.993007    1.138904
   H     0.032905   -2.496383    0.804411
   H    -0.347913   -1.550937    2.105057
   H     1.211027   -1.623112    1.551680
   H    -2.543223   -0.963360   -0.371709
   H    -2.546132    0.605813   -0.864170
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   H    -2.624277    0.250472    0.748696
```

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TS1-2.xyz
   33
 SCF Done:  E(RmPW+HF-PW91) =  -862.266453138     A.U. after    9 cycles
   C     0.377233    2.954947    0.447877
   N     0.330397    1.621310    0.344050
   N     1.452170    1.116663    0.927247
   C     2.202839    2.139185    1.395230
   C     1.553079    3.333979    1.111787
   B     1.772826   -0.391472    0.931085
   N     0.586176   -1.139854    1.566799
   N    -0.688393   -0.984894    1.117955
   C    -1.476364   -1.764458    1.868448
   C    -0.704660   -2.448214    2.821597
   C     0.596724   -2.020431    2.593890
   Pt   -1.107235    0.395160   -0.452730
   N     1.993711   -0.864291   -0.501447
   N     1.021735   -0.670013   -1.437107
   C     1.497964   -1.159771   -2.585953
   C     2.796803   -1.683205   -2.402373
   C     3.072175   -1.472089   -1.060194
   H     0.910332   -1.113899   -3.481803
   H     3.944394   -1.706288   -0.482586
   H     3.431828   -2.138348   -3.135563
   H     2.753444   -0.583331    1.588123
   H     1.510638   -2.280039    3.089313
   H     3.136257    1.955661    1.888213
   H    -1.043853   -3.141190    3.564119
   H     1.878886    4.325994    1.348622
   H    -2.535548   -1.791754    1.708934
   H    -0.415939    3.556941    0.054531
   H    -1.924029   -1.248012   -2.053133
   H    -1.405384    1.466217   -1.550856
   C    -2.653685   -0.854714   -1.348362
   H    -3.003528   -1.662482   -0.713094
   H    -2.704849    0.223274   -0.423259
   H    -3.475695   -0.431660   -1.918202
```

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TS10a-11.xyz
   15
 SCF Done:  E(RmPW+HF-PW91) =  -273.111314789     A.U. after    1 cycles
   H     2.683672    0.408882   -0.055037
   Pt   -0.003154   -0.177488   -0.062161
   C     2.060536   -0.393310    0.329365
   N     0.188984    2.028752    0.011277
   H    -0.101635   -1.725029   -0.133227
   N    -2.124415   -0.163406    0.246736
   H     1.977597   -0.331155    1.414668
   H     2.473219   -1.354601    0.050812
   H    -2.559559    0.752222    0.248165
   H     1.110011   -0.393147   -1.120031
   H    -0.350968    2.453581    0.757826
   H     1.166645    2.257800    0.157723
   H    -0.103983    2.422360   -0.877276
   H    -2.531072   -0.715115   -0.503230
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   H    -2.333090   -0.629330    1.125850


TS10a-15.xyz
   15
 SCF Done:  E(RmPW+HF-PW91) =  -273.113405310     A.U. after    1 cycles
   C    -2.040077   -0.355259    0.005038
   Pt   -0.008157   -0.176507   -0.001148
   N     2.207960   -0.030966    0.004068
   N    -0.293429    1.947709    0.001087
   H     0.043033   -1.594705   -0.666658
   H     2.563719    0.878391   -0.268633
   H     0.049421   -1.597557    0.659218
   H    -2.371251   -1.386735   -0.045862
   H    -2.436702    0.180712   -0.858699
   H    -2.420096    0.086505    0.927727
   H    -0.040400    2.340750   -0.901500
   H     0.246717    2.413076    0.724215
   H    -1.278718    2.134589    0.164055
   H     2.549036   -0.251360    0.934387
   H     2.570231   -0.721770   -0.645061


TS11-11.xyz
   15
 SCF Done:  E(RmPW+HF-PW91) =  -273.131540100     A.U. after    1 cycles
   H     3.186084   -1.055949    0.000053
   Pt   -0.058858   -0.197080   -0.000001
   C     2.391037   -0.312227    0.000002
   N     0.264478    1.991635   -0.000001
   H    -0.320209   -1.734433    0.000007
   N    -2.089543   -0.040482    0.000002
   H     2.480756    0.274187   -0.906291
   H     1.534116   -1.072379   -0.000041
   H    -2.447645   -0.515817   -0.824179
   H     2.480680    0.274218    0.906284
   H    -0.137912    2.417122   -0.828708
   H     1.260720    2.184535   -0.000017
   H    -0.137883    2.417103    0.828731
   H    -2.430942    0.914747    0.000007
   H    -2.447643   -0.515823    0.824180


TS19a-20.xyz
   34
 SCF Done:  E(RmPW+HF-PW91) =  -862.843999836     A.U. after   15 cycles
   C    -2.657355   -0.360983   -1.563030
   N    -1.597964   -0.117082   -0.779617
   N    -2.035869    0.566774    0.315065
   C    -3.372322    0.751118    0.218884
   C    -3.808629    0.174341   -0.967211
   B    -1.025636    0.946856    1.385739
   N    -0.320186   -0.347489    1.880148
   N     0.330040   -1.213172    1.039554
   C     0.753124   -2.265712    1.750903
   C     0.373674   -2.094154    3.086262
   C    -0.297003   -0.877314    3.124344
   Pt    0.479573   -0.563655   -0.850017
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   H     0.275805   -1.967956   -1.432877
   N     0.031942    1.918601    0.769815
   N     0.772807    1.629145   -0.354500
   C     1.753459    2.559861   -0.459917
   C     1.635060    3.470530    0.581905
   C     0.548197    3.022793    1.336389
   H     2.456781    2.534215   -1.269664
   H     0.132567    3.423461    2.239931
   H     2.243714    4.331252    0.767379
   H    -1.540856    1.487258    2.308835
   H    -0.756917   -0.370376    3.949058
   H    -3.922277    1.267500    0.980289
   H     0.557852   -2.760249    3.903472
   H    -4.810279    0.141586   -1.343330
   H     1.290286   -3.070361    1.290693
   H    -2.555451   -0.895062   -2.486721
   C     2.486782   -1.019844   -0.915812
   H     0.562709    0.180934   -2.382329
   H     0.525266    0.996975   -1.651574
   H     2.908289   -0.734992   -1.874530
   H     2.965001   -0.469369   -0.108332
   H     2.633680   -2.085286   -0.767262


TS2-2.xyz
   33
 SCF Done:  E(RmPW+HF-PW91) =  -862.273926084     A.U. after   11 cycles
   C    -0.166960    3.015274    0.193122
   N    -0.020585    1.682628    0.202287
   N     1.133644    1.381838    0.858299
   C     1.708000    2.535550    1.263948
   C     0.913481    3.602566    0.861548
   B     1.689630   -0.058050    1.053278
   N     0.564705   -0.923774    1.634070
   N    -0.687952   -0.945607    1.107668
   C    -1.420183   -1.786379    1.851199
   C    -0.630431   -2.331111    2.875409
   C     0.620049   -1.753532    2.700192
   Pt   -1.164461    0.273247   -0.563417
   N     2.239007   -0.646868   -0.236063
   N     1.431229   -1.163410   -1.211168
   C     2.248881   -1.556583   -2.192983
   C     3.601060   -1.301076   -1.865934
   C     3.547865   -0.722563   -0.610388
   H     1.846482   -2.002433   -3.081864
   H     4.334631   -0.374042    0.029354
   H     4.472534   -1.512236   -2.452761
   H     2.573909    0.024965    1.858081
   H     1.527022   -1.875590    3.257245
   H     2.632170    2.524237    1.805313
   H    -0.926960   -3.030374    3.630167
   H     1.088928    4.645717    1.025614
   H    -2.456624   -1.952253    1.637811
   H    -1.014680    3.465011   -0.280620
   H    -3.009446   -1.986550   -2.269529
   H    -1.501656    1.259133   -1.742028
   C    -2.527545   -1.615588   -1.366986
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   H    -1.742104   -2.299528   -1.073792
   H    -3.278437   -1.489875   -0.596634
   H    -2.151574   -0.632212   -1.806654


TS2-4.xyz
   33
 SCF Done:  E(RmPW+HF-PW91) =  -862.259979085     A.U. after    1 cycles
   C    -1.905382   -2.104781   -1.404919
   N    -1.183846   -1.208810   -0.727153
   N    -2.052687   -0.358370   -0.092417
   C    -3.320341   -0.744620   -0.372396
   C    -3.274910   -1.852811   -1.207294
   B    -1.569637    0.785752    0.848754
   N    -0.647868    0.157944    1.903852
   N     0.474913   -0.483261    1.485775
   C     1.105707   -0.946545    2.568967
   C     0.378752   -0.598367    3.722538
   C    -0.726592    0.100485    3.253281
   Pt    0.717892   -0.446751   -0.625524
   N    -0.791466    1.909301    0.120607
   N     0.473454    1.740940   -0.389801
   C     0.844157    2.910483   -0.917742
   C    -0.175272    3.867526   -0.746561
   C    -1.188373    3.190475   -0.085150
   H     1.801061    3.013681   -1.388470
   H    -2.146739    3.533596    0.250143
   H    -0.169706    4.893168   -1.055267
   H    -2.533651    1.264750    1.368891
   H    -1.543145    0.548136    3.783371
   H    -4.160227   -0.219570    0.036292
   H     0.621802   -0.824088    4.740802
   H    -4.103142   -2.398982   -1.610350
   H     2.021781   -1.494835    2.479048
   H    -1.423622   -2.862919   -1.987572
   H     2.846660   -1.256910   -0.838024
   H     0.807857   -0.391387   -2.187675
   C     3.836674   -0.935573   -0.482767
   H     3.739108   -0.119239    0.227867
   H     4.322740   -1.783562   -0.006420
   H     4.417807   -0.605892   -1.339292


TS20-20.xyz
   34
 SCF Done:  E(RmPW+HF-PW91) =  -862.864897625     A.U. after   14 cycles
   Pt   -0.612395   -0.000001   -0.946111
   B     1.291977    0.000002    1.584794
   N     1.512257    0.000000   -0.914008
   N     2.129843    0.000001    0.300821
   N     0.371319   -1.235283    1.560937
   N    -0.548734   -1.388875    0.567412
   N    -0.548736    1.388876    0.567409
   N     0.371318    1.235287    1.560934
   C    -2.686450   -0.000002   -0.906476
   C     2.464267   -0.000001   -1.858955
   C     3.725264    0.000000   -1.250654
   C     3.468186    0.000001    0.115258
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   C    -1.238614   -2.517197    0.803379
   C    -0.759961   -3.109263    1.974486
   C     0.254382   -2.267174    2.420932
   C     0.254380    2.267179    2.420928
   C    -0.759964    3.109266    1.974480
   C    -1.238616    2.517197    0.803374
   H    -0.677171   -1.242053   -1.979045
   H     1.979794    0.000003    2.551278
   H     2.219959   -0.000002   -2.902929
   H     4.680838    0.000000   -1.732853
   H     4.145138    0.000003    0.946219
   H    -2.017459   -2.845957    0.145062
   H    -1.099164   -4.016615    2.429657
   H     0.883626   -2.341391    3.285277
   H    -2.017462    2.845955    0.145057
   H    -1.099168    4.016618    2.429650
   H     0.883624    2.341398    3.285273
   H    -3.063177   -0.887594   -1.404569
   H    -2.968047   -0.000001    0.141075
   H    -3.063178    0.887588   -1.404571
   H    -0.677172    1.242049   -1.979047
   H    -0.712191   -0.000003   -2.567887


TS24-24.xyz
   39
 SCF Done:  E(RmPW+HF-PW91) =  -977.918822513     A.U. after    1 cycles
   C    -0.271210   -2.356093   -1.654700
   N     0.117945   -1.247189   -1.013384
   N     1.375660   -0.946756   -1.434541
   C     1.773330   -1.870061   -2.339522
   C     0.749499   -2.792257   -2.512613
   Pt   -0.892665   -0.059021    0.335705
   C    -1.827065   -1.712071    1.119890
   B     2.206758    0.217064   -0.858136
   N     2.618248   -0.077573    0.578082
   N     1.682331   -0.293752    1.547752
   C     2.362711   -0.515814    2.676188
   C     3.756967   -0.445764    2.448763
   C     3.873406   -0.164379    1.097653
   N     0.109706    1.605010   -0.453276
   N     1.375624    1.510640   -0.939255
   C     1.771169    2.720484   -1.399376
   C     0.735793    3.625728   -1.209204
   C    -0.287697    2.873918   -0.609868
   O    -3.594700    0.715092    0.062933
   C    -4.881001    0.092518    0.379592
   H    -1.662705    0.867901    1.441671
   H     3.186768    0.351812   -1.534922
   H    -1.263092    3.182497   -0.292578
   H     0.723050    4.666228   -1.462320
   H     2.746562    2.857179   -1.821149
   H     1.838355   -0.713201    3.590721
   H     4.547951   -0.579737    3.159406
   H     4.743306   -0.023803    0.486839
   H    -1.237113   -2.779787   -1.471623
   H     0.742751   -3.647126   -3.157490
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   H     2.743627   -1.814631   -2.790303
   H    -2.375974   -1.499419    2.039838
   H    -1.041975   -2.431276    1.362737
   H    -2.515921   -2.201104    0.418530
   H    -2.912524    0.202006   -0.514193
   H    -2.864104    0.881208    0.824116
   H    -4.713416   -0.865574    0.860262
   H    -5.421147   -0.020575   -0.551516
   H    -5.404741    0.775067    1.035716


TS25-25.xyz
   36
 SCF Done:  E(RmPW+HF-PW91) =  -938.632556913     A.U. after    1 cycles
   C     0.556555   -2.268668    1.733101
   N     0.123770   -1.199350    1.054010
   N    -1.121703   -0.895656    1.508311
   C    -1.468278   -1.777767    2.472920
   C    -0.423130   -2.675176    2.650918
   Pt    1.044699   -0.069341   -0.393807
   C     1.938823   -1.749678   -1.166044
   B    -1.982511    0.234990    0.908092
   N    -2.402535   -0.116139   -0.513286
   N    -1.467772   -0.347093   -1.480387
   C    -2.147074   -0.622191   -2.597532
   C    -3.540827   -0.572173   -2.364700
   C    -3.657073   -0.246255   -1.023351
   N     0.084514    1.623630    0.397957
   N    -1.164004    1.538754    0.928957
   C    -1.544182    2.757152    1.378753
   C    -0.515951    3.658037    1.135426
   C     0.487201    2.894743    0.516345
   O     3.711182    0.751000   -0.311800
   H     4.560914    0.336837   -0.523602
   H     1.752344    0.818473   -1.587054
   H    -2.954027    0.378529    1.593632
   H     1.451865    3.197045    0.162037
   H    -0.494570    4.703087    1.368229
   H    -2.504144    2.902541    1.831930
   H    -1.622866   -0.840710   -3.507185
   H    -4.332188   -0.746555   -3.065978
   H    -4.527124   -0.102022   -0.413676
   H     1.521854   -2.686273    1.533484
   H    -0.377110   -3.495995    3.337004
   H    -2.420795   -1.713821    2.959107
   H     2.396903   -1.571867   -2.140619
   H     1.152550   -2.495250   -1.297684
   H     2.701683   -2.182720   -0.507708
   H     3.031431    0.245725    0.308137
   H     2.917555    0.861434   -1.063152
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