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Evaluating Transition Metal Barrier Heights with the Latest DFT Exchange–Correlation Functionals – the MOBH35 Benchmark Dataset

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Evaluating Transition Metal Barrier Heights with the Latest DFT Exchange–Correlation Functionals – the MOBH35 Benchmark Dataset

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A new database of transition metal reaction barrier heights – MOBH35 – is presented. Benchmark energies (forward and reverse barriers and reaction energy) are calculated using DLPNO-CCSD(T) extrapolated to the complete basis set limit using a Weizmann1-like scheme. Using these benchmark energies, the performance of a wide selection of density functional theory (DFT) exchange–correlation functionals, including the latest from the Truhlar and Head-Gordon groups, is evaluated. It was found, using the def2-TZVPP basis set, that the ωB97M-V (MAD 1.8 kcal/mol), ωB97X-V (MAD 2.1 kcal/mol) and SCAN0 (MAD 2.1 kcal/mol) hybrid functionals are recommended. The double-hybrid functionals PWPB95 (MAD 1.6 kcal/mol) and B2K-PLYP (MAD 1.8 kcal/mol) did perform slightly better but this has to be balanced by their increased computational cost.

Introduction

Transition metal complexes form a vital class of compounds in various fields of chemistry, notably catalysis of industrially relevant reactions.[1] Given the size of transition metal complexes, density functional theory (DFT) is well-suited to study their reaction mechanisms. For main-group systems, there are a myriad of studies on the performance of DFT functionals, such as Truhlar and coworkers' DATABASE2015 benchmarks,[2] Goerigk and coworkers' GMTKN55 (and related) benchmarks,[3] and Mardirossian and Head-Gordon's evaluation of the Minnesota family of functionals.[4] However, it is known that transition metals behave differently from their main group counterparts. Quintal *et al.* in 2006 considered a number of the functionals available at the time for a set of small model complexes.[5] Modrzejewski *et al.* recently considered some model reactions and how well selected hybrid-meta-GGA functionals perform.[6] More recently, Dohm *et al.* presented a benchmark set of "real life" transition metal reactions – MOR41 – based on highly-accurate yet computationally relatively efficient DLPNO-CCSD(T) energies;[7] they compared the accuracy of a wide selection of GGA, meta-GGA, hybrid and double-hybrid DFT functionals and found that of the functionals tested, the double-hybrid PWPB95$_{D3BJ}$ and the ωB97X-V and mPW1B95$_{D3BJ}$ hybrid functionals performed the best.

By evaluating the accuracy of functionals with respect to reaction energy, MOR41 represents an important step forward, but in order to predict reaction mechanisms involving transition metal complexes, reaction barrier heights must also be known accurately. For main group reactions, it has been shown that functionals that perform well for thermodynamics are often less accurate in predicting reaction barrier heights. For the former, hybrid functionals with low amounts of Hartree–Fock exchange (15-25%) were found to be advantageous, while "kinetic functionals" – such as the aforementioned mPW1K, BB1K and BMK – have significantly higher percentages

(>40%), which tends to be detrimental to thermodynamic predictions. This catch-22 is in part offset by the kinetic energy density (τ) component of the latter hybrid meta-GGA functional.[8]

In this study, we present a complementary benchmark dataset to MOR41, which we shall term MOBH35 (metal–organic barrier heights with 35 members). This dataset is composed of reactions, including both early and late and 3*d*, 4*d* and 5*d* transition metals, taken from the literature for which computational studies have been reported. The geometries of all species were reoptimized at a consistent level of theory ($TPSS_{D3BJ}$/def2-SVP/W06), both to ensure consistency in the method and also to include dispersion that may play a significant role in determining the reactivity of the species. Benchmark energies for all species were then calculated using a level of theory very similar to that used by Dohm *et al.*:[7] DLPNO-CCSD(T)[9] energies were extrapolated to the basis set limit but following the philosophy of Martin's Weizmann1 (W1) thermochemical composite method.[10] The Hartree–Fock and CCSD correlation energies were extrapolated from basis sets of triple-ζ and quadruple-ζ quality, while the (T) triples corrections, which converges faster with the size of the basis set[11] but are computationally more expensive, were extrapolated to the basis set limit using basis sets of double-ζ and triple-ζ quality (see Computational Methods for details). Finally, a wide variety of DFT functionals was evaluated to determine which perform well, ideally for both thermodynamics (*i.e.*, MOR41) and kinetics (*i.e.*, MOBH35). As part of this study, MOR41 was used to evaluate some of the newer functionals that were not part of Dohm *et al.*'s original study, including the latest functionals from the Truhlar (*e.g.*, MN15,[12] MN15-L[13]) and Head-Gordon (*e.g.*, ωB97M-V,[14] B97M-V[15]) groups.

Computational Methods

A selection of DFT functionals were considered and these are summarized in Table 1. Two codes were used to calculate the DFT energies: GAUSSIAN16 REV. B01[16] and ORCA versions 4.0.1, 4.1.0

and 4.1.1;[17] in general, GAUSSIAN16 was used, but for functionals not implemented therein ORCA was used. For double-hybrid functionals the preference was to use ORCA due to its ability to use RIJCOSX (*vide infra*) to markedly increase computational efficiency. Certain functionals implemented in ORCA use the XCFUN DFT library.[18] In addition, semiempirical models (see Table 1) were calculated with MOPAC2016 version 19.024L.[19]

With these functionals the def2-TZVPP (and in some cases, def2-QZVPP) basis set was used.[20] With GAUSSIAN16, density fitting (DF, also termed resolution-of-identity or RI) was used to improve the performance of GGA and meta-GGA functionals; the Weigend06 (W06) density fitting basis set[20g,21] was used. With ORCA, RI with the def2-TZVPP/C[22] and def2/J[21] auxiliary basis sets was used in conjunction with the resolution of identity–chain of spheres exchange (RIJCOSX) approximation[23] to improve the performance of all functionals. All DDFT calculations used the (99,590) "ultrafine" integration grid in GAUSSIAN16 and the equivalent "GRID6" in ORCA (see the respective user manuals for details). For ease of notation, the "def2-" prefix will be dropped from the notation but these versions of the basis sets were used in all cases.

Dispersion corrections (an empirical correction[24] added *a posteriori* to the calculated energies, specifically the third version of Grimme's dispersion[24a,25] – D3 – preferably with Becke-Johnson dampening – D3BJ[25-26]) were calculated using the DFTD3 program (version 2.1rev6) by Grimme and coworkers, locally modified to read GAUSSIAN output (*i.e.,* .log) files; parameters for functionals not included in the standard version were taken from the Supporting Information of the study by Goerigk *et al*.[3c] (D3BJ parameters for B2K-PLYP from Karton and Georigk[27]). For certain functionals, dispersion is included using a nonlocal (NL) correlation correction, specifically Vydrov and Van Voorhis's VV10 functional;[28] all such calculations were done using ORCA. VV10 has a single parameter *b*; for Head-Gordon's B97M-V, B97X-V, ωB97M-V and ωB97X-V, *b* is

optimized as part of the functional parameterization (see Table 1), while for SCAN, TPSS, M06-L, PBE and PBE0 *b* was taken from Brandenberg *et al.*,[29] for BLYP, B3LYP, B3PW91, revPBE, revPBE0 and revPBE38 from Hujo and Grimme,[30] PWPB95, DSD-BLYP, DSD-PBEP86 and DOD-PBEP86 from Yu,[31] and rPW86PBE (which the authors define as VV10) from Vydrov and Van Voorhis.[28] Note that by default ORCA adds the NL dispersion as a non-self-consistent correction to the final SCF energy rather than self-consistently as in the original implementation; Najibi and Goerigk have shown, using their extensive GMTKN55 database,[3c] that there is no improvement in accuracy when the NL correction is added self-consistently and skipping this iterative process represents a significant saving in computational effort.[32] One functional – APFD – has a unique dispersion correction defined as part of its functional development.[33]

Table 1. Summary of exchange-correlation functionals included in this study.

Functional	Program	%HF	%MP2	reference
		LSDA		
SVWN5	GAUSSIAN			Slater $\left(\rho^{\frac{4}{3}}\right)$ exchange,[34] VWN5 correlation[35]
		GGA		
BLYP	GAUSSIAN			Becke88 exchange,[36] Lee–Yang–Parr correlation[37]
BP86	GAUSSIAN			Becke88 exchange,[36] Perdew86 correlation[38]

GLYP	GAUSSIAN	Gill96 exchange,[39] Lee–Yang–Parr correlation[37]
HCTH[a]	GAUSSIAN	[40]
mPWLYP	GAUSSIAN	modified Perdew–Wang exchange,[41] Lee–Yang–Parr correlation[37]
mPWPW91	GAUSSIAN	modified Perdew–Wang exchange,[41] PW91 correlation[42]
N12	GAUSSIAN	[43]
OLYP	GAUSSIAN	OPTX exchange,[44] Lee–Yang–Parr correlation[37]
PBE	GAUSSIAN	[45]
revPBE	ORCA	[46]
rPW86PBE[d]	ORCA	revised Perdew–Wang86 exchange, Perdew–Burke–Ernzerhof correlation[45]
SOGGA11	GAUSSIAN	[47]
XLYP	GAUSSIAN	X exchange,[48] Lee–Yang–Parr correlation[37]
ωB97	ORCA	[49]

meta-GGA			
B97M-D3BJ	ORCA		32
B97M-V	ORCA		15
M06-L	GAUSSIAN		50
M11-L	GAUSSIAN		51
MN12-L	GAUSSIAN		52
MN15-L	GAUSSIAN		13
PKZB	GAUSSIAN		53
revTPSS	GAUSSIAN		54
SCAN	ORCA		55
TPSS	GAUSSIAN		56
VSXC	GAUSSIAN		57
τHCTH	GAUSSIAN		58
hybrid-GGA			
APFD	GAUSSIAN	22.945	33
B1LYP	GAUSSIAN	25	59
B3LYP[b]	GAUSSIAN	20	60

B3PW91	GAUSSIAN	20	[61]
B97-1	GAUSSIAN	21	[62]
B97-2	GAUSSIAN	21	[63]
B98	GAUSSIAN	21.98	[64]
BH&HLYP	GAUSSIAN	50	[65]
CAM-B3LYP	GAUSSIAN	19-65[c]	[66]
HISS	GAUSSIAN	[c]	[67]
HSE03	GAUSSIAN	[c]	[68]
HSE06	GAUSSIAN	25-0[c]	[68]
LC-ωHPBE	GAUSSIAN	0-100[c]	[68g]
LC-ωPBE	GAUSSIAN	0-10[c]	[69]
mPW1PW91	GAUSSIAN	25	[41]
N12-SX	GAUSSIAN	25-0[c]	[70]
O3LYP	GAUSSIAN	20	OPTX exchange,[44] Lee–Yang–Parr correlation,[37] hybrid[71]
PBE0	GAUSSIAN	25	[72]
revPBE0	ORCA	25	[46,72]

revPBE38	ORCA	38	[30]
SOGGA11-X	GAUSSIAN	40.15	[73]
X3LYP	GAUSSIAN	21.8	[48]
ωB97X	ORCA	15.7706	[49]
ωB97X-D[f]	ORCA	19.5728	[74]
ωB97X-D3[f]	ORCA	16.7	[75]
ωB97X-D3BJ[f]	ORCA	16.7	[32]
ωB97X-V	ORCA	16.7	[76]
hybrid-meta-GGA			
B1B95	GAUSSIAN	28	[77]
BB1K	GAUSSIAN	42	[8]
BMK	GAUSSIAN	42	[78]
M06	GAUSSIAN	27	[79]
M06-2X	GAUSSIAN	54	[79]
M06-HF	GAUSSIAN	100	[80]
M08-HX	GAUSSIAN	52.23	[81]

M11	GAUSSIAN	42.8-100[c]	[82]
MN12-SX	GAUSSIAN	25-0[c]	[70]
MN15	GAUSSIAN	44	[12]
mPW1B95	GAUSSIAN	31	[83]
mPW1K	GAUSSIAN	42.8	[84]
mPW1KCIS	GAUSSIAN	15	[85]
mPWB1K	GAUSSIAN	44	[83]
mPWKCIS1K	GAUSSIAN	41	[85]
PBE1KCIS	GAUSSIAN	22	[86]
PW6B95	GAUSSIAN	28	[87]
PWB6K	GAUSSIAN	46	[87]
revTPSS0	GAUSSIAN	25	[54,88]
revTPSSh	GAUSSIAN	10	[54,56]
SCAN0	ORCA	25	[89]
TPSS0	GAUSSIAN	25	[88]
TPSS1KCIS	GAUSSIAN	13	[90]

TPSSh	GAUSSIAN	10		[56]
τHCTHhyb	GAUSSIAN	15		[58]
ωB97M-D3BJ	ORCA	15		[32]
ωB97M-V	ORCA	15		[14]
		double hybrid		
B2GP-PLYP	ORCA	65	36	[91]
B2K-PLYP	ORCA	72	42	[92]
B2PLYP	ORCA	53	27	[93]
B2T-PLYP	ORCA	60	31	[94]
DOD-PBEB95	ORCA[e]	65	0/54[g]	[95]
DOD-PBEP86	ORCA[e]	65	0/47[g]	[95]
DOD-SVWN5	ORCA[e]	69	0/58[g]	[95]
DSD-BLYP	ORCA[e,h]	71	40/47[g]	[95-96]
DSD-PBEB95	ORCA[e]	66	9/46[g]	[95]
DSD-PBEP86	ORCA[e]	72	36/51[g]	[95,97]
mPW2K-PLYP	ORCA	72	42	[92]

mPW2PLYP	ORCA	55	25	[98]
PBE0-2	ORCA	79.3701	50	[99]
PBE0-DH	ORCA	50	12.5	[100]
PBE-QIDH	ORCA	69	33.34	[101]
PWPB95	ORCA	50	26.9	[3b]
SCAN-2	ORCA	79.370	50	[89]
SCAN-DH	ORCA	50	12.5	[89]
SCAN-QIDH	ORCA	69.336	33.333	[89]
low-cost methods				
B97-3c	ORCA			[102]
HF-3c	ORCA	100		[103]
PBEh-3c	ORCA	42		[104]
PM6[i]	MOPAC			[105]
PM7[j]	MOPAC			[106]

[a] Refers to the /407 variant. [b] Using VWN3 as defined in Stephens *et al.*[60] [c] Range-separated hybrid functional. [d] When used with NL dispersion, this is what Vydrov and Van Voorhis term VV10.[28] [e] Run using the parameters from Kozuch and Martin.[95] [f] One should not confuse ωB97X-D3BJ with ωB97X-D and ωB97X-D3; the former is a D3BJ variant of Head-Gordon's ωB97X-V

functional, Head-Gordon's survival-of-the-fittest functional, while the latter two are dispersion-variants of the older ωB97 functional. [g] DSD functionals use separate scale factors for same spin and opposite spin contributions to the MP2 energy; these two numbers are the same spin and opposite spin SCS-MP2-type scale factors, respectively. [h] Using the parameters, including for dispersion, from the later paper[95] and not the initial communication. [i] A few dispersion-corrected variants were tested, namely PM6-D3,[107] PM6-DH+,[108] PM6-DH2,[109] PM6-DH2X,[110] PM6-D3H4[111] and PM6-D3H4X.[112] [j] Also tested the PM7-TS variant; see MOPAC online manual.

Accurate benchmark energies were calculated with ORCA using coupled cluster with all singles and doubles and a quasiperturbative triples correction (*i.e.*, CCSD(T)) using domain-localized pair natural orbitals (DLPNO)[9] and the RIJCOSX approximation.[23] In the original MOR41 study, the benchmark energies were calculated using this level of theory extrapolated to the complete basis set limit (CBS) using the def2-TZVPP and def2-QZVPP basis sets.[7] Here, because the (T) component proved to be too computationally demanding to calculate using the available computer hardware, the coupled-cluster energies are extrapolated to the basis set limit using a W1-like extrapolation scheme.[10] The Hartree–Fock (HF) energies are extrapolated using the equation proposed by Zhong *et al.*:[113]

$$E_n \approx E_{CBS} + A \cdot \exp\left(-\alpha\sqrt{L}\right)$$

where E_n is the energy calculated with the *n*-tuple-ζ basis set, E_{CBS} is the energy at the complete basis set (CBS) limit, L is the highest angular momentum of the basis set (which for the basis sets in question equals *n*), and *A* and α are parameters. For two basis sets (*e.g.,* def2-TZVPP and def2-QZVPP, *n* = 3 and 4, respectively) this equation can be rewritten in a more convenient form (where $n_2 > n_1$):

$$E_{CBS}^{HF} = E_{n_2} + \frac{E_{n_2} - E_{n_1}}{\exp\left(\alpha(\sqrt{n_2} - \sqrt{n_1})\right) - 1}$$

CCSD, (T) and MP2 correlation energies are extrapolated using Helgaker *et al.*'s inverse-cubic extrapolation (β = 3):[114]

$$E_{CBS}^{corr} = \frac{n_1^\beta E_{n_1}^{corr} - n_2^\beta E_{n_2}^{corr}}{n_1^\beta - n_2^\beta}$$

The parameters α and β are taken from Neese and Valeev,[115] specifically α = 10.390 and β = 2.400 for CBS(SVP/TZVP) extrapolations and α = 7.880 and β = 2.970 for CBS(TZVPP/QZVPP) extrapolations. The SCF and CCSD correlation energies are extrapolated, in a similar manner as in the original W1 theory,[10] using the def2-TZVPP and def2-QZVPP basis sets, while the (T) correlation energy, which is known to converge faster with basis set,[11] is extrapolated using the def2-SVP and def2-TZVP basis sets. For convenience, these extrapolated DLPNO-CCSD(T) energies are denoted as CCSD(T)/CBS_{W1}. All DLPNO calculations used the "*tightPNO*" option as recommended by Liakos *et al.*[116]

Results and Discussion

MOR41 – Additional Functionals

Since the initial publication by Dohm *et al.* of the MOR41 database, newer functionals have been made available, notably from the Truhlar (*e.g.*, MN15 and MN15-L) and Head-Gordon (*e.g.*, B97M-V and ωB97M-V) groups; likewise many functionals were not tested. Therefore, we tested the performance of several functionals against the MOR41 database. While Dohm *et al*. chose to use the def2-QZVPP basis set, we opted here for the smaller def2-TZVPP basis set since this basis set is more commonly used in computational studies of transition metal systems. Nevertheless, for a number of functionals the larger basis was used; a comparison in the Supporting Information (Table S1) shows that there is little to be gained by using the larger basis set. It should also be

noted that a number of the functionals tested by Dohm *et al.* were also evaluated here to ensure consistency in the results between values computed with different codes, basis sets, *et cetera*.

The comparison of functionals is given in Table 2. From these results, it is clear that the best non-double hybrid functionals are ωB97M-V, ωB97X-V (which was the best in Dohm *et al.*'s study) and mPW1B95$_{D3BJ}$; the best GGA/meta-GGA functionals, which are computationally less costly than hybrids, are MN15-L, SCAN$_{D3BJ}$ and TPSS$_{D3BJ}$. It is interesting to note that the dispersion correction, which generally improves (in some cases quite drastically) the performance of the underlying functional, has little effect on the highly-parameterized MN15-L functional (maximum correction is 0.17 kcal/mol, *c.f.* 535.4 kcal/mol for HCTH).

Table 2. Evaluation of several functionals using Dohm *et al.*'s MOR41 transition metal reaction energy database with the def2-TZVPP basis set both with and without an empirical dispersion correction (all values in kcal/mol).

Functional	**no dispersion**		**with dispersion**			**Dohm *et al.*[a]**
	MAD	**RMSD**	**Type**	**MAD**	**RMSD**	**MAD**
			GGA			
B97-D3BJ	—[b]	—[b]	D3BJ	5.8	7.1	5.9
BLYP	13.2	17.3	D3BJ	5.2	6.9	5.2
BP86	9.2	12.2	D3BJ	5.1	6.5	4.9
HCTH	15.4	19.5	D3BJ	13.0	16.8	

mPWPW91	9.0	12.0	D3BJ	4.9	6.3	
N12	10.1	12.9	D3	4.0	5.5	
OLYP	17.7	23.3	D3BJ	4.9	7.2	
PBE	7.8	10.1	D3BJ	3.8	5.1	3.8
XLYP	12.4	16.2	D3BJ	11.1	13.5	
ωB97	4.7	5.8	none			
meta-GGA						
B97M-D3BJ	—[b]	—[b]	D3BJ	5.6	7.0	
B97M-V	—[b]	—[b]	NL	3.8	4.6	
M06-L	5.7	6.9	D3	5.2	6.4	4.9
M11-L	7.7	8.8	D3	4.9	6.2	
MN12-L	3.8	4.9	D3BJ	6.4	8.3	
MN15-L	3.2	4.5	D3	3.2	4.5	
mPWB95	7.6	9.6	N/A[c]			
PKZB	10.1	12.9	D3	7.5	8.6	
revTPSS	6.8	9.2	D3BJ	4.7	5.4	
SCAN	3.9	5.3	D3BJ	3.3	4.5	

TPSS	7.8	10.5	D3BJ	3.6	4.7	3.3
VSXC	15.4	23.3	N/A[c]			
τHCTH	12.6	16.4	D3	5.7	6.9	
hybrid-GGA						
APFD	—[b]	—[b]	PFD	7.5	9.1	
B3LYP	11.0	14.4	D3BJ	4.9	6.0	4.9
B97-1	7.9	10.3	D3BJ	4.4	5.6	
B97-2	10.6	13.8	D3BJ	12.0	15.0	
B98	8.6	11.2	D3BJ	6.2	7.7	
HISS	5.7	7.2	D3BJ	6.0	7.3	
HSE06	6.3	8.3	D3BJ	2.9	3.7	
mPW1PW91	7.6	10.0	D3BJ	3.8	4.9	
N12-SX	6.3	8.1	D3BJ	3.6	4.7	
O3LYP	15.6	20.5	D3BJ	7.4	8.6	
PBE0	6.4	8.4	D3BJ	2.6	3.5	2.6
X3LYP	10.1	13.2	D3BJ	5.3	6.7	
ωB97X-D	—[b]	—[b]	D2	3.9	5.0	

ωB97X-D3	—[b]	—[b]	D3	5.2	6.3	
ωB97X-D3BJ	—[b]	—[b]	D3BJ	5.5	6.8	
ωB97X	5.5	6.8	D3	4.1	5.0	4.2
	—[b]	—[b]	D3BJ	5.5	6.8	
ωB97X-V	—[b]	—[b]	NL	2.1	2.6	2.2
hybrid-meta-GGA						
M06	6.5	8.0	D3	5.4	7.1	5.6
M11	4.3	5.3	D3BJ	3.8	4.7	
MN12-SX	3.9	4.9	D3BJ	3.4	4.1	
MN15	2.6	3.3	D3BJ	2.6	3.3	
mPW1B95	5.8	7.2	D3BJ	2.3	3.0	2.4
PW6B95	6.3	7.7	D3BJ	2.6	3.3	2.7
SCAN0	3.5	4.6	N/A[b]			
TPSSh	7.2	9.7	D3BJ	7.6	9.0	2.8
τHCTHhyb	8.0	10.4	D3BJ	7.2	8.9	
ωB97M-D3BJ			D3BJ	3.0	3.7	
ωB97M-V			NL	2.0	2.5	

double hybrid						
B2GP-PLYP	5.0	6.2	D3BJ	3.4	4.8	3.5
B2K-PLYP	4.7	5.7	D3BJ	3.2	4.6	
B2T-PLYP	5.4	6.7	N/A[c]			
PWPB95	4.5	5.5	D3BJ	2.9	6.4	1.9
SCAN0-2	4.8	6.5	N/A[c]			
SCAN0-DH	2.6	3.1	N/A[c]			
SCAN0-QIDH	2.9	4.2	N/A[c]			
low-cost methods						
B97-3c			D3	4.4	5.9	4.4
HF-3c			D3	18.9	22.9	
PBEh-3c			D3	4.9	6.4	4.9

[a] Where available[7] [b] By definition, a dispersion correction is part of the functional form. [c] Not available.

The MOBH35 Database

In order to build a benchmark database, we selected reactions that have already been studied computationally. Reactions were chosen to include a wide range of transition metals (both early and late transition metals from each of the three rows of the periodic table) as well as a broad selection of reactions types (*e.g.*, oxidative addition, ligand dissociation, σ-bond metathesis; Table

3). Starting from the reported structures for the transition states and the connecting minima, the geometries were reoptimized at the $TPSS_{D3BJ}$/def2-SVP/W06 level of theory; this is close to the level of theory used by Dohm *et al.* in their study.[7] Reoptimizing the geometries was essential since the original studies used different levels of theory, and in many cases the functionals did not include a dispersion correction. Table 4 lists the reactions included in our MOBH35 dataset with the relevant citations. The reaction energies and barrier heights of all the reactions (Table 4) were calculated at the $CCSD(T)/CBS_{W1}$ level of theory (see Computational Methods section for full details), which again is similar to that used by Dohm *et al.*[7]

Table 3. Periodic table of the elements representation of the number of reactions for each particular transition metal in the MOBH35 barrier height database.

2 Sc	2 Ti			1 Mn	4 Fe				
		2 Nb	1 Mo		2 Ru	1 Rh	5 Pd		
		2 Ta	1 W	2 Re	2 Os	2 Ir	6 Pt		

The following nomenclature is used in identifying structures in the MOBH35 dataset: each complex is identified according to its role in the reaction ("**r**" for reactant, "**p**" for product or "**ts**" for transition state) and the reaction in which it participates. Note that in a few cases, the product of one reaction is the reactant for the next. In these cases, two complexes may have the structure.

These complexes are **p6/r7**, **p8/r9** and **p34/r35**. In addition, in one case (**r30/r31**) the same reactant is involved in two separate reactions.

One issue that arises whenever one uses energies not calculated at the same level as the geometry optimizations is small barrier heights. Using higher level methods, be it larger basis sets, a more robust method or adding corrections (*e.g.*, solvation or basis set superposition error), is common in order to obtain more reliable reaction energies and barrier heights, especially when the use of the higher level of theory would make the geometry optimizations intractable with the available computational resources. However, when using such an approach, one may on occasion obtain a negative barrier height, something that on the face of it would seem nonsensical. This is a result of the approximations made by using this approach that the changes in geometry obtained were one to do the geometry optimizations at the higher level of theory would be negligible; at the level of theory used for the geometry optimization one does obtain a positive barrier height. When studying a particular reaction, especially when part of a complex reaction mechanism, one would just state that this particular step has a very small barrier height – on the order of a few kcal/mol – that will not affect the reaction kinetics given that other steps have significantly higher barriers. In our MOBH35 dataset, there are two reactions with negative barriers (#10 and #35) and another three with barriers >23 kcal/mol. It was decided to include these reactions despite the negative or small barriers since the main point is how well the various DFT exchange–correlation functionals perform compared to the CCSD(T)/CBS_{W1} numbers.

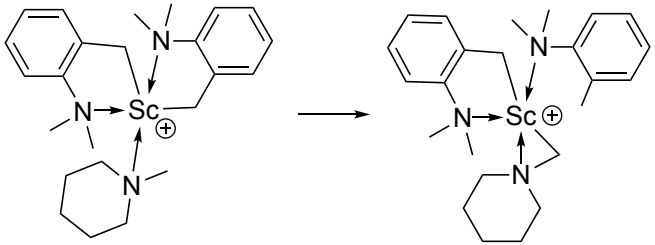
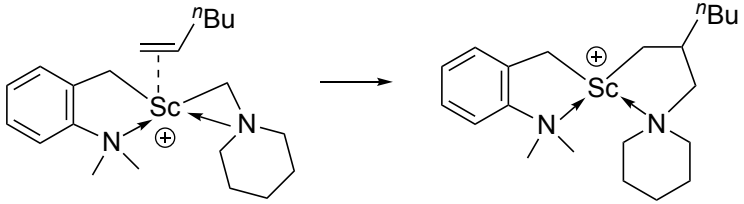
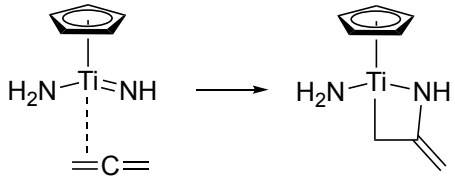
Figure 1 shows the mean absolute deviations (MAD) for each reaction step over all methods tested (DFT and wavefunction theory, excluding the semiempirical methods since they gave dramatically larger errors, *vide infra*). The average MAD of 4.0 kcal/mol is less than the 2σ (where σ is the standard deviation) confidence interval of 6.1 kcal/mol. This indicates that the MOBH35

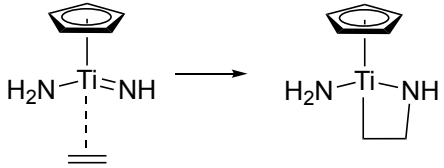
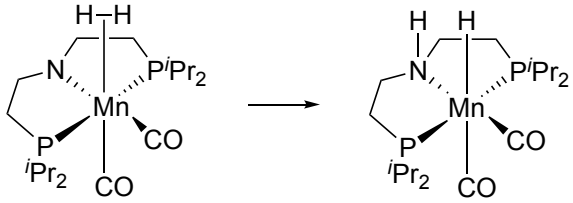
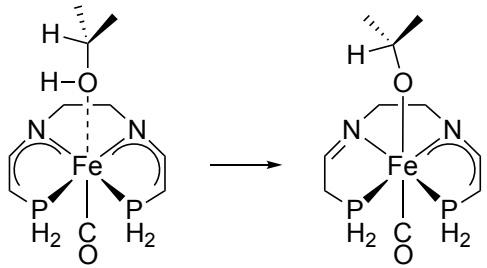
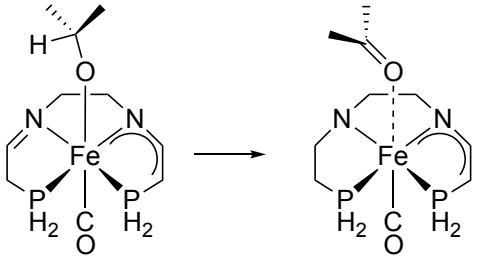
dataset is well balanced, has reliable reference values and that most of the methods tested have reasonable performances for this dataset. The reaction steps with MAD >10 kcal/mol involve association or dissociation of a ligand, and the geometry of such a transition state is probably more sensitive to the computational method.

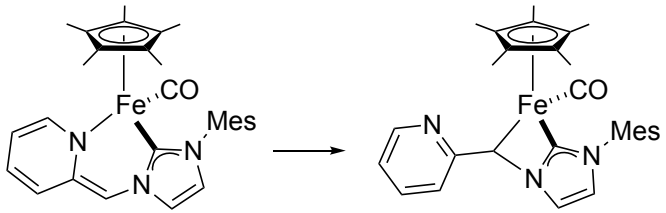
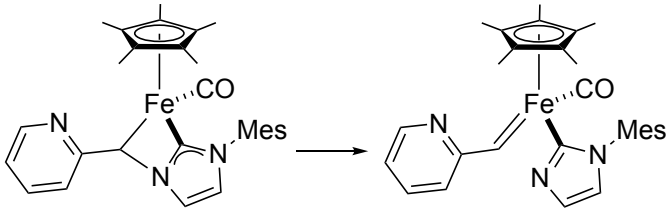
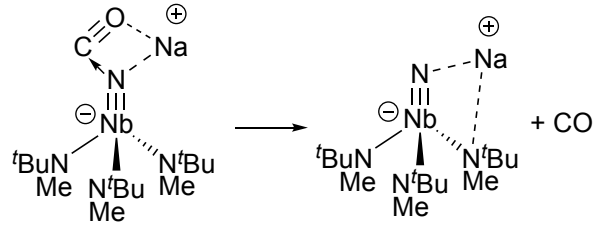
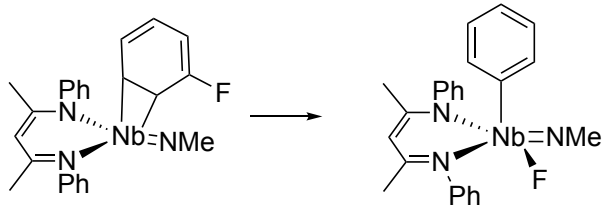
Performance of DFT Functionals Against the MOBH35 Database

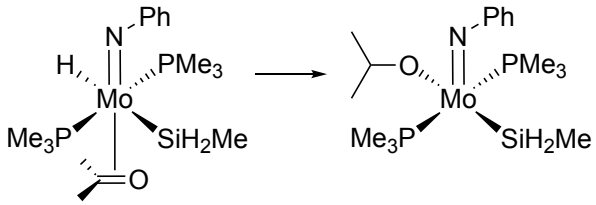
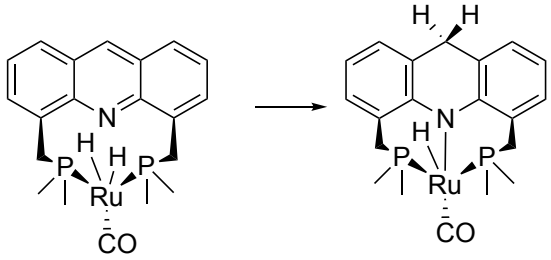
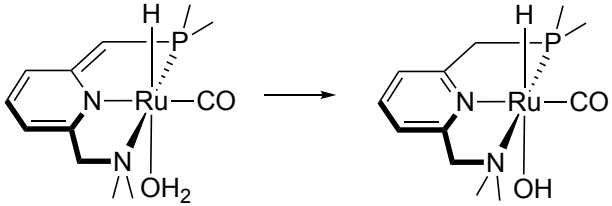
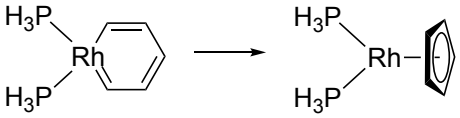
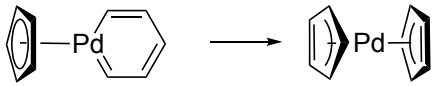
When assessing each method against the benchmark values, the mean absolute deviation (MAD) and root mean squared deviation (RMSD) of three energies for each reaction were considered: (*i*) the forward barrier height, as defined by the direction the reaction is written in Table 4, (*ii*) the reverse barrier height, and (*iii*) the overall reaction energy. This is the same approach taken by Truhlar and coworkers with their main-group barrier heights database.[90,117] A wide selection of DFT exchange–correlation functionals were tested and the results are summarized in Table 5; also included are the evaluations of a selection of low-cost and semiempirical methods as well as various wavefunction methods obtained as part of the benchmarking of the MOBH35 dataset.

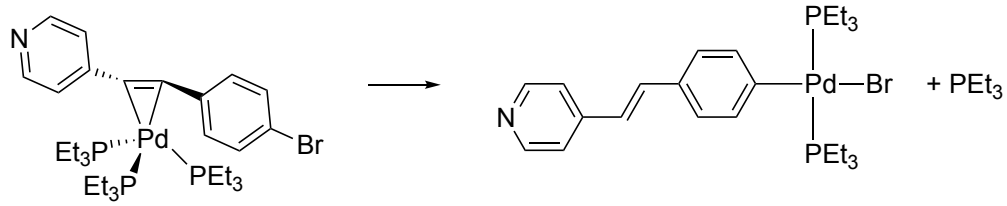
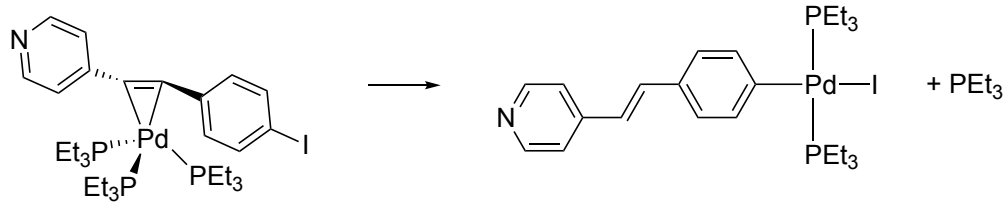
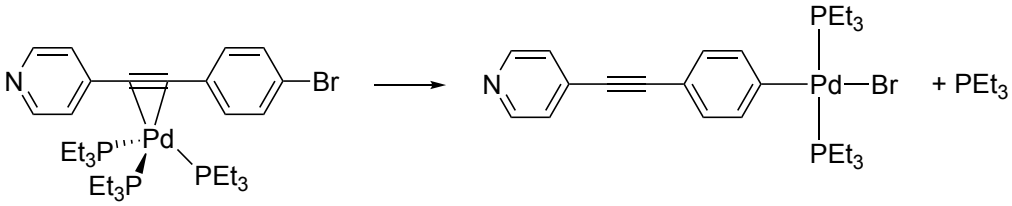
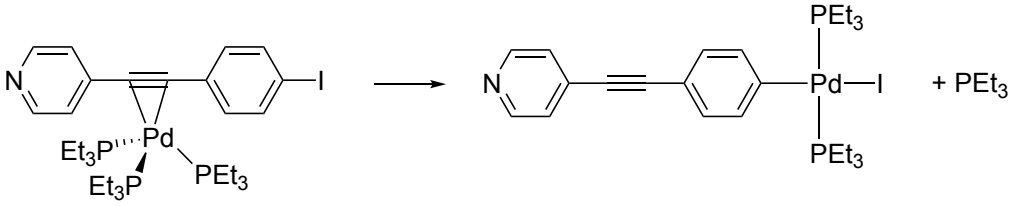
Table 4. Components of the MOBH35 database, including barrier heights and reaction energy (ΔE_{rxn}) in kcal/mol calculated at the CCSD(T)/CBS_{W1} level of theory, sorted according to the atomic number of the transition metal.

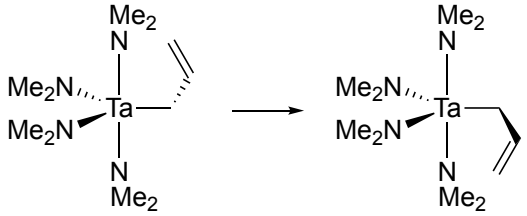
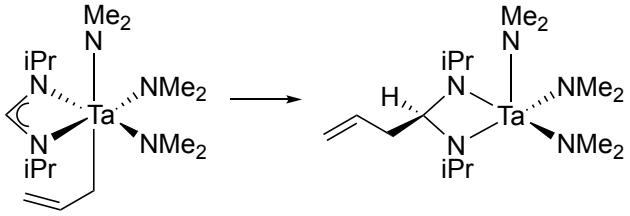
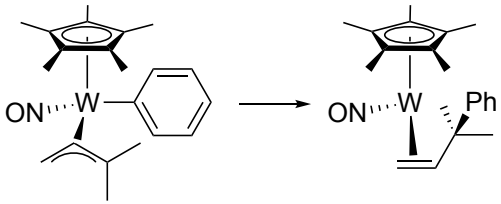
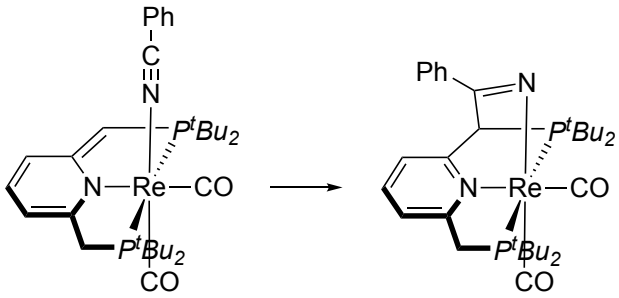
Reaction		**Barrier Height**		ΔE_{rxn}	**ref.**
		forward	**reverse**		
1		26.2	15.9	10.3	[118]
2		5.5	22.4	-16.9	[118]
3		1.0	28.4	-27.4	[119]

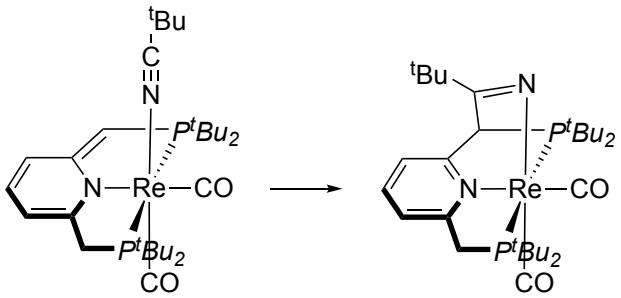
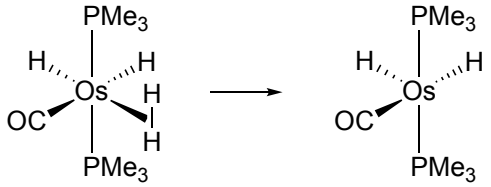
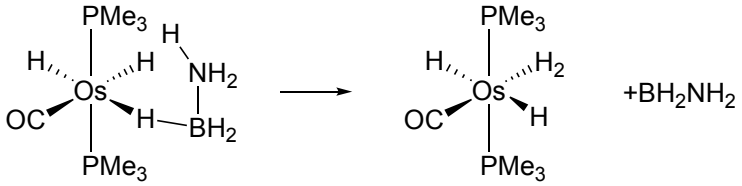
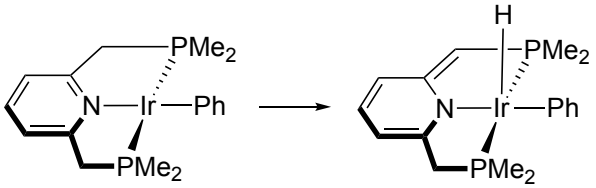
4		1.3	9.9	-8.6	[119]
5		4.36	22.4	-17.8	[120]
6		16.0	14.1	1.9	[121]
7		28.2	18.7	9.5	[121]

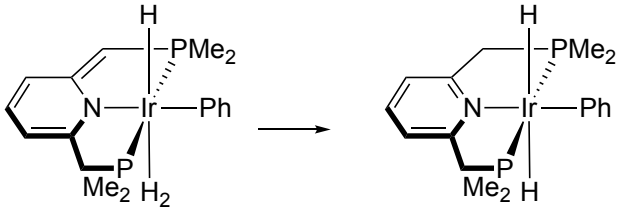
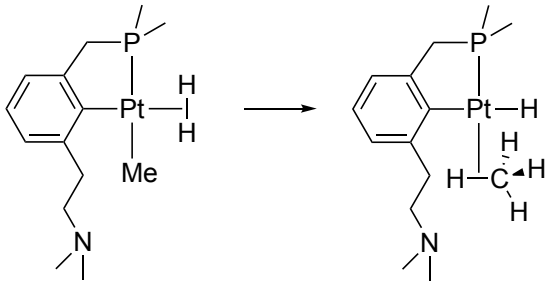
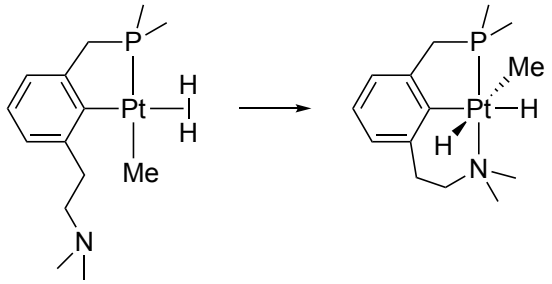
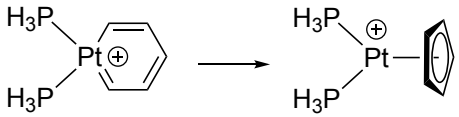
8		36.4	35.2	1.1	[122]
9		33.8	4.2	29.7	[122]
10		-5.4	7.7	13.1	[123]
11		35.1	90.2	-55.1	[124]

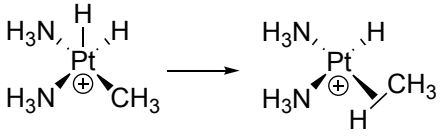
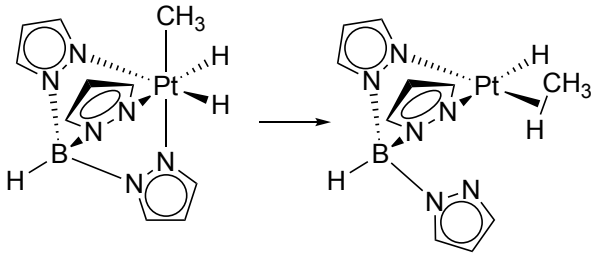
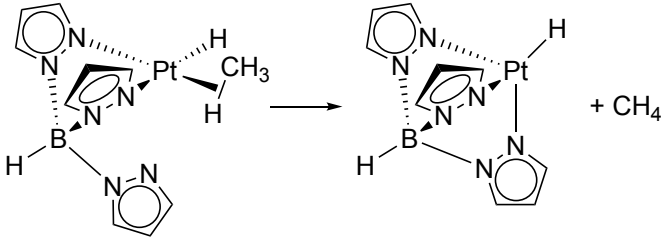
12		0.3	32.0	-31.7	[125]
13		23.1	50.5	-27.5	[126]
14		10.4	14.4	-4.0	[127]
15		20.5	78.8	-58.3	[128]
16		33.4	56.1	-22.7	[128]

17		20.1	37.1	-17.0	[129]
18		23.6	37.9	-14.2	[129]
19		11.1	37.4	-26.3	[129]
20		12.5	39.5	-27.0	[129]

21		9.4	9.4	0.0	[130]
22		14.3	29.6	-15.3	[130]
23		31.2	22.1	9.1	[131]
24		2.9	16.9	-14.0	[132]

25		2.9	11.9	-9.1	[132]
26		25.2	0.2	25.3	[133]
27		13.5	2.4	11.1	[133]
28[a]		27.9	17.3	10.6	[134]

29[a]		15.1	30.7	-15.6	[134]
30		9.8	17.5	-7.6	[135]
31		3.1	13.6	-10.5	[135]
32		19.0	64.9	-45.9	[128]

33		1.5	8.1	-6.6	[136]
34		29.0	2.8	26.2	[136]
35		18.8	-1.2	-20.0	[136]

[a] Two bridging water molecules (see[134]) not shown.

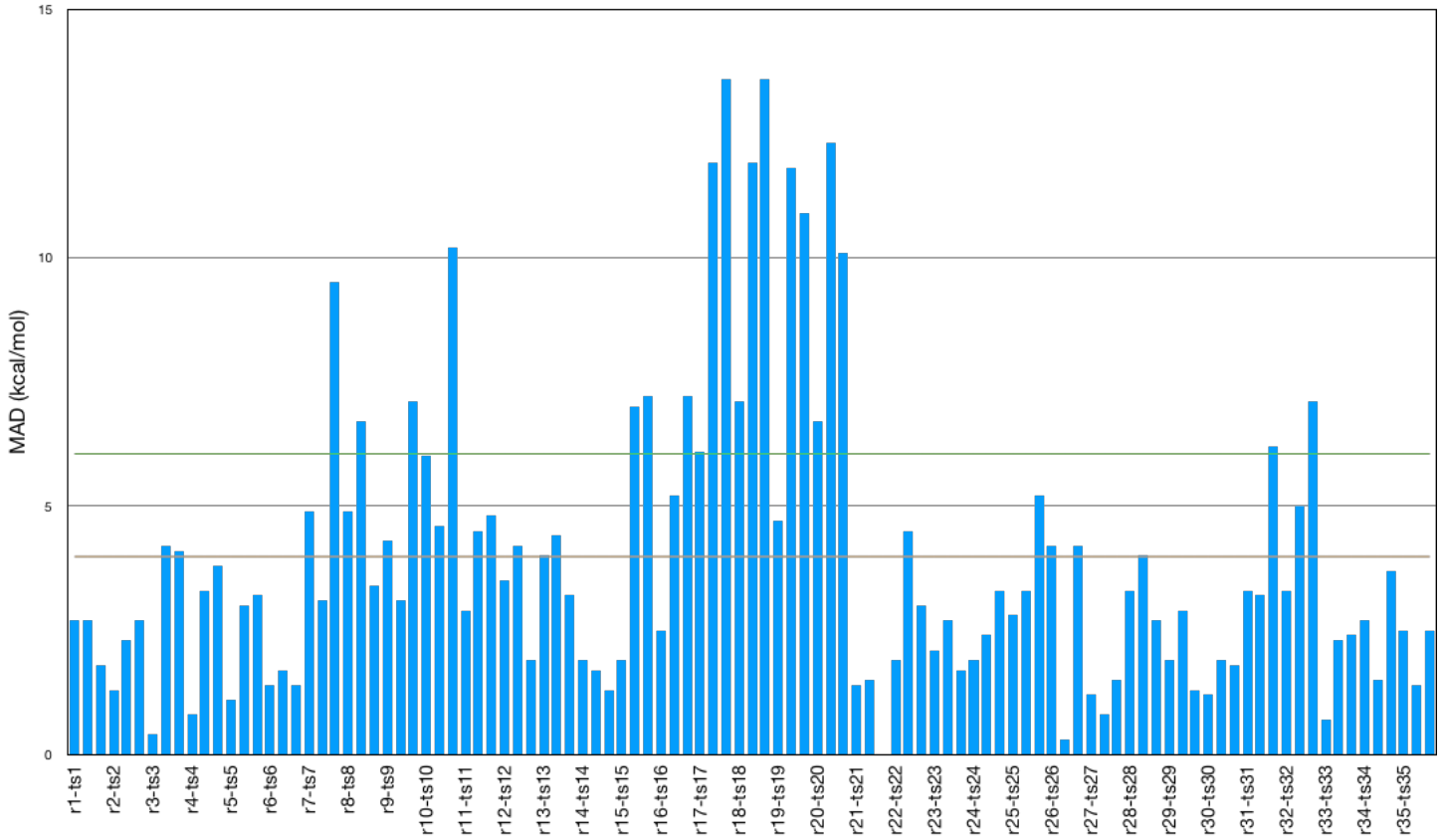


Figure 1. Mean absolute deviation (MAD, kcal/mol) for all methods tested (excluding semiempirical methods, see text) for each reaction step (forward barrier, reverse barrier and reaction energy); the orange and green lines (at 4.0 and 6.1 kcal/mol) mark the average error and the 2σ interval.

Table 5. Evaluation of the MOBH35 database for a wide variety of exchange–correlation functionals (ordered by class alphabetically), low-cost methods and wavefunction methods.

Functional	No Dispersion		With Dispersion		
	MAD	RMSD	Type	MAD	RMSD
LSDA					
SVWN5	7.2	10.0	N/A[b]		
GGA					
BLYP	6.8	9.6	D3BJ	6.3	8.7
			NL	5.5	7.4
BP86	4.6	6.5	D3BJ	6.0	8.7
GLYP	7.1	10.9	N/A[b]		
HCTH	6.0	8.6	D3	5.0	7.2
mPWLYP	6.3	8.7	D3BJ	5.7	7.8
mPWPW91	4.7	6.3	D3BJ	5.6	8.0
N12	4.4	5.9	D3	5.3	8.0
OLYP	6.9	11.0	D3BJ	5.4	7.8

PBE	4.3	5.6	D3BJ	5.0	7.0
			NL	5.2	7.2
revPBE	5.4	7.8	D3BJ	5.4	7.6
revPBE-NL	—[a]	—[a]	NL	5.4	7.5
rPW86PBE	5.2	7.1	D3BJ	5.6	7.7
			NL	5.4	7.3
			SCNL(*i.e.*,VV10)	5.4	7.3
SOGGA11	5.4	6.9	N/A[b]		
XLYP	6.6	9.1	D3BJ	6.4	8.9
ωB97	2.9	3.8	none		
meta-GGA					
B97M-D3BJ	—[a]	—[a]	D3BJ	3.6	5.2
B97M-V	—[a]	—[a]	NL	3.1	4.4
M06-L	4.0	5.5	D3	4.4	6.1
			NL	4.4	6.2
M11-L	4.1	5.6	D3	4.2	6.2
MN12-L	4.2	6.2	D3BJ	5.0	7.7

MN15-L	3.8	5.9	D3	3.8	5.9
PKZB	4.0	5.4	D3	5.9	8.4
revTPSS	3.8	5.0	D3BJ	4.8	6.6
SCAN[c]	3.4	4.6	D3BJ	4.1	5.6
			NL	4.1	5.6
			SCNL	4.1	5.6
TPSS	4.4	5.9	D3BJ	4.8	6.6
			NL	5.0	6.9
VSXC	13.1	24.5	N/A[b]		
τHCTH	5.6	8.1	D3BJ	5.3	7.2
hybrid-GGA					
APFD	—[a]	—[a]	PFD	4.0	6.0
B1LYP	5.3	8.2	D3BJ	4.0	5.5
B3LYP	5.1	7.7	D3BJ	4.0	5.5
			NL	3.1	4.2
B3PW91	3.8	5.9	D3BJ	3.6	5.7
			NL	3.6	5.1

B97-1	3.5	5.1	D3BJ	3.0	4.1
B97-2	4.2	6.6	D3BJ	3.7	5.3
B98	3.9	5.8	D3BJ	3.1	4.3
BH&HLYP	5.8	8.6	D3BJ	3.6	4.6
CAM-B3LYP	3.8	5.8	D3	2.4	3.1
HISS	3.5	4.9	D3BJ	3.2	4.4
HSE03	3.0	4.2	D3BJ	3.1	4.5
HSE06	2.9	4.1	D3BJ	2.9	4.3
LC-ωHPBE	3.8	5.4	D3BJ	3.3	4.6
LC-ωPBE	3.8	5.4	D3	3.2	4.4
mPW1K	4.0	5.9	N/A[b]		
mPW1PW91	3.3	5.0	D3BJ	3.1	4.7
N12-SX	3.2	4.5	D3BJ	3.2	4.9
O3LYP	6.0	10.0	D3BJ	3.4	4.6
PBE0	2.9	4.2	D3BJ	2.8	4.1
			NL	3.4	4.9
revPBE0	4.1	6.6	NL	3.1	4.5

			SCNL	3.2	4.6
revPBE38	4.3	6.9	NL	3.0	4.1
SOGGA11-X	3.7	5.5	D3BJ	2.9	4.1
ωB97X	2.8	3.7	D3	2.3	3.0
			D3BJ	2.3	3.3
			NL(*i.e.*,ωB97X-V)	2.1	2.7
hybrid-meta-GGA					
B1B95	2.7	3.8	D3BJ	3.5	5.4
BB1K	3.2	4.5	N/A[b]		
BMK	3.3	5.2	D3BJ	3.1	4.5
M06	3.4	4.6	D3	5.9	7.9
M06-2X	3.0	4.1	D3	3.0	4.0
M06-HF	4.7	6.5	D3	4.3	6.0
M08-HX	3.3	4.7	D3	3.2	4.6
M11	2.9	6.7	D3BJ	2.7	3.9
MN12-SX	2.7	3.8	D3BJ	2.8	4.3
MN15	2.6	3.9	D3BJ	2.6	4.0

mPW1B95	2.5	3.3	D3BJ	3.0	4.2
mPW1KCIS	4.1	5.9	D3BJ	4.1	5.7
mPWB1K	3.1	4.2	D3BJ	3.3	4.4
mPWKCIS1K	4.3	6.5	D3BJ	3.1	4.1
PBE1KCIS	3.5	4.9	D3BJ	3.2	4.4
PW6B95	2.4	3.3	D3BJ	2.6	3.8
PWB6K	2.7	3.7	D3BJ	2.9	3.9
revTPSS0	2.7	4.2	D3BJ	2.7	4.1
revTPSSh	3.1	4.2	D3BJ	3.7	5.5
SCAN0	2.1	3.1	N/A[b]		
TPSS0	3.6	5.2	D3BJ	3.5	5.1
TPSS1KCIS	3.8	5.6	D3BJ	3.7	5.3
TPSSh	3.6	5.2	D3BJ	3.9	5.3
τHCTHhyb	3.8	5.4	D3BJ	3.8	5.3
ωB97M-D3BJ	—[a]	—[a]	D3BJ	2.0	2.8
ωB97M-V	—[a]	—[a]	NL	1.8	2.6

double hybrid					
B2GP-PLYP	2.0	3.0	D3BJ	2.7	4.4
B2K-PLYP	1.8	2.6	D3BJ	2.4	4.0
B2PLYP	6.8	9.6	D3BJ	5.5	7.7
B2T-PLYP	2.2	3.4	N/A[b]		
DOD-PBEP86			D3BJ	2.4	4.3
DOD-PBEP86	—[a]	—[a]	D3BJ	2.5	4.6
			NL	2.1	3.6
DOD-SVWN5	—[a]	—[a]	D3BJ	2.0	4.0
DSD-BLYP	—[a]	—[a]	D3BJ	3.1	5.3
			NL	2.9	4.7
DSD-PBEB95	—[a]	—[a]	D3BJ	2.6	4.4
DSD-PBEP86	—[a]	—[a]	D3BJ	2.7	4.5
			NL	2.6	4.3
mPW2K-PLYP	3.8	9.4	N/A[b]		
mPW2PLYP	2.5	3.6	D3BJ	2.8	4.2
PBE0-2	3.2	4.7	N/A[b]		

PBE0-DH	2.2	2.9	N/A[b]		
PBE-QIDH	2.4	3.10	N/A[b]		
PWPB95	1.6	2.5	D3BJ	2.4	3.9
			NL	2.4	3.8
SCAN0-2	3.3	5.1	N/A[b]		
SCAN0-DH	1.7	2.5	N/A[b]		
SCAN0-QIDH	2.5	3.5	N/A[b]		
wave function methods					
HF/QZVPP	13.1	18.8	N/A[b]		
DLPNO-MP2/TZVP	6.3	10.0	N/A[b]		
DLPNO-MP2/QZVPP	6.4	9.9	N/A[b]		
DLPNO-CCSD(T)/SVP	2.1	2.8	N/A[b]		
DLPNO-CCSD(T)/TZVP	1.5	2.3	N/A[b]		
DLPNO-CCSD/QZVPP	2.4	3.1	N/A[b]		
DLPNO-CCSD(T)/CBS(SVP/TZVP)	1.9	2.8	N/A[b]		
DLPNO-MP2/CBS(SVP/TZVP)	6.9	11.2	N/A[b]		
DLPNO-MP2/CBS(TZVPP/QZVPP)	6.3	9.7	N/A[b]		

low cost/semi-empirical methods					
B97-3c	—[a]	—[a]	D3	4.8	6.9
HF-3c	—[a]	—[a]	D3	13.5	17.5
PBEh-3c	—[a]	—[a]	D3	5.0	9.6
PM6	21.5	28.8	D3	20.2	27.7
			DH+	20.8	28.2
			DH2	20.9	28.4
			DH2X	20.9	28.4
			D3H4	18.9	25.7
			D3H4X	18.9	25.7
PM7	106.4	146.1	N/A[b]		
PM7-TS	67.8	141.8	N/A[b]		

[a] By definition, a dispersion correction is part of the functional form. [b] Not available. [c] SCAN has been reported to have significant grid dependence.[29] Therefore, the calculations were repeated with other integration grids, yielding (MAD, RMSD – both in kcal/mol) of GRID4 (3.3, 4.6), GRID5 (3.3, 4.6), GRID6 (3.4, 4.6), GRID7 (3.4, 4.7). Clearly, this is not an issue here.

Reviewing the results in Table 5, one can conclude that the top nonlocal (*i.e.*, non-hybrid) functionals are ωB97, B97M-V, SCAN and MN15-L, while the top hybrids are ωB97M-V, ωB97X-V, SCAN0 and MN15. Like with the MOR41 database, most nonlocal functionals do not

perform well, although the top nonlocal functionals perform better than many hybrid functionals. Nevertheless, their use would not be recommended. On the other hand, the top three hybrid functionals perform on par with the top double-hybrid functionals – PWPB95, SCAN0-DH and B2K-PLYP; given the significant computational expense of double hybrids, this makes ωB97M-V or ωB97X-V very enticing, especially given that these are the top performing hybrid functionals for both the MOBH35 and MOR41 databases. However, if these functionals are not available, one should use a double-hybrid functional like PWPB95 or B2K-PLYP, which are more widely available.

Najibi and Goerigk had previously noted that the NL dispersion correction can be applied noniteratively as the self-consistent form (*i.e.*, SCNL) did not have any significant impact on their evaluation of their GMTKN55 database.[32] Just to be sure, this was again tested here for a few functionals, and it was found that indeed the self-consistent application of the NL correction did not impact the results (Table 6).

One functional that did surprisingly well is M06-2X. It was generally accepted that M06-2X is not suitable for transition metal complex and one should rather use M06.[79] Moreover, Quintal *et al.* found that "kinetics" functionals with high percentages of "exact" Hartree–Fock exchange do not perform as well as they do for main group reactions.[5] Nonetheless, for the MOBH35 dataset, M06-2X actually outperforms M06 and the kinetics functionals only perform slightly poorer than their non-kinetics versions. That being said, these are not the top performers.

From the calculations done in order to obtain the benchmark energies, one can extract numbers for some lower-level wavefunction methods. DLPNO-CCSD(T)/def2-TZVP has a MAD of 1.5 kcal/mol, yet despite its significant cost this is only marginally better than the MADs for the top double-hybrid and hybrid functionals; this makes the use of the more expensive method

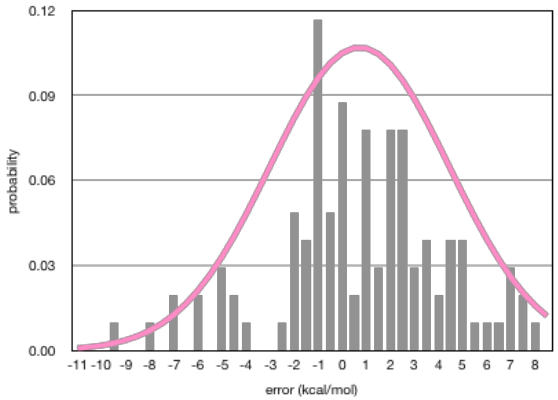
unappealing compared to its cheaper competitors. Even more notable is that MP2, either with a large quadruple-ζ basis set or using basis-set extrapolation, does very poorly and a large portion of the DFT functionals – and even the low-cost B97-3c – outperform it.

In Figure 2 are plotted the error distributions of the top functionals, superimposed with a normal (Gaussian) distribution based on the mean error and standard deviation for each functional (Table 6); in panel (f) is plotted an overlay of all eight normal distributions. As can be expected, CCSD(T)/def2-TZVP, which was already found to have the lowest MAD (*vide supra*), has the tightest distribution (*i.e.*, smallest standard deviation). The double-hybrid PWPB95 and the hybrid ωB97M-V both have similar distributions. MN15, which has a MAD smaller than the GGAs, nevertheless has a distribution that is similar to the latter. This is significant as a narrow error distribution is preferred – whereas one can account for a systematic error, it is harder to account for a larger error.

Table 6. Mean error and standard deviation (both in kcal/mol) and the ratio of MAD and RMSD (unitless) for selected methods.

Method	Mean	Standard Deviation
CCSD(T)/def2-TZVP	0.19	2.30
ωB97	0.72	3.73
SCAN	-1.65	4.36
B97M-V	-1.14	4.30
MN15	-0.36	3.91
SCAN0	-0.49	3.05
ωB97M-V	0.18	2.62
PWPB95	-0.41	2.44

a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0.06
0.03
0.00
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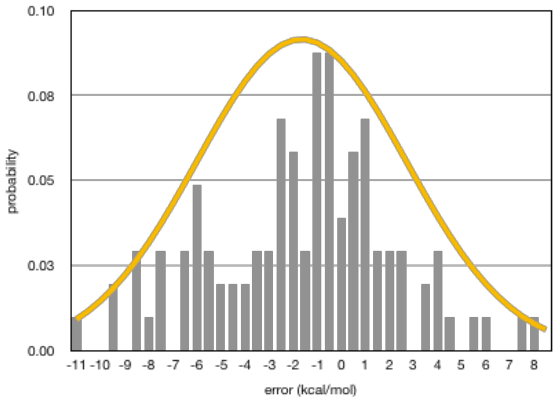
error (kcal/mol)

b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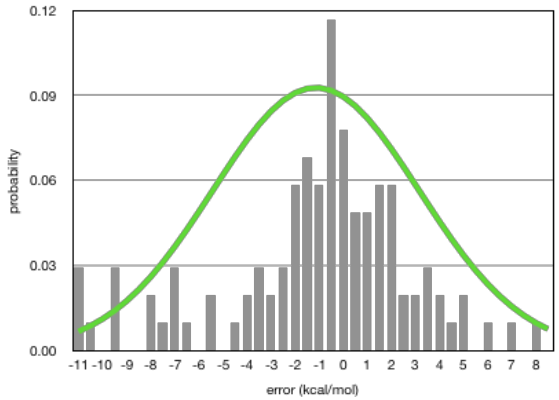
error (kcal/mol)

c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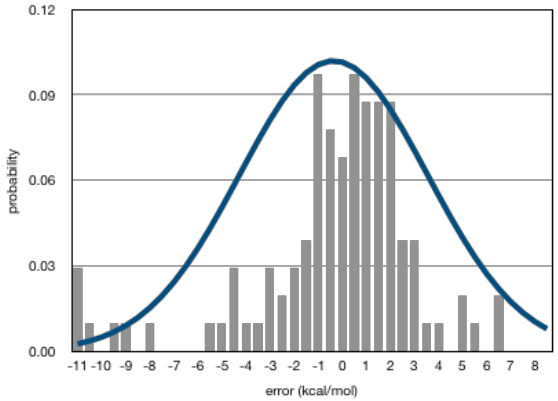
error (kcal/mol)

d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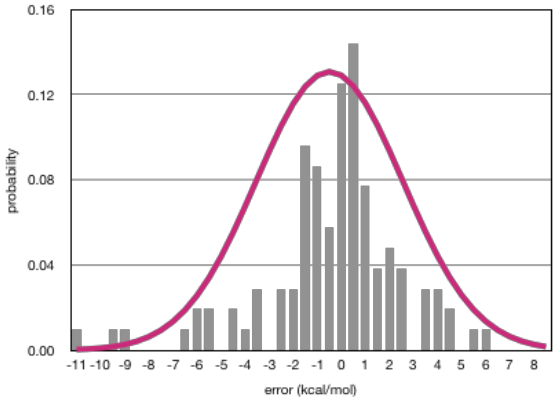
error (kcal/mol)

e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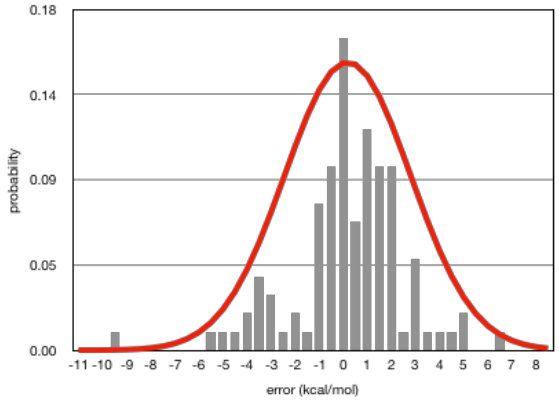
error (kcal/mol)

f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error (kcal/mol)

g h i

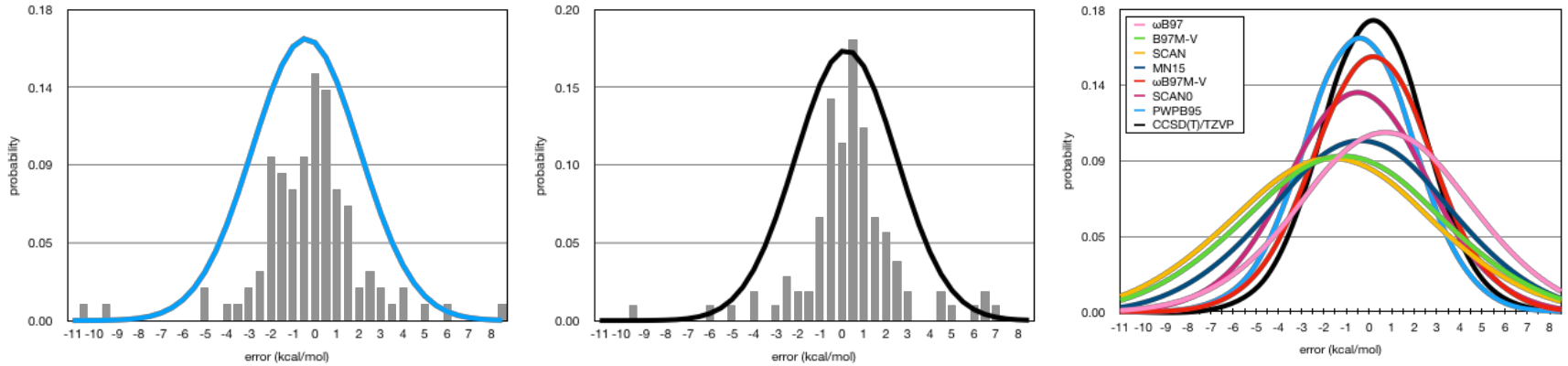

Figure 2. Error distribution and corresponding normal distribution of (a) ωB97, (b) SCAN, (c) B97M-V, (d) MN15, (e) SCAN0, (f) ωB97M-V, (g) PWPB95 and (h) DLPNO-CCSD(T)/def2-TZVP, and (i) an overlay of all the normal distribution curves.

The low-cost methods and semiempirical methods considered here are intended for use as the size of the systems being studied grow beyond the feasibility of standard DFT methods. One would not expect these methods to perform well, and as a general rule this is true. Only Grimme and coworkers' B97-3c and PBEh-3c have MADs that may be considered acceptable. In general, their use would not be recommended except for cases where there are no better options.

One surprising observation from the data in Table 5 it that the dispersion correction does not always improve the results. For many functionals (*e.g.,* B3LYP, HCTH, O3LYP and B2PLYP) there indeed are lower errors when dispersion is included, while for some (*e.g.*, MN15-L, MN15 and HSE06) dispersion has a negligible impact. However, there are a number of functionals (*e.g.*, BP86, PBE, TPSS, SCAN, B2K-PLYP and PWPB95) where the dispersion correction is actually detrimental. This was rather unexpected given the repeated observation that including these dispersion corrections generally improves accuracy,[137] often correcting an otherwise repulsive interaction, although Kozuch and Martin observed that dispersion-corrections can also be detrimental.[138] It is possible that these deviations are within the expected error associated with the CCSD(T)/CBS_{W1} benchmark level of theory. Another possibility is that this is a consequence of fitting the dispersion parameters using only dimers are equilibrium distance. For instance, in their initial parameterization of D3BJ parameters for several functionals, including PB86, PBE and TPSS, Grimme *et al.* fitted against a set of databases that are primarily equilibrium geometries with a small number of nonequilibrium distances included via the S22+ dataset.[24a,25] It is possible that as a consequence the dispersion parameters are ill-fitted to describe transition states, which by definition are nonequilibrium structures. In contrast, the parameters used here for a number of functionals were taken from the Supporting Information of Goerigk *et al.*'s GMTKN55 paper,

where the parameters were fit against a much larger dataset that includes a significant number of nonequilibrium structures, including reaction transition states.

Conclusions

A new database – MOBH35 – of thirty-five transition metals reactions is presented. The geometries were reoptimized at a consistent level of theory – $TPSS_{D3BJ}$/def2-SVP – and the reaction energies and barrier heights were calculated at the $CCDS(T)/CBS_{W1}$ level of theory, a composite, basis set extrapolation method akin to Martin and coworkers' Weizmann-1 (W1). After evaluating a wide range of density-functional exchange–correlation functionals from all rungs of Perdew's ladder,[139] we found that Head-Gordon and coworkers' ωB97M-V and ωB97X-V functionals, as well as SCAN0, are recommended; the first two are the top performers for both our MOBH35 dataset and Dohm *et al.*'s MOR41 dataset. Alternatively, one could calculate energies using either the PWPB95 or B2K-PLYP double hybrid functional, whose slightly improved accuracy is counterbalanced by their significantly increased computational cost. It is interesting to note that these functionals have similar accuracies for the MOBH35 dataset as coupled-cluster methods. The use of the results presented here should be beneficial to any future mechanistic studies involving transition metal complexes.

Supporting Information. Table comparing MOR41 with the def2-TZVPP and def2-QZVPP basis sets and Cartesian coordinates of all structures in the MOBH35 dataset. The following files are available free of charge.

Table S1 and Cartesian coordinates of MOBH35 (PDF file)

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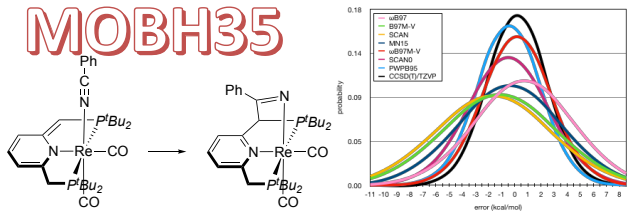
Table of Contents Graphic



Evaluating Transition Metal Barrier Heights with the Latest DFT Exchange–Correlation Functionals – the MOBH35 Benchmark Dataset

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Supporting Information

Table S1. Evaluation of several functionals using Dohm *et al.*'s MOR41 transition metal reaction energy database with the def2-TZVPP and def2-QZVPP basis sets without an empirical dispersion correction (all values in kcal/mol)

Functional	TZVPP		QZVPP	
	MAD	**RMSD**	**MAD**	**RMSD**
MN15-L	3.2	4.5	3.3	4.6
HCTH	15.4	19.5	15.7	20.0
τHCTH	12.6	16.4	12.7	16.6
VSXC	15.4	23.3	17.0	26.8
TPSS	7.8	10.5	7.9	10.7
M11-L	7.7	8.8	7.7	8.8
MN12-L	3.8	4.9	3.8	4.9
N12	10.1	12.9	10.3	13.2
revTPSS	6.8	9.2	6.9	9.4
BLYP	13.2	17.3	13.5	17.6
OLYP	17.7	23.3	18.1	23.8
XLYP	12.4	16.2	12.6	16.5
PBE	7.8	10.1	8.0	10.4
BP86	9.2	12.2	9.4	12.5

M06-L	5.7	6.9	5.9	7.2
PKZB	10.1	12.9	10.4	13.2
mPWPW91	9.0	12.0	9.3	12.2
ωB97M-V	2.0	2.5	2.1	2.6
SCAN	3.9	5.3	4.0	5.4
PWPB95	4.5	5.5	4.8	5.9
SCAN0	3.5	3.8	4.6	4.8
B2T-PLYP	5.4	6.7	5.5	7.2
B2K-PLYP	4.7	5.7	4.8	6.2
SCAN0-DH	2.6	3.1	2.9	3.6
B2GP-PLYP	5.0	6.2	5.2	6.7

Cartesian Coordinates (in Å) of all Structures in MOBH35

```
5
Structure: CH4 Stoichiometry: CH4+
   C     0.000000    0.000000    0.000000
   H     0.636184    0.636184    0.636184
   H    -0.636184   -0.636184    0.636184
   H    -0.636184    0.636184   -0.636184
   H     0.636184   -0.636184   -0.636184
2
Structure: CO Stoichiometry: CO+
   C     0.000000    0.000000   -0.651214
   O     0.000000    0.000000    0.488410
22
Structure: PEt3 Stoichiometry: C6H15P+
   P    -0.152692   -0.191307   -0.524975
   C     1.023862   -1.419449    0.274350
   C     2.502358   -1.192202   -0.066758
   H     0.705332   -2.415434   -0.088794
   H     0.871248   -1.415087    1.372031
   H     3.129004   -2.008507    0.335243
   H     2.658105   -1.149325   -1.159397
   H     2.876677   -0.247009    0.363444
   C    -1.727367   -0.776424    0.317820
   C    -2.975828   -0.003000   -0.125866
   H    -1.601876   -0.725436    1.417639
   H    -1.835568   -1.846547    0.058500
   H    -3.882304   -0.397896    0.367051
   H    -2.902373    1.069515    0.130104
   H    -3.120009   -0.075462   -1.218184
   C     0.176520    1.344636    0.513627
   C     1.213381    2.300150   -0.093859
   H     0.464897    1.040701    1.539447
   H    -0.794642    1.867353    0.600623
   H     1.326160    3.207386    0.527124
   H     2.207406    1.828079   -0.178118
   H     0.910761    2.615001   -1.107968
65
Structure: P1 Stoichiometry: C24H37N3Sc+
   N     0.560616    2.108690    0.286735
   N     1.488178   -1.892091   -0.468372
   C    -0.539714    0.654672   -1.904338
   H     0.438162    0.987788   -2.297092
   H    -1.100095    0.123164   -2.688495
   C    -1.341787    1.677894   -1.217438
   C    -0.835431    2.367628   -0.067236
   C    -1.652841    3.232597    0.685735
   H    -1.246645    3.755986    1.554066
   C    -2.987931    3.428183    0.330382
   H    -3.615824    4.102292    0.920326
   C    -3.512284    2.766505   -0.796829
   H    -4.554278    2.928692   -1.090572
   C    -2.707177    1.911619   -1.545222
   H    -3.118052    1.401825   -2.422955
   C     0.929178    2.483623    1.672317
   H     0.888582    3.579532    1.815270
   H     1.964781    2.156623    1.848152
   H     0.253906    1.984480    2.381834
```

```
   C     1.516856    2.758377   -0.654475
   H     1.196606    2.595877   -1.691578
   H     2.519668    2.330398   -0.503918
   H     1.545421    3.846471   -0.461987
   C     2.260675   -0.734916    2.194035
   H     2.452978    0.054080    2.936657
   H     2.626399   -1.683299    2.626386
   C     2.960748   -0.402288    0.892149
   C     2.610892   -0.957700   -0.374663
   C     3.325914   -0.570838   -1.528375
   H     3.063068   -0.985721   -2.502140
   C     4.395021    0.326526   -1.445651
   H     4.939426    0.600606   -2.354182
   C     4.767706    0.856711   -0.204160
   H     5.608690    1.551906   -0.125794
   C     4.048043    0.495254    0.938777
   H     4.332772    0.912986    1.910532
   C     1.724070   -3.162567    0.278891
   H     0.833089   -3.798517    0.175105
   H     1.903012   -2.971448    1.342453
   H     2.597036   -3.690560   -0.145410
   C     1.114563   -2.257225   -1.863648
   H     0.905194   -1.354982   -2.452353
   H     0.201382   -2.867953   -1.820260
   H     1.914589   -2.849564   -2.345070
   Sc   -0.001421   -0.133662    0.126638
   C    -1.709238   -2.482905    1.284612
   C    -2.102448   -3.412411    0.133719
   N    -1.855249   -1.054437    0.911667
   C    -3.519452   -3.108196   -0.374340
   C    -3.653724   -1.615646   -0.708435
   C    -3.248930   -0.758435    0.489272
   C    -1.282131   -0.125141    1.918740
   H    -0.662182   -2.649663    1.598969
   H    -2.340047   -2.680808    2.176386
   H    -1.386082   -3.279809   -0.699358
   H    -2.016252   -4.460466    0.470195
   H    -3.751985   -3.732408   -1.254071
   H    -4.252725   -3.375116    0.410357
   H    -3.006441   -1.357734   -1.568480
   H    -4.690224   -1.368776   -0.995998
   H    -3.306885    0.314087    0.254599
   H    -3.918796   -0.955379    1.351991
   H    -1.955794    0.733972    2.063568
   H     1.153833   -0.825056    2.124255
   H    -1.104728   -0.629677    2.886073
60
Structure: P2 Stoichiometry: C21H36N2Sc+
   N     2.144054    1.329209    1.038690
   C     1.955150    1.133625   -1.837415
   H     3.023499    0.959910   -1.618970
   H     1.774821    1.146200   -2.921145
   C     1.307539    2.237970   -1.113149
   C     1.331325    2.323996    0.323132
   C     0.553582    3.274755    1.017197
   H     0.605470    3.336010    2.106863
   C    -0.280929    4.144101    0.319492
   H    -0.879828    4.880147    0.863348
```

C	-0.345472	4.066644	-1.085877
H	-1.001167	4.745657	-1.639795
C	0.423665	3.136910	-1.776449
H	0.370035	3.085818	-2.868630
C	1.734022	1.074169	2.441499
H	1.953682	1.934258	3.099582
H	2.296047	0.202820	2.815477
H	0.651096	0.866423	2.485420
C	3.608457	1.581130	0.958687
H	3.885360	1.829994	-0.074625
H	4.155072	0.680410	1.282829
H	3.878639	2.428644	1.613843
Sc	0.946455	-0.064631	-0.257004
C	1.427498	-2.850928	1.135920
C	2.853261	-2.600678	0.631612
N	0.445250	-2.244024	0.195359
C	3.052364	-3.163269	-0.782698
C	1.962054	-2.629515	-1.720935
C	0.559963	-2.876493	-1.152570
C	-0.958875	-2.279314	0.720355
H	1.266640	-2.397237	2.129643
H	1.234493	-3.938373	1.235474
H	3.055782	-1.502805	0.624306
H	3.579715	-3.029715	1.342227
H	4.054996	-2.909346	-1.165738
H	2.992423	-4.266894	-0.745111
H	2.115723	-1.534524	-1.894645
H	2.035949	-3.081504	-2.724244
H	-0.214357	-2.436310	-1.803527
H	0.346892	-3.961891	-1.074415
H	-1.345506	-3.316849	0.675369
H	-0.900698	-1.995999	1.787802
C	-1.871083	-1.281328	-0.015940
H	-1.971442	-1.616762	-1.068784
C	-1.210837	0.114492	-0.011135
H	-1.329720	0.573969	0.999650
H	-1.698959	0.809990	-0.719372
C	-3.287868	-1.334586	0.601400
H	-3.639051	-2.385862	0.618219
H	-3.223692	-1.010486	1.659891
C	-4.320115	-0.472527	-0.134841
H	-4.361671	-0.782927	-1.198198
H	-3.984903	0.582158	-0.135075
C	-5.726698	-0.556794	0.475866
H	-6.061578	-1.612321	0.474339
H	-5.677011	-0.254276	1.540157
C	-6.754506	0.310918	-0.258874
H	-7.752460	0.229980	0.204754
H	-6.460762	1.376321	-0.242796
H	-6.849180	0.006647	-1.317042

23

Structure: P3 Stoichiometry: C8H12N2Ti+

C	1.091054	-1.265254	1.140693
C	2.174988	-0.408848	0.794069
C	2.274110	-0.374322	-0.624992
C	1.257064	-1.220838	-1.159670
C	0.533141	-1.775809	-0.067688
Ti	0.165443	0.550921	-0.076726

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   C    -2.162712    0.038533    0.015841
   N    -1.461363    0.574251   -1.092433
   N     0.946663    2.279159    0.008195
   C    -1.457779    0.450784    1.274066
   H     2.791184    0.158464    1.493996
   H     0.746612   -1.492047    2.149653
   H     2.984390    0.217523   -1.204887
   H     1.056432   -1.396604   -2.218333
   H    -0.347911   -2.417090   -0.140870
   H    -1.631500   -0.198192    2.141809
   C    -3.221433   -0.817159   -0.072640
   H    -1.863413    0.353191   -2.006219
   H     1.906253    2.584269    0.184158
   H     0.370093    3.098542   -0.213986
   H    -1.619093    1.518807    1.508509
   H    -3.728411   -1.167755    0.830685
   H    -3.632090   -1.115757   -1.044958
22
Structure: P4 Stoichiometry: C7H12N2Ti+
   C     1.373320   -1.030121    1.050513
   C     1.949769    0.263717    0.903978
   C     2.089123    0.530238   -0.486051
   C     1.601686   -0.601155   -1.202514
   C     1.167716   -1.568277   -0.251535
   Ti   -0.257909    0.319736   -0.077590
   N    -1.650216   -0.167366   -1.199655
   C    -2.475089   -0.673691   -0.041464
   C    -1.672942   -0.454012    1.265786
   N    -0.354234    2.209902    0.135047
   H     2.202195    0.946413    1.717663
   H     1.130815   -1.519742    1.993868
   H     2.469423    1.451770   -0.929480
   H     1.551399   -0.700192   -2.288611
   H     0.712968   -2.533322   -0.483177
   H    -1.495474   -1.387814    1.818193
   H    -2.684131   -1.752375   -0.183804
   H    -2.028496   -0.427724   -2.110798
   H     0.359630    2.856528    0.479031
   H    -1.163056    2.749852   -0.187353
   H    -2.109388    0.316065    1.919373
   H    -3.442239   -0.131609   -0.017940
62
Structure: P5 Stoichiometry: C18H38MnNP2O2+
   P    -2.185602   -0.136110   -0.035707
   N    -0.005573   -1.844021   -1.082361
   C     0.976156   -1.720032   -2.187019
   C    -1.359992   -2.342855   -1.454648
   C    -2.364883   -1.195946   -1.572078
   H    -3.386229   -1.583497   -1.737472
   H    -2.104967   -0.550806   -2.428367
   C     2.365539   -1.438491   -1.597837
   H     3.026069   -1.004973   -2.367331
   P     2.205889   -0.251913   -0.128388
   C     0.106192    1.254879    1.408268
   O     0.168089    1.984576    2.329940
   Mn    0.022216    0.079911    0.100046
   C     0.037025    1.244437   -1.241930
   O     0.055223    2.063308   -2.097622
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   C    -3.328622    1.338115   -0.315144
   H    -4.312107    1.043073    0.098225
   C    -2.804368    2.553893    0.469649
   H    -3.538340    3.378985    0.415223
   H    -2.621532    2.322912    1.531160
   H    -1.852018    2.907327    0.040865
   C    -3.509871    1.686449   -1.801767
   H    -4.014566    0.881191   -2.361868
   H    -4.131135    2.596313   -1.892740
   H    -2.538667    1.897411   -2.281242
   C     3.285037    1.179891   -0.707365
   H     2.895234    1.333272   -1.732939
   C     3.018112    2.476287    0.073812
   H     3.593844    3.305720   -0.376210
   H     1.950639    2.742150    0.045468
   H     3.318158    2.391735    1.131649
   C     4.781513    0.845726   -0.792995
   H     5.323326    1.660927   -1.306667
   H     5.227473    0.735690    0.211157
   H     4.971684   -0.087071   -1.353660
   H     0.995468   -2.644052   -2.802693
   H     0.649539   -0.886260   -2.830028
   H     2.837203   -2.378091   -1.258757
   H    -1.682050   -3.037650   -0.660254
   H    -1.304235   -2.924189   -2.395647
   C     3.212037   -1.138220    1.196720
   H     4.219627   -1.324553    0.777649
   C     2.554880   -2.481020    1.549706
   H     3.110511   -2.974536    2.367658
   H     1.513947   -2.308720    1.880533
   H     2.541926   -3.181026    0.693936
   C     3.327298   -0.250467    2.446480
   H     3.845887   -0.797168    3.255268
   H     3.895615    0.672953    2.247392
   H     2.325600    0.036545    2.810612
   C    -3.069229   -1.137461    1.291521
   H    -2.409038   -2.021223    1.385163
   C    -4.490549   -1.599708    0.943277
   H    -4.900749   -2.216774    1.764068
   H    -5.174705   -0.742721    0.806408
   H    -4.521526   -2.208551    0.023107
   C    -3.015025   -0.383111    2.629927
   H    -3.359590   -1.037856    3.451040
   H    -1.986242   -0.055526    2.853319
   H    -3.672049    0.505087    2.616068
   H     0.381514   -2.478474   -0.377405
   H    -0.048181   -0.974132    1.404090
37
Structure: P6/R7 Stoichiometry: C10H20FeP2O2N2+
   Fe   -0.349696   -0.507952   -0.226251
   P     1.164825   -1.411166   -1.508936
   P    -1.739418    0.577585   -1.566452
   N     0.820364   -1.015066    1.239388
   N    -1.215013    0.541814    1.190996
   H     0.938504   -0.852203    3.368640
   H    -1.389478    0.446430    3.316255
   H    -0.491081   -1.707151    2.688802
   C     0.188912   -0.846638    2.555701
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   H     0.056468    1.308936    2.719041
   C    -0.626494    0.456035    2.511255
   H     2.688205   -1.572710    1.961490
   H    -2.745870    1.872632    1.731934
   C     2.045415   -1.383931    1.084184
   C    -2.259916    1.331260    0.901658
   H     3.120781   -2.547593   -0.376249
   C     2.599596   -1.574702   -0.298299
   H     3.340478   -0.786931   -0.520140
   H    -1.120373    1.455000   -2.505222
   H    -2.627897   -0.082023   -2.469483
   H     1.731627   -0.716229   -2.601084
   H     1.163291   -2.731157   -2.067589
   C    -1.446373   -1.856105   -0.067456
   O    -2.176280   -2.764649    0.017373
   O     0.986925    0.872659   -0.744460
   C     1.435599    1.906009    0.096710
   C     2.925759    2.161575   -0.186854
   C     0.608530    3.181452   -0.128706
   H     1.347643    1.623418    1.171352
   H     3.538167    1.280519    0.076742
   H     3.066893    2.368494   -1.263090
   H     3.307303    3.024122    0.389778
   H    -0.464349    2.970152    0.006952
   H     0.903857    3.989518    0.567281
   H     0.756412    3.540938   -1.163677
   C    -2.727363    1.486737   -0.396879
   H    -3.594188    2.104838   -0.642283
37
Structure: P7 Stoichiometry: C10H20O2FeN2P2+
   Fe   -0.333441    0.182147   -0.260506
   P     1.089889    1.333928   -1.597975
   P    -0.987905   -1.614413   -1.331503
   N     0.079651    1.580478    1.025790
   N    -1.325500   -0.593249    1.237372
   H    -0.595216    2.231971    2.936380
   H    -1.950567    0.001055    3.177703
   H     0.363767    0.711192    2.932539
   C    -0.393169    1.299656    2.370772
   H    -2.497055    1.096549    1.871957
   C    -1.647958    0.447408    2.204529
   H     1.158034    3.304179    1.509207
   C     0.933292    2.562716    0.721874
   H    -1.321499   -3.211863    0.457997
   C    -2.009093   -2.519773   -0.059362
   H    -2.834121   -3.097734   -0.508908
   H    -1.872417   -1.498522   -2.441723
   H    -0.179427   -2.657051   -1.882200
   H     0.597166    1.844060   -2.839903
   H     2.298329    0.793939   -2.157193
   C    -1.638188    1.066200   -0.924582
   O    -2.530304    1.673299   -1.376320
   C    -2.469065   -1.428314    0.916704
   H    -3.328441   -0.863882    0.469708
   H    -2.867944   -1.904220    1.839934
   O     1.357005   -0.725890    0.690867
   C     2.389378   -1.345405    0.430847
   C     2.674398   -1.924908   -0.934696
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   H     2.549260   -3.023211   -0.886990
   H     1.976460   -1.511063   -1.674838
   H     3.718208   -1.730335   -1.235934
   C     3.422819   -1.548349    1.514705
   H     3.792257   -2.588955    1.524386
   H     4.291647   -0.896769    1.302264
   H     3.000470   -1.276901    2.492974
   C     1.534181    2.679445   -0.529221
   H     2.168570    3.527106   -0.799977
67
Structure: P8/R9 Stoichiometry: C29H33ON3Fe+
   Fe   -0.772465    0.665003   -0.021624
   O    -1.514303   -0.117793   -2.725971
   N    -4.218254   -0.700195    0.664219
   N    -0.652720   -1.695818    0.854036
   C     0.553239    2.232687    0.271529
   C    -0.136134    1.924452    1.512982
   C    -1.546208    2.116433    1.295352
   C    -2.640354    1.963015    2.313407
   H    -2.270541    1.475077    3.230210
   H    -3.473138    1.355919    1.916951
   H    -3.031975    2.957040    2.601438
   C    -1.748675    2.508164   -0.068853
   C    -3.073417    2.834227   -0.697457
   H    -3.349632    3.892497   -0.521540
   H    -3.869979    2.198475   -0.277911
   H    -3.051366    2.669339   -1.787246
   C    -0.439228    2.601659   -0.696744
   C    -0.172194    3.077470   -2.096954
   H    -0.972144    2.770774   -2.790183
   H     0.778643    2.673759   -2.481980
   H    -0.105579    4.182002   -2.124870
   C     0.517328    1.550676    2.812969
   H     0.651808    2.434941    3.465787
   H     1.513167    1.111740    2.640702
   H    -0.083152    0.813424    3.372607
   C     2.041130    2.282179    0.075157
   H     2.318099    2.069384   -0.969656
   H     2.560409    1.544915    0.707396
   H     2.437686    3.284476    0.331176
   C    -1.219901    0.145225   -1.620542
   C    -5.361560   -1.034871    0.051356
   H    -6.259142   -0.492810    0.381742
   C    -5.457617   -2.013248   -0.947896
   H    -6.421697   -2.248180   -1.409588
   C    -4.279164   -2.673667   -1.328495
   H    -4.298092   -3.445403   -2.106074
   C    -3.076910   -2.331177   -0.708602
   H    -2.138566   -2.813967   -0.998616
   C    -3.075745   -1.329009    0.290941
   C    -1.846979   -0.849701    0.951279
   H    -2.034091   -0.558769    1.995100
   C     0.310118   -0.890978    0.349217
   C    -0.171453   -2.954082    1.200450
   H    -0.793354   -3.747931    1.610018
   C     1.165384   -2.925448    0.895571
   H     1.936739   -3.688224    0.978705
   N     1.455477   -1.645910    0.379215
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   C     2.764982   -1.184442    0.014468
   C     3.735854   -1.023245    1.027173
   C     4.998253   -0.528828    0.657813
   H     5.755829   -0.384563    1.437350
   C     5.306930   -0.198691   -0.672381
   C     6.678967    0.312079   -1.049936
   H     6.616558    1.096212   -1.823894
   H     7.302713   -0.504457   -1.460702
   H     7.208365    0.727362   -0.176314
   C     4.311604   -0.375348   -1.649002
   H     4.531583   -0.120855   -2.692745
   C     3.033982   -0.866689   -1.334317
   C     1.979042   -1.006353   -2.402752
   H     1.359926   -1.905877   -2.250905
   H     2.439348   -1.053374   -3.402792
   H     1.287695   -0.146189   -2.376623
   C     3.431908   -1.345195    2.472783
   H     3.531259   -2.427292    2.677056
   H     2.400881   -1.061810    2.740492
   H     4.129647   -0.815678    3.141517
67
Structure: P9 Stoichiometry: C29H33FeON3+
   Fe    1.283662    0.170943   -0.208804
   O    -0.729201   -0.556799   -2.164434
   N    -1.384287    2.045768   -0.811974
   N     1.197675   -0.475310    2.638334
   C     2.970730   -1.205317    0.106713
   C     3.373008    0.160525    0.382593
   C     3.181386    0.918033   -0.816187
   C     3.579234    2.348214   -1.041636
   H     3.583915    2.923330   -0.101769
   H     2.898009    2.851377   -1.746933
   H     4.601423    2.394894   -1.462269
   C     2.618085    0.042150   -1.817021
   C     2.342647    0.396807   -3.250370
   H     3.231982    0.189479   -3.876360
   H     2.095060    1.465112   -3.357247
   H     1.500586   -0.185821   -3.656095
   C     2.533360   -1.286866   -1.247841
   C     2.149214   -2.519796   -2.016208
   H     1.195090   -2.388997   -2.553636
   H     2.050614   -3.392761   -1.353164
   H     2.926722   -2.755419   -2.767303
   C     3.963804    0.639513    1.674817
   H     4.968987    0.203786    1.830717
   H     3.300796    0.334954    2.504099
   H     4.067987    1.736996    1.685806
   C     3.125385   -2.341463    1.070511
   H     2.513424   -3.210107    0.779800
   H     2.820099   -2.021259    2.079448
   H     4.184036   -2.662285    1.103728
   C    -0.075959   -0.192094   -1.268193
   C    -2.530348    2.697102   -0.996641
   H    -3.239331    2.236686   -1.698381
   C    -2.852466    3.900225   -0.340762
   H    -3.811053    4.394942   -0.527011
   C    -1.911337    4.442615    0.545621
   H    -2.118445    5.376830    1.078549
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   C    -0.698671    3.773471    0.730398
   H     0.064924    4.169319    1.407838
   C    -0.459443    2.555384    0.039860
   C     0.786973    1.828571    0.229659
   H     1.534187    2.442602    0.768533
   C     0.518640   -0.530248    1.489837
   C     0.385860   -0.957805    3.641923
   H     0.728290   -1.023520    4.676910
   C    -0.837745   -1.315155    3.122294
   H    -1.741777   -1.739017    3.558090
   N    -0.755476   -1.040821    1.758006
   C    -1.847025   -1.247660    0.856748
   C    -1.850977   -2.395533    0.036623
   C    -2.918432   -2.572309   -0.854190
   H    -2.919223   -3.449430   -1.512289
   C    -3.975936   -1.648430   -0.931416
   C    -5.081522   -1.825748   -1.947185
   H    -4.766321   -1.440688   -2.935839
   H    -5.993414   -1.279380   -1.652481
   H    -5.341684   -2.890260   -2.079511
   C    -3.965507   -0.546628   -0.059801
   H    -4.796605    0.168926   -0.087977
   C    -2.917589   -0.329875    0.850316
   C    -2.952622    0.823012    1.823710
   H    -3.267999    0.478691    2.826155
   H    -3.662705    1.597683    1.493264
   H    -1.956318    1.277043    1.944225
   C    -0.713341   -3.380427    0.122853
   H    -0.652484   -3.826950    1.131880
   H     0.245979   -2.866849   -0.052665
   H    -0.828171   -4.189107   -0.616450
68
Structure: P19 Stoichiometry: C25H38PdBrP2N+
   C    -7.920823    0.112030   -1.202216
   C    -7.179262   -0.000001    0.000000
   C    -7.920823   -0.112032    1.202216
   C    -9.317656   -0.106244    1.140422
   N   -10.022047    0.000000    0.000000
   C    -9.317656    0.106243   -1.140422
   C    -5.757438   -0.000001    0.000000
   C    -4.528326   -0.000001    0.000000
   C    -3.105665   -0.000001    0.000000
   C    -2.376852   -0.119339    1.210736
   C    -0.978468   -0.117561    1.203670
   C    -0.244251   -0.000001    0.000000
   C    -0.978468    0.117559   -1.203670
   C    -2.376852    0.119338   -1.210737
   H    -9.904475   -0.192379    2.065455
   H    -7.402461   -0.201360    2.161373
   H    -9.904476    0.192378   -2.065454
   H    -7.402461    0.201358   -2.161373
   H    -2.925814   -0.213624    2.153541
   H    -2.925814    0.213622   -2.153542
   H    -0.445965   -0.211454    2.157512
   H    -0.445965    0.211453   -2.157513
   Pd    1.761721    0.000000    0.000000
   Br    4.305071    0.000001    0.000000
   P     1.797818   -2.331691   -0.049350
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   P     1.797817    2.331691    0.049349
   C     2.574753    2.897210   -1.543363
   C     2.399934    4.351856   -1.996887
   H     2.156762    2.212462   -2.303553
   H     3.637851    2.611034   -1.444197
   H     2.923142    4.505554   -2.957545
   H     1.336801    4.599891   -2.158039
   H     2.813511    5.071358   -1.272578
   C     0.148006    3.178420    0.186967
   C     0.100419    4.642854    0.641958
   H    -0.432979    2.547535    0.882835
   H    -0.338109    3.043330   -0.796966
   H    -0.949077    4.984972    0.681472
   H     0.522775    4.761921    1.654274
   H     0.647214    5.317116   -0.036275
   C     2.837029    2.953504    1.460562
   C     3.545758    4.306702    1.319685
   H     3.583545    2.152305    1.603011
   H     2.171364    2.934656    2.344371
   H     4.126026    4.516701    2.235840
   H     4.257987    4.291754    0.477644
   H     2.845631    5.143928    1.166500
   C     2.837031   -2.953503   -1.460562
   C     3.545762   -4.306701   -1.319685
   H     3.583547   -2.152304   -1.603010
   H     2.171367   -2.934655   -2.344371
   H     4.126030   -4.516699   -2.235839
   H     4.257991   -4.291753   -0.477644
   H     2.845635   -5.143927   -1.166500
   C     2.574755   -2.897210    1.543363
   C     2.399936   -4.351855    1.996887
   H     2.156763   -2.212461    2.303553
   H     3.637852   -2.611033    1.444198
   H     2.923144   -4.505553    2.957545
   H     1.336803   -4.599891    2.158038
   H     2.813514   -5.071357    1.272578
   C     0.148008   -3.178421   -0.186968
   C     0.100422   -4.642855   -0.641959
   H    -0.432977   -2.547536   -0.882836
   H    -0.338107   -3.043331    0.796965
   H    -0.949073   -4.984974   -0.681473
   H     0.522780   -4.761922   -1.654275
   H     0.647217   -5.317116    0.036274
57
Structure: P10 Stoichiometry: C15H36N4NaNb+
   Nb    0.118271    0.042264   -0.050482
   N    -0.997917    1.678849    0.454578
   N     2.054012   -0.070696    0.630090
   N    -0.811196   -1.861842    0.383413
   N     0.234936   -0.043002   -1.783001
   Na    0.268458   -2.329744   -1.787836
   C    -2.252341   -2.149315    0.099722
   C    -0.376029   -2.332710    1.707190
   H    -0.998697   -1.952890    2.549080
   H    -0.367855   -3.439952    1.789510
   H     0.661324   -1.998248    1.881858
   C    -1.433234    2.879250   -0.317058
   C    -1.175331    1.776540    1.902181
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   H    -0.661771    2.652147    2.355815
   H    -2.241494    1.815220    2.204004
   H    -0.762127    0.870118    2.390112
   C     3.349300   -0.142185   -0.106951
   C     2.191695    0.329057    2.032043
   H     1.194069    0.513897    2.470577
   H     2.671463   -0.448522    2.661670
   H     2.769876    1.269092    2.159580
   C    -2.526112   -1.949886   -1.405174
   H    -2.120824   -0.986007   -1.761625
   H    -2.082078   -2.773115   -2.007682
   H    -3.609322   -1.979701   -1.611135
   C    -3.163844   -1.175569    0.887333
   H    -2.959383   -1.240038    1.970564
   H    -2.968582   -0.139296    0.559962
   H    -4.233444   -1.406568    0.732184
   C    -2.622313   -3.605013    0.461747
   H    -3.647374   -3.833047    0.120749
   H    -1.930790   -4.317493   -0.027817
   H    -2.585411   -3.786427    1.548858
   C     3.213852   -1.099702   -1.306794
   H     2.961393   -2.117633   -0.944283
   H     2.423643   -0.732884   -1.983676
   H     4.167070   -1.164322   -1.860575
   C    -1.779715    2.464872   -1.756680
   H    -2.652509    1.787260   -1.756863
   H    -2.029599    3.357134   -2.358398
   H    -0.937595    1.927557   -2.221476
   C    -2.687341    3.533652    0.306489
   H    -2.489261    3.964816    1.302948
   H    -3.037278    4.352784   -0.345291
   H    -3.507012    2.798836    0.399630
   C    -0.270469    3.898925   -0.335592
   H    -0.557064    4.829972   -0.858358
   H     0.033710    4.166235    0.692761
   H     0.600805    3.458570   -0.850347
   C     4.489181   -0.677492    0.790924
   H     5.403080   -0.812620    0.186893
   H     4.736843    0.013722    1.613721
   H     4.218704   -1.656147    1.226977
   C     3.709162    1.267908   -0.629064
   H     2.925345    1.609502   -1.326371
   H     3.769368    1.986909    0.207435
   H     4.682997    1.272353   -1.152501
54
Structure: P11 Stoichiometry: C24H25NbN3F+
   Nb   -0.259356   -0.151027   -0.916901
   N    -1.370290   -1.517906   -1.236799
   N    -1.749274    0.940447    0.154856
   N     1.111838    1.445296   -0.000829
   C    -2.206305   -2.667497   -1.239558
   C    -3.020573    0.261461    0.247470
   C    -3.953478    0.338973   -0.802286
   C    -5.183209   -0.324152   -0.699060
   H    -5.901352   -0.260860   -1.523458
   C    -5.494517   -1.068479    0.449951
   H    -6.455781   -1.586575    0.527089
   C    -4.559393   -1.155764    1.491358
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H	-4.785714	-1.745388	2.386063
C	-3.326938	-0.493092	1.392937
C	-3.010140	2.832216	1.137130
H	-3.447327	2.245172	1.963128
H	-3.762223	2.840753	0.329829
H	-2.839572	3.862175	1.482763
C	-1.710713	2.210722	0.662279
C	-0.558071	2.986781	0.793014
H	-0.706696	3.989655	1.200081
C	0.788908	2.614264	0.544100
C	1.867638	3.607882	0.930046
H	2.390757	3.280966	1.845528
H	1.432675	4.601619	1.115970
H	2.629614	3.680937	0.136235
C	2.495352	1.085906	-0.103982
C	3.113435	1.032245	-1.366508
C	4.438563	0.585335	-1.476396
H	4.912092	0.544030	-2.463143
C	5.149169	0.183877	-0.337477
H	6.178205	-0.178793	-0.429463
C	4.530902	0.238693	0.921997
H	5.071630	-0.090400	1.815360
C	3.213304	0.689590	1.041754
H	-3.698682	0.911291	-1.699716
H	-2.588716	-0.561061	2.198084
H	-3.171923	-2.453046	-0.739312
H	-2.420721	-3.011669	-2.271048
H	-1.717641	-3.498473	-0.691032
H	2.712832	0.695244	2.014068
H	2.540836	1.320982	-2.251715
F	0.333455	0.368177	-2.655839
C	2.787119	-3.086977	1.776297
C	1.719874	-2.415184	2.390989
C	0.852397	-1.622832	1.621920
C	1.030256	-1.485751	0.228051
C	2.095453	-2.188087	-0.375533
C	2.970018	-2.974319	0.389599
H	3.471403	-3.698518	2.374817
H	1.565393	-2.504364	3.472947
H	0.034102	-1.092132	2.127873
H	2.268381	-2.105576	-1.456415
H	3.800703	-3.497165	-0.098191

57

Structure: P12 Stoichiometry: C16H35NMoSiOP2+

Mo	0.348587	0.004939	-0.163936
Si	0.308406	0.056368	2.315152
P	0.191572	2.489677	-0.205660
P	0.537903	-2.479563	-0.091599
N	-1.434129	-0.105634	-0.231418
H	3.434078	1.478247	-1.586236
C	0.351157	3.364765	-1.840042
H	0.238124	4.459866	-1.742113
H	-0.421962	2.977719	-2.525472
H	1.340411	3.138804	-2.273987
C	1.422721	3.414215	0.821353
H	1.300914	4.507543	0.722316
H	2.440702	3.128067	0.508782
H	1.288357	3.122268	1.875894

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   C    -1.422585    3.125894    0.416623
   H    -1.455152    4.229422    0.406725
   H    -1.569703    2.753540    1.443600
   H    -2.231550    2.723172   -0.214643
   C     0.792875   -3.411531   -1.680765
   H     0.837118   -4.504276   -1.521480
   H     1.732583   -3.072838   -2.148958
   H    -0.038710   -3.176119   -2.366584
   C     1.897114   -3.167234    0.958634
   H     1.936475   -4.270021    0.911584
   H     1.731401   -2.847707    2.000845
   H     2.857812   -2.748067    0.615828
   C    -0.970861   -3.287225    0.593570
   H    -0.865427   -4.385656    0.629699
   H    -1.834040   -3.014684   -0.035638
   H    -1.144588   -2.890877    1.607301
   C     2.070022    0.204548    3.069103
   H     2.554167    1.147972    2.759419
   H     2.718292   -0.621980    2.727541
   H     2.036532    0.183430    4.174327
   H    -0.475618    1.190857    2.945094
   H    -0.300096   -1.152612    2.998182
   C    -2.799897   -0.133538   -0.278703
   C    -4.894911   -0.170268   -1.538084
   C    -3.496874   -0.144623   -1.515715
   C    -3.550204   -0.149546    0.927818
   C    -4.946406   -0.174534    0.889127
   C    -5.628133   -0.185099   -0.340115
   H    -5.419623   -0.178484   -2.500091
   H    -2.915416   -0.132351   -2.443047
   H    -3.005255   -0.139713    1.876704
   H    -5.511696   -0.185716    1.827716
   H    -6.722591   -0.204846   -0.363820
   C     3.475881    0.453272   -1.152108
   O     2.214902    0.146458   -0.622064
   C     3.819559   -0.529794   -2.279051
   H     3.899166   -1.555490   -1.876391
   H     4.780178   -0.266956   -2.756366
   H     3.028718   -0.518870   -3.048346
   C     4.520225    0.445219   -0.029758
   H     4.586368   -0.561056    0.419954
   H     4.235095    1.153868    0.764867
   H     5.516064    0.725880   -0.416032
50
Structure: P13 Stoichiometry: C20H25P2ORuN+
   C     2.233404   -3.314857    0.873067
   C     1.356297   -2.215843    0.854432
   C     1.735344   -1.036315    0.152508
   C     3.015579   -0.975674   -0.462316
   C     3.881629   -2.072630   -0.389684
   C     3.492471   -3.252935    0.262760
   C     3.342796    0.292762   -1.220700
   C     2.806697    1.498204   -0.481514
   C     1.541849    1.333976    0.131140
   C     0.938763    2.428637    0.809252
   C     1.584309    3.675993    0.801347
   C     2.831275    3.841376    0.181257
   C     3.444350    2.744725   -0.443765
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   H     1.928282   -4.222660    1.407474
   H     4.866260   -2.007320   -0.867884
   H     4.168082   -4.113369    0.302555
   H     4.425424    0.380019   -1.412133
   H     1.115391    4.521272    1.319325
   H     3.326620    4.817608    0.195059
   H     4.421031    2.862475   -0.928118
   N     0.889968    0.089304    0.096231
   Ru   -1.013539    0.020583   -0.762083
   C     0.032026   -2.275560    1.570081
   H    -0.074122   -1.422053    2.267527
   H    -0.074728   -3.217911    2.135649
   C    -0.337764    2.210934    1.580370
   H    -0.197015    1.395571    2.316398
   H    -0.639304    3.124936    2.122583
   P    -1.342955   -2.071105    0.334458
   P    -1.760900    1.632727    0.532411
   C    -2.391905    3.151063   -0.291949
   H    -3.200433    2.877295   -0.989469
   H    -2.767594    3.877329    0.449943
   H    -1.562791    3.591224   -0.868447
   C    -3.075347    1.266530    1.776623
   H    -3.330138    2.170606    2.357672
   H    -3.975039    0.895264    1.259173
   H    -2.711898    0.485303    2.463508
   C    -1.160669   -3.579194   -0.721837
   H    -1.228058   -4.505093   -0.123468
   H    -1.948651   -3.579895   -1.493379
   H    -0.175920   -3.540687   -1.216898
   C    -2.884830   -2.448780    1.281101
   H    -3.751315   -2.364483    0.603956
   H    -2.850561   -3.465466    1.710616
   H    -3.007421   -1.715351    2.093691
   C    -2.600019   -0.049111   -1.728931
   O    -3.603795   -0.095487   -2.335651
   H    -0.560675    1.378238   -1.550520
   H     2.841177    0.246115   -2.214054
39
Structure: P14 Stoichiometry: C12H21O2PRuN2+
   C    -2.100649    1.470461    0.574209
   C    -2.301929    0.031222    0.181088
   N    -1.153206   -0.626725   -0.114396
   C    -1.145161   -1.963864   -0.347797
   C    -2.340830   -2.695021   -0.294325
   C    -3.543091   -2.025968   -0.026683
   C    -3.527286   -0.644227    0.208227
   C     0.198686   -2.559860   -0.682776
   P     1.568819   -1.457803   -0.005696
   H    -4.447777   -0.096803    0.431013
   H    -2.325479   -3.773900   -0.473403
   H    -4.486761   -2.580075    0.002421
   C    -1.407565    2.389024   -1.590938
   C    -0.544986    3.321853    0.499748
   H     0.270733   -3.613875   -0.359785
   H    -1.731196    1.453725    1.618936
   H    -3.035480    2.058977    0.489802
   C     3.030969   -1.950659   -1.011109
   C     1.924693   -2.166047    1.663491
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   H     3.907668   -1.390252   -0.645087
   H     3.235269   -3.033801   -0.944877
   H     2.847420   -1.659820   -2.058032
   H     2.836359   -1.684811    2.057494
   H     1.082265   -1.882532    2.316171
   H     2.066086   -3.261132    1.645121
   H    -1.379238    4.046666    0.603089
   H    -0.179585    2.999904    1.487655
   H     0.273059    3.783235   -0.073259
   H    -2.233631    3.131520   -1.604926
   H    -0.542611    2.777891   -2.146952
   H    -1.738798    1.455872   -2.070719
   C     2.157075    1.510412   -0.193310
   O     3.169322    2.100213   -0.283425
   Ru    0.593949    0.533661   -0.100154
   H     0.333188   -2.532046   -1.781723
   N    -0.990441    2.096364   -0.203338
   H     0.660071    0.418656   -1.742771
   O     0.150058    0.682876    1.987780
   H     0.973313    0.912424    2.452394
19
Structure: P15 Stoichiometry: C5H11P2Rh+
   C    -1.807108    1.145325    0.384096
   C    -1.866847    0.706428   -1.003207
   C    -1.866890   -0.705464   -1.003937
   C    -1.807018   -1.145719    0.382906
   C    -1.867055   -0.000614    1.239437
   Rh    0.073045   -0.000001    0.005312
   H    -1.899093   -1.355489   -1.879309
   H    -1.899038    1.357344   -1.877920
   H    -1.827111    2.186322    0.714098
   H    -1.826993   -2.187043    0.711882
   H    -1.906769   -0.001174    2.328586
   P     1.618656    1.582736   -0.006101
   P     1.618669   -1.582716   -0.006102
   H     3.000616   -1.229789   -0.045656
   H     1.726051   -2.526950    1.065466
   H     1.674152   -2.567768   -1.044352
   H     3.000603    1.229808   -0.045672
   H     1.674134    2.567793   -1.044346
   H     1.726056    2.526963    1.065471
21
Structure: P16 Stoichiometry: C10H10Pd+
   C    -1.888913    1.141084    0.503150
   C    -2.518746    0.688732   -0.747738
   C    -2.518747   -0.688731   -0.747738
   C    -1.888914   -1.141083    0.503152
   C    -1.691382    0.000001    1.347312
   Pd   -0.000045   -0.000001   -0.000122
   H    -1.407307    0.000002    2.400983
   H    -1.819384   -2.183366    0.824022
   H    -2.840046   -1.346776   -1.557640
   H    -1.819381    2.183367    0.824020
   H    -2.840044    1.346776   -1.557641
   C     2.518928    0.688716    0.747855
   C     1.888891    1.141083   -0.502955
   C     1.691325    0.000003   -1.347125
   C     1.888892   -1.141080   -0.502959
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   C     2.518929   -0.688717    0.747852
   H     1.819369   -2.183370   -0.823810
   H     2.840339   -1.346770    1.557705
   H     2.840337    1.346766    1.557710
   H     1.819367    2.183373   -0.823802
   H     1.407242    0.000005   -2.400796
70
Structure: P17 Stoichiometry: C25H40PdP2NBr+
   C    -5.498113   -0.044949    0.446861
   H    -5.171693   -0.124186    1.491636
   C    -4.558748    0.025681   -0.534740
   H    -4.898368    0.106805   -1.575995
   C    -6.947714   -0.024050    0.258111
   C    -7.804094   -0.101658    1.381041
   C    -7.586335    0.071751   -1.001825
   C    -9.191990   -0.080694    1.202772
   H    -7.380556   -0.177773    2.389048
   C    -8.981651    0.084539   -1.067886
   H    -7.002852    0.136054   -1.925729
   H    -9.857322   -0.140841    2.075472
   H    -9.480039    0.158939   -2.044490
   C    -3.107368    0.009407   -0.372792
   C    -2.284101    0.106062   -1.520122
   C    -2.459392   -0.097168    0.882663
   C    -0.887337    0.099218   -1.422491
   H    -2.758720    0.189978   -2.505893
   C    -1.065202   -0.101872    0.978017
   H    -3.056517   -0.177884    1.797792
   C    -0.241637   -0.002810   -0.170274
   H    -0.290426    0.177508   -2.338869
   H    -0.604188   -0.184562    1.969584
   N    -9.792239    0.010581    0.004633
   Pd    1.758498   -0.000340   -0.017781
   Br    4.295745    0.007035    0.180121
   P     1.785961    2.330826    0.034224
   P     1.802240   -2.331061   -0.052581
   C     2.711633    2.908840   -1.472218
   C     2.575732    4.366324   -1.929999
   H     2.371432    2.228322   -2.273842
   H     3.761187    2.624959   -1.273058
   H     3.188286    4.528972   -2.834773
   H     1.532146    4.612538   -2.190923
   H     2.914983    5.081842   -1.164252
   C     0.129704    3.176425    0.015166
   C     0.036656    4.634980    0.482107
   H    -0.519068    2.537237    0.639842
   H    -0.253688    3.054710   -1.014860
   H    -1.011579    4.978067    0.421883
   H     0.356580    4.740213    1.532888
   H     0.648285    5.317382   -0.129427
   C     2.683659    2.946064    1.542387
   C     3.400301    4.300964    1.479455
   H     3.414762    2.145111    1.750740
   H     1.936472    2.920273    2.358247
   H     3.889688    4.505149    2.448488
   H     4.190115    4.292703    0.709613
   H     2.716631    5.138529    1.265785
   C     2.474513   -2.887228    1.590187
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   C     2.279289   -4.341470    2.036596
   H     2.002920   -2.202506    2.318433
   H     3.540018   -2.594516    1.560621
   H     2.741840   -4.489506    3.028769
   H     1.209550   -4.595371    2.131464
   H     2.741596   -5.060682    1.342083
   C     2.935447   -2.954488   -1.388838
   C     3.635139   -4.306589   -1.199546
   H     3.688942   -2.152457   -1.481425
   H     2.331260   -2.937326   -2.315829
   H     4.275207   -4.516720   -2.074977
   H     4.290055   -4.289789   -0.312227
   H     2.927610   -5.144771   -1.092330
   C     0.168128   -3.184774   -0.293908
   C     0.155371   -4.651021   -0.745082
   H    -0.368681   -2.558141   -1.027992
   H    -0.380924   -3.047726    0.656085
   H    -0.888055   -4.997960   -0.850258
   H     0.642008   -4.772160   -1.727909
   H     0.660424   -5.320479   -0.030673
70
Structure: P18 Stoichiometry: C25H40INPdP2+
   C     5.738084    0.041184    0.453968
   H     5.409367    0.118040    1.498203
   C     4.801131   -0.027456   -0.529849
   H     5.142905   -0.106338   -1.570524
   C     7.188275    0.021053    0.268380
   C     8.041894    0.095802    1.393480
   C     7.829417   -0.071132   -0.990449
   C     9.430238    0.075652    1.218198
   H     7.616088    0.169060    2.400730
   C     9.224906   -0.083399   -1.053506
   H     7.247960   -0.132959   -1.915790
   H    10.093706    0.133560    2.092434
   H     9.725533   -0.154955   -2.029150
   C     3.349178   -0.011506   -0.370856
   C     2.528751   -0.105775   -1.520344
   C     2.698552    0.092748    0.883352
   C     1.131632   -0.098525   -1.426048
   H     3.005495   -0.187859   -2.505188
   C     1.303997    0.097620    0.975727
   H     3.293528    0.171562    1.800000
   C     0.484682    0.001297   -0.174987
   H     0.536781   -0.173973   -2.343956
   H     0.840687    0.178093    1.966342
   N    10.032927   -0.012186    0.021086
   Pd   -1.522318    0.001071   -0.031254
   P    -1.515945   -2.337442    0.025193
   P    -1.526474    2.339439   -0.068842
   C    -2.425800   -2.949165   -1.479697
   C    -2.225141   -4.394878   -1.949973
   H    -2.124377   -2.246459   -2.277670
   H    -3.487546   -2.720003   -1.275849
   H    -2.829768   -4.574662   -2.856781
   H    -1.171967   -4.594260   -2.212030
   H    -2.535394   -5.130714   -1.191158
   C     0.160437   -3.146382    0.000115
   C     0.286301   -4.604485    0.460916
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   H     0.795782   -2.497527    0.628064
   H     0.541588   -3.011941   -1.028956
   H     1.342769   -4.921292    0.400545
   H    -0.031590   -4.722499    1.510934
   H    -0.307159   -5.299275   -0.154163
   C    -2.373174   -2.993682    1.542190
   C    -3.080047   -4.352309    1.457008
   H    -3.105230   -2.208604    1.799131
   H    -1.603548   -2.986637    2.337300
   H    -3.551112   -4.584948    2.428628
   H    -3.882620   -4.331145    0.700706
   H    -2.392554   -5.177781    1.210989
   C    -2.219608    2.924576    1.557182
   C    -1.962129    4.364344    2.018137
   H    -1.807206    2.212171    2.294659
   H    -3.298374    2.691185    1.499281
   H    -2.439863    4.527566    3.000641
   H    -0.883904    4.565390    2.139391
   H    -2.373793    5.109727    1.319255
   C    -2.590072    3.012483   -1.440804
   C    -3.279061    4.368118   -1.239751
   H    -3.350462    2.228546   -1.600495
   H    -1.941420    3.016870   -2.337350
   H    -3.883057    4.611133   -2.132051
   H    -3.966531    4.335915   -0.377832
   H    -2.564388    5.192302   -1.083453
   C     0.135452    3.153652   -0.266261
   C     0.194320    4.620434   -0.712305
   H     0.675680    2.518019   -0.989651
   H     0.658380    3.001555    0.695917
   H     1.248527    4.940265   -0.792911
   H    -0.266266    4.756839   -1.705588
   H    -0.308966    5.301088   -0.007610
   I    -4.242802   -0.003596    0.154092
68
Structure: P20 Stoichiometry: C25H38NP2PdI+
   C    -8.142132   -0.000002    1.219531
   C    -7.422416   -0.000002   -0.000979
   C    -8.185012    0.000000   -1.195069
   C    -9.580590    0.000001   -1.108109
   N   -10.264296    0.000001    0.049651
   C    -9.539855   -0.000001    1.182386
   C    -6.000650   -0.000003   -0.025320
   C    -4.771788   -0.000003   -0.044057
   C    -3.349086   -0.000004   -0.060355
   C    -2.632532   -0.000002   -1.284227
   C    -1.233825   -0.000002   -1.290621
   C    -0.489378   -0.000002   -0.087526
   C    -1.210251   -0.000004    1.128460
   C    -2.608545   -0.000005    1.148967
   H   -10.183934    0.000003   -2.026463
   H    -7.683857    0.000001   -2.167423
   H   -10.110106   -0.000002    2.121663
   H    -7.606630   -0.000004    2.173416
   H    -3.190508   -0.000002   -2.226413
   H    -3.148281   -0.000006    2.101727
   H    -0.709772   -0.000001   -2.253628
   H    -0.669055   -0.000005    2.082165
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   Pd    1.523175    0.000000   -0.092800
   P     1.523614    2.338729   -0.032748
   P     1.523618   -2.338729   -0.032750
   C     2.268713   -2.859469    1.592153
   C     2.025951   -4.279744    2.116783
   H     1.878376   -2.118637    2.313406
   H     3.345004   -2.629521    1.491479
   H     2.531368   -4.403886    3.091097
   H     0.951800   -4.475647    2.276000
   H     2.418873   -5.052005    1.436639
   C    -0.145535   -3.155068   -0.139194
   C    -0.222198   -4.638596   -0.523311
   H    -0.709900   -2.548778   -0.869044
   H    -0.634797   -2.961720    0.833324
   H    -1.279287   -4.957076   -0.557555
   H     0.206363   -4.816631   -1.524319
   H     0.301298   -5.292369    0.192018
   C     2.536852   -3.070849   -1.412464
   C     3.234506   -4.416499   -1.177439
   H     3.289458   -2.294813   -1.635383
   H     1.855151   -3.114885   -2.283034
   H     3.805561   -4.698567   -2.079851
   H     3.953075   -4.346684   -0.343574
   H     2.526919   -5.232680   -0.959067
   C     2.268715    2.859472    1.592151
   C     2.025954    4.279746    2.116781
   H     3.345006    2.629525    1.491472
   H     1.878383    2.118639    2.313406
   H     2.531374    4.403890    3.091092
   H     2.418872    5.052007    1.436635
   H     0.951803    4.475648    2.276002
   C     2.536840    3.070850   -1.412467
   C     3.234492    4.416501   -1.177448
   H     1.855135    3.114883   -2.283035
   H     3.289447    2.294816   -1.635389
   H     3.805543    4.698569   -2.079862
   H     2.526904    5.232681   -0.959074
   H     3.953065    4.346689   -0.343585
   C    -0.145542    3.155065   -0.139185
   C    -0.222209    4.638593   -0.523304
   H    -0.634797    2.961718    0.833337
   H    -0.709910    2.548774   -0.869030
   H    -1.279298    4.957072   -0.557541
   H     0.301292    5.292367    0.192021
   H     0.206347    4.816626   -1.524314
   I     4.247480    0.000003   -0.012121
45
Structure: P21 Stoichiometry: C11H29N4Ta+
   Ta   -0.025541    0.072788   -0.091932
   N     0.139915   -0.700153    1.763702
   N     2.016840    0.264207   -0.328698
   N    -2.079175   -0.300198   -0.179383
   N    -0.264917    2.078191   -0.135027
   C     1.015057   -2.980210   -0.888100
   H     2.041660   -2.615562   -1.000245
   H     0.876791   -3.917074   -0.337925
   C    -0.039824   -2.327383   -1.444860
   H    -1.036150   -2.772593   -1.304139
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   C    -0.000594   -1.000696   -2.086612
   H     0.949070   -0.783767   -2.601820
   H    -0.851260   -0.793879   -2.753801
   H     3.611557   -1.157565   -0.328035
   C     3.063174   -0.476883    0.360456
   H     2.632327   -1.084577    1.170358
   H     3.818474    0.215127    0.793411
   H     3.390489    1.689061   -1.112810
   C     2.570881    1.017205   -1.446656
   H     2.996443    0.343629   -2.224095
   H     1.790019    1.634115   -1.922960
   H    -3.565135   -1.740534   -0.668737
   C    -3.028919   -0.873050   -1.114399
   H    -2.536086   -1.215154   -2.035726
   H    -3.809761   -0.134145   -1.403959
   H    -3.594863    0.877345    0.758052
   C    -2.800841    0.143561    1.016603
   H    -3.293509   -0.709926    1.531788
   H    -2.118003    0.625414    1.735602
   H    -0.857927   -2.513022    1.397799
   C    -0.254596   -2.034203    2.184208
   H    -0.861450   -1.991572    3.113678
   H     0.627368   -2.681690    2.383834
   H     1.624507   -0.347187    3.257983
   C     0.697734    0.104123    2.841546
   H     0.954525    1.113289    2.476685
   H    -0.024828    0.214980    3.678594
   C     0.694222    3.038136    0.407009
   H     1.596723    2.517946    0.761883
   H     0.252965    3.605866    1.254113
   H     0.997406    3.778611   -0.363390
   H    -1.156561    3.481498   -1.459631
   C    -1.444315    2.766670   -0.660228
   H    -1.955850    3.349717    0.135529
   H    -2.154962    2.040189   -1.078946
60
Structure: P22 Stoichiometry: C16H38TaN5+
   Ta    0.655272   -0.143630    0.079470
   N     1.768767   -1.094894   -1.307251
   N     0.695930   -0.916488    1.954614
   N     2.030719    1.347908    0.424702
   N    -1.188442   -0.891590   -0.489500
   N    -0.712117    1.258506   -0.499701
   C     3.030449   -1.752011   -1.000977
   H     3.872486   -1.315137   -1.580543
   H     3.271284   -1.645391    0.070705
   H     2.988647   -2.837366   -1.234393
   C     1.376422   -1.216502   -2.703328
   H     0.408548   -0.715832   -2.868707
   H     2.128197   -0.754229   -3.378492
   H     1.268444   -2.282286   -3.001714
   H     2.798346   -0.685868    2.069715
   C     1.955672   -1.043660    2.684702
   H     2.148961   -2.099509    2.969750
   H     1.942612   -0.442613    3.619769
   H    -0.559331   -0.660701    3.658337
   C    -0.441716   -1.321427    2.771731
   H    -0.306950   -2.357654    3.150595
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   H    -1.368025   -1.274522    2.182375
   C     1.900676    2.232452    1.578287
   H     1.587322    3.257985    1.284359
   H     1.149509    1.836210    2.282780
   H     2.868308    2.327221    2.116801
   H     2.695043    2.863563   -0.931091
   C     2.998173    1.869509   -0.530802
   H     3.993370    2.004217   -0.054047
   H     3.105878    1.176428   -1.380015
   C    -1.907287   -2.148708   -0.637479
   H    -2.766045   -2.163554    0.073078
   C    -0.974759   -3.311858   -0.272406
   H    -0.552018   -3.174473    0.736362
   H    -1.516635   -4.273296   -0.298023
   H    -0.133458   -3.364823   -0.986193
   C    -2.479127   -2.340633   -2.056282
   H    -3.018392   -3.302177   -2.128197
   H    -3.187711   -1.538695   -2.326287
   H    -1.663537   -2.342387   -2.801471
   H    -1.220443    4.646327   -0.064638
   C    -1.405573    3.580076    0.161563
   H    -2.496956    3.417517    0.143024
   H    -1.046621    3.375328    1.183967
   C    -0.670265    2.677102   -0.851088
   H     0.397055    2.957615   -0.806430
   C    -1.147489    2.942916   -2.290198
   H    -0.598052    2.306235   -3.005659
   H    -2.227184    2.738029   -2.406191
   H    -0.978916    3.999626   -2.563769
   H    -2.021956    0.415411   -1.955844
   C    -1.820486    0.372893   -0.859213
   C    -3.933584   -0.055471    2.152495
   H    -4.775100   -0.635436    1.750776
   H    -3.817562   -0.043932    3.242609
   C    -3.086913    0.605614    1.347265
   H    -2.251761    1.168708    1.786244
   C    -3.172364    0.646454   -0.150312
   H    -3.921815   -0.082424   -0.510651
   H    -3.525336    1.642316   -0.484029
53
Structure: P23 Stoichiometry: C21H29OWN+
   C    -2.422595    0.929151    0.311165
   C    -1.274755    1.722501    0.647168
   C    -0.520137    1.005218    1.667427
   C    -1.184533   -0.223108    1.923185
   C    -2.333456   -0.313366    1.037176
   W    -0.523196   -0.239471   -0.439253
   N    -1.307667   -0.337070   -2.063918
   O    -2.003802   -0.303288   -3.051558
   C     2.291289   -1.608967   -0.126360
   C     0.934809   -1.892338   -0.807631
   C    -0.253316   -2.411322   -0.163342
   H    -0.201106   -2.711975    0.891659
   H    -0.929562   -3.044078   -0.753004
   H     1.038056   -2.117771   -1.879015
   C     2.270077   -2.019611    1.359885
   H     1.476054   -1.478542    1.899281
   H     2.079563   -3.101949    1.453623
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   H     3.231015   -1.794040    1.852878
   C     3.418330   -2.380245   -0.853567
   H     3.462162   -2.090564   -1.917722
   H     4.406867   -2.180064   -0.401514
   H     3.223443   -3.465841   -0.798486
   C     0.686462    1.545280    2.383011
   H     0.384264    2.264622    3.168277
   H     1.264108    0.741621    2.866418
   H     1.363891    2.071806    1.691602
   C    -0.892675   -1.194377    3.030494
   H     0.091745   -1.012497    3.489307
   H    -1.655321   -1.085874    3.824989
   H    -0.927777   -2.243260    2.690867
   C    -3.366613   -1.405863    1.059466
   H    -2.902858   -2.389103    1.241263
   H    -4.115195   -1.231225    1.857209
   H    -3.903953   -1.462703    0.099163
   C    -3.541403    1.336046   -0.605184
   H    -3.934095    0.477623   -1.172571
   H    -4.374278    1.769321   -0.019329
   H    -3.209262    2.091863   -1.334125
   C    -1.044251    3.151741    0.233138
   H    -1.302164    3.318116   -0.826112
   H    -1.668376    3.835699    0.840672
   H     0.006510    3.445942    0.379282
   C     2.562916   -0.093525   -0.221005
   C     1.658451    0.735669   -0.933822
   C     3.658576    0.527623    0.406713
   C     1.895179    2.118095   -1.088380
   H     0.966486    0.249281   -1.694399
   C     3.876674    1.907658    0.283662
   H     4.362948   -0.074243    0.990712
   C     3.001812    2.708345   -0.471846
   H     1.207045    2.712950   -1.695897
   H     4.745848    2.362351    0.771253
   H     3.189489    3.781548   -0.579802
86
Structure: P24 Stoichiometry: C32H47O2P2ReN2+
   C     1.213776    0.432994    2.460922
   C     0.941132    0.950750    3.732240
   C    -0.392111    1.140176    4.130510
   C    -1.422945    0.833982    3.240417
   C    -1.104457    0.296868    1.981556
   N     0.196191    0.070927    1.627275
   H    -0.618943    1.546764    5.121248
   H     1.769242    1.221692    4.392887
   H    -2.470126    1.006685    3.503735
   C    -2.103610    0.090460    0.885558
   H    -3.133716    0.142257    1.267269
   C     2.613809    0.314996    1.912871
   H     2.979994   -0.722789    2.032245
   H     3.301301    0.983881    2.458305
   P    -1.700772   -1.480335   -0.112223
   P     2.589393    0.568792    0.041071
   C     0.966223   -1.143629   -2.234788
   O     1.247658   -1.388544   -3.350421
   C    -1.714376    1.204494   -0.162464
   C    -2.968611   -1.452485   -1.569898
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C	-4.294345	-0.786526	-1.148160
C	-2.365273	-0.677304	-2.762853
C	-3.230917	-2.887210	-2.074727
H	-4.753989	-1.268641	-0.270487
H	-4.156934	0.284677	-0.929537
H	-5.012579	-0.861829	-1.986077
H	-1.451710	-1.166825	-3.132817
H	-3.112829	-0.679317	-3.578371
H	-2.114106	0.363132	-2.516798
H	-3.857100	-2.820645	-2.983377
H	-2.292110	-3.393900	-2.355128
H	-3.770806	-3.512493	-1.347043
C	-2.098811	-2.939385	1.062546
C	-1.590536	-4.254896	0.429189
C	-1.310564	-2.728980	2.375739
C	-3.594605	-3.039139	1.419869
H	-2.143006	-4.535994	-0.477729
H	-0.519174	-4.187447	0.184530
H	-1.717777	-5.069886	1.166182
H	-1.715795	-1.898346	2.974110
H	-1.398026	-3.651313	2.979210
H	-0.241588	-2.545187	2.191413
H	-3.731391	-3.843446	2.167004
H	-3.967924	-2.102283	1.869718
H	-4.226752	-3.283887	0.552202
C	2.502143	2.464865	-0.217290
C	2.039580	2.694990	-1.674508
C	1.406125	3.010034	0.724372
C	3.802856	3.234168	0.074040
H	2.774499	2.335844	-2.411566
H	1.073752	2.187729	-1.841891
H	1.902092	3.781283	-1.835273
H	1.704815	2.957829	1.785189
H	1.233608	4.073929	0.476925
H	0.455716	2.475247	0.583065
H	3.600151	4.316136	-0.036463
H	4.159513	3.070332	1.106342
H	4.615621	2.980063	-0.624688
C	4.308895	-0.071059	-0.507970
C	4.276136	-1.611854	-0.513461
C	4.573304	0.396750	-1.954327
C	5.446873	0.375073	0.434248
H	4.056089	-2.034030	0.480475
H	3.528328	-1.996892	-1.222577
H	5.273994	-1.977845	-0.820215
H	4.728499	1.484855	-2.026317
H	5.490532	-0.097021	-2.325239
H	3.742874	0.112395	-2.622732
H	6.401888	-0.029883	0.050292
H	5.551611	1.466547	0.503436
H	5.309079	-0.028133	1.452121
C	1.392185	-2.324538	0.230958
O	1.784581	-3.334215	0.703401
Re	0.577004	-0.692382	-0.400906
N	-0.633204	1.038931	-0.827733
C	-2.574640	2.414124	-0.286647
C	-3.663051	2.691205	0.568447
C	-2.277109	3.341209	-1.312284

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   C    -4.428912    3.854406    0.403942
   H    -3.916566    2.000588    1.378536
   C    -3.042837    4.496975   -1.478441
   H    -1.426551    3.116141   -1.962988
   C    -4.124695    4.761000   -0.620130
   H    -5.267247    4.051753    1.081048
   H    -2.798728    5.200150   -2.282484
   H    -4.724919    5.667921   -0.749940
88
Structure: P25 Stoichiometry: C30H51ReN2P2O2+
   C     1.184011    0.683265    2.346299
   C     1.057817    1.457880    3.504156
   C    -0.172303    2.073137    3.793881
   C    -1.242239    1.917887    2.911329
   C    -1.080278    1.114148    1.768680
   N     0.112881    0.491192    1.521665
   H    -0.283917    2.682711    4.696309
   H     1.921568    1.591170    4.161269
   H    -2.204638    2.403680    3.095338
   C    -2.105056    0.986937    0.682848
   H    -3.082304    1.364172    1.015409
   C     2.495755    0.077130    1.908337
   H     2.534524   -0.987363    2.209586
   H     3.343096    0.597530    2.386753
   P    -2.111071   -0.801298    0.010661
   P     2.576805    0.010238    0.020530
   C     0.539540   -1.506893   -2.046953
   O     0.744109   -1.999739   -3.095442
   C    -1.440862    1.783091   -0.521174
   C    -3.333163   -0.796707   -1.481826
   C    -4.466108    0.225525   -1.274448
   C    -2.544836   -0.451146   -2.765301
   C    -3.933025   -2.199797   -1.709007
   H    -5.041205    0.043908   -0.352690
   H    -4.073484    1.252322   -1.241849
   H    -5.167581    0.165560   -2.127686
   H    -1.844642   -1.259695   -3.023769
   H    -3.269616   -0.345610   -3.594674
   H    -1.965479    0.476918   -2.676877
   H    -4.502366   -2.174902   -2.656528
   H    -3.145079   -2.963815   -1.815710
   H    -4.629008   -2.509310   -0.913920
   C    -2.850391   -1.863453    1.426595
   C    -2.708111   -3.363742    1.079978
   C    -2.026687   -1.616276    2.711240
   C    -4.319453   -1.509350    1.730872
   H    -3.334331   -3.670738    0.232137
   H    -1.661356   -3.623954    0.861724
   H    -3.024409   -3.954054    1.960399
   H    -2.200528   -0.613640    3.130556
   H    -2.345758   -2.356381    3.468143
   H    -0.947837   -1.749029    2.542247
   H    -4.651385   -2.086602    2.614294
   H    -4.439020   -0.438036    1.970655
   H    -4.998761   -1.758483    0.900604
   C     3.073885    1.776743   -0.524765
   C     2.647589    1.916717   -2.004179
   C     2.222566    2.746740    0.317296
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   C     4.551613    2.162584   -0.337043
   H     3.200534    1.231603   -2.666233
   H     1.564773    1.722290   -2.102059
   H     2.855362    2.951314   -2.338488
   H     2.547384    2.777121    1.371076
   H     2.333427    3.765933   -0.096376
   H     1.157615    2.478051    0.271507
   H     4.671238    3.225012   -0.622065
   H     4.874668    2.066336    0.714490
   H     5.234044    1.575099   -0.971158
   C     4.032024   -1.183550   -0.331194
   C     3.560172   -2.631559   -0.099005
   C     4.416392   -1.052631   -1.820407
   C     5.248668   -0.932594    0.584195
   H     3.235746   -2.809927    0.938718
   H     2.729840   -2.898201   -0.769583
   H     4.410348   -3.308411   -0.306173
   H     4.870689   -0.078258   -2.059295
   H     5.156514   -1.836307   -2.066930
   H     3.537561   -1.201404   -2.470632
   H     6.043637   -1.655503    0.321599
   H     5.669595    0.076784    0.482648
   H     4.994285   -1.100312    1.644925
   C     0.622066   -2.327302    0.593763
   O     0.722730   -3.310683    1.243231
   Re    0.285629   -0.671591   -0.326586
   N    -0.435297    1.248122   -1.086901
   C    -1.955263    3.212308   -0.876283
   C    -0.808347    4.210535   -0.600025
   C    -2.281735    3.257981   -2.385485
   C    -3.185214    3.653955   -0.059977
   H    -0.514854    4.195572    0.464446
   H     0.071546    3.947530   -1.206813
   H    -1.126092    5.237886   -0.857245
   H    -3.152306    2.627567   -2.634201
   H    -2.510258    4.293740   -2.696473
   H    -1.415383    2.892997   -2.961091
   H    -3.489963    4.669507   -0.369948
   H    -4.053401    2.989351   -0.211505
   H    -2.963219    3.692307    1.021186
33
Structure: P26 Stoichiometry: C7H22OsP2O+
   Os    0.013873   -0.002533    0.046404
   H    -1.367450   -4.122864    1.414393
   H    -0.993673   -3.531872    1.115448
   P     2.337245   -0.279283   -0.048460
   P    -2.317773   -0.205467   -0.071214
   C    -3.270862    1.285731   -0.607845
   H    -4.356983    1.089503   -0.650970
   H    -3.069214    2.110552    0.095664
   H    -2.910458    1.591833   -1.604034
   C    -2.917520   -1.497294   -1.247600
   H    -2.509703   -2.471673   -0.934692
   H    -4.020980   -1.539096   -1.276595
   H    -2.528442   -1.266910   -2.252975
   C    -3.189618   -0.676321    1.495907
   H    -3.003793    0.097871    2.259524
   H    -4.278353   -0.778044    1.338274
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   H    -2.780354   -1.633873    1.857911
   C     2.905117   -1.457779   -1.353183
   H     4.004916   -1.560819   -1.356162
   H     2.432467   -2.435724   -1.168358
   H     2.564664   -1.089730   -2.334978
   C     3.375020    1.212886   -0.390183
   H     3.197550    1.960527    0.400700
   H     4.451125    0.968173   -0.436174
   H     3.053722    1.650384   -1.350059
   C     3.143284   -0.972064    1.470479
   H     2.676408   -1.942920    1.705964
   H     4.230132   -1.109290    1.327469
   H     2.972513   -0.285910    2.317374
   C     0.032718    1.902170    0.159589
   O     0.048264    3.072774    0.266756
   H     0.011010   -1.746730    0.042199
   H     0.023505    0.144246   -1.538576
39
Structure: P27 Stoichiometry: C7H26OOsBP2N+
   Os   -0.070467   -0.315695   -0.246587
   H     0.101753    1.310380    0.374923
   H    -0.000465    0.730360   -1.742858
   P    -2.405086    0.028362   -0.197795
   P     2.287278   -0.358670   -0.237859
   C     3.162490   -1.904507   -0.743857
   H     4.260307   -1.799755   -0.678745
   H     2.826580   -2.725866   -0.089309
   H     2.871526   -2.153126   -1.777866
   C     3.061141    0.943593   -1.291863
   H     2.664138    1.912313   -0.940315
   H     4.162474    0.933066   -1.211967
   H     2.769485    0.792243   -2.344778
   C     3.019432    0.005263    1.416295
   H     2.701110   -0.769662    2.133027
   H     4.122292    0.040008    1.375350
   H     2.621782    0.975665    1.755111
   C    -3.042426    1.227188   -1.449656
   H    -4.130788    1.378600   -1.342344
   H    -2.519139    2.186874   -1.304044
   H    -2.825548    0.849658   -2.463152
   C    -3.497570   -1.441542   -0.436824
   H    -3.253604   -2.186982    0.338261
   H    -4.567906   -1.175605   -0.373095
   H    -3.279164   -1.888932   -1.420423
   C    -3.015133    0.741454    1.388484
   H    -2.469758    1.680640    1.576227
   H    -4.102408    0.931081    1.357015
   H    -2.787139    0.037403    2.206069
   C    -0.139327   -1.131075    1.443994
   O    -0.189085   -1.652230    2.490752
   H     2.147327    3.529716    1.127181
   H     1.489049    4.007021   -0.359865
   H    -0.880784    3.183000    0.190381
   H    -0.067236    2.575141    2.029938
   B     0.086373    2.897448    0.870406
   N     1.334203    3.517392    0.517357
   H    -0.067433   -0.084205   -2.040915
   H    -0.214089   -1.854988   -0.957392
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51
Structure: P28 Stoichiometry: C17H28P2IrO2N+

C	4.044093	-1.022816	-0.526471
C	2.610919	-1.071529	-0.472616
N	1.915514	0.139509	-0.513190
C	2.584115	1.327573	-0.561856
C	3.976646	1.399803	-0.561994
C	4.708929	0.189413	-0.556399
C	1.895189	-2.283520	-0.296188
P	0.121528	-2.215598	-0.336640
Ir	-0.237376	0.069433	-0.280692
P	0.009478	2.340869	-0.042559
C	1.745253	2.585496	-0.689479
C	-2.272048	-0.028183	-0.088992
C	-3.064981	-0.395360	-1.207516
C	-4.466724	-0.446933	-1.145806
C	-5.133037	-0.143533	0.051033
C	-4.376462	0.216229	1.177174
C	-2.976066	0.274830	1.104475
O	2.365969	-1.613287	2.563142
O	0.313811	0.022962	3.119965
H	4.596684	-1.967193	-0.518019
H	4.478186	2.370310	-0.598067
H	5.804216	0.212865	-0.579801
C	-0.519687	-3.172520	-1.788097
C	-0.564992	-3.176987	1.082157
H	2.251440	3.452379	-0.229617
H	1.622231	2.818911	-1.765788
H	2.181980	-1.944279	1.632985
H	2.441703	-3.230793	-0.383772
C	-0.988899	3.578787	-0.976218
C	-0.001442	2.990624	1.677702
H	-2.574337	-0.647930	-2.159216
H	-5.040830	-0.731637	-2.036171
H	-6.226367	-0.188714	0.105856
H	-4.882286	0.455791	2.120833
H	-2.409913	0.564271	1.999315
H	-0.047647	0.025376	1.269989
H	-0.412657	-0.557457	3.408661
H	1.085382	-0.603421	2.966490
H	3.147377	-1.046170	2.427145
H	0.452486	3.995095	1.735879
H	-1.052266	3.040769	2.010582
H	0.520188	2.273389	2.331402
H	-0.616521	4.607628	-0.826848
H	-0.966595	3.328301	-2.049740
H	-2.032619	3.508333	-0.626950
H	-0.171305	-4.219778	-1.748036
H	-1.623054	-3.150008	-1.786000
H	-0.147928	-2.704678	-2.714295
H	-0.219795	-4.225404	1.061942
H	-0.229783	-2.700480	2.016399
H	-1.666812	-3.143086	1.038125

53
Structure: P29 Stoichiometry: C17H30P2IrO2N+

C	4.074682	-1.113001	-0.031868
C	2.676013	-1.049826	-0.126497
N	2.041380	0.158649	-0.185365

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   C     2.759283    1.318797   -0.153967
   C     4.153924    1.298121   -0.027905
   C     4.821267    0.068188    0.029804
   C     1.817452   -2.288781   -0.117286
   P     0.150634   -1.950992   -0.876766
   Ir   -0.117704    0.231059   -0.227901
   P     0.220632    2.420980    0.288948
   C     1.982650    2.605167   -0.321492
   C    -2.180534    0.238994   -0.203500
   C    -2.948609   -0.092889   -1.348752
   C    -4.351065   -0.143618   -1.321893
   C    -5.052560    0.151710   -0.143018
   C    -4.324349    0.500068    1.003862
   C    -2.920047    0.539117    0.970622
   O     0.831922   -3.410259    2.693457
   O    -1.378356   -1.813337    2.731662
   H     4.563580   -2.090532    0.010843
   H     4.706955    2.241325    0.005305
   H     5.911662    0.032006    0.118811
   C     0.364284   -2.290213   -2.675324
   C    -0.933165   -3.313706   -0.299650
   H     2.521037    3.462561    0.119023
   H     1.870528    2.796221   -1.407205
   H     1.573934   -2.576846    0.935195
   H     2.347765   -3.143123   -0.574609
   C    -0.697133    3.766960   -0.561100
   C     0.277034    2.968871    2.047515
   H    -2.427898   -0.307076   -2.289818
   H    -4.901037   -0.410113   -2.233189
   H    -6.147431    0.115249   -0.120015
   H    -4.851135    0.741088    1.935801
   H    -2.379711    0.800269    1.889217
   H    -0.913698   -1.121681    2.170740
   H    -2.272392   -1.834476    2.343995
   H    -0.057622   -2.967264    2.750678
   H     1.350447   -2.916613    3.353557
   H    -0.170318    0.708843   -1.834249
   H    -0.102529   -0.188093    1.422612
   H     0.639586    4.006675    2.154134
   H    -0.739607    2.887398    2.467790
   H     0.932222    2.276883    2.601154
   H    -0.287355    4.767020   -0.335488
   H    -0.666936    3.571554   -1.644839
   H    -1.748935    3.713303   -0.233167
   H    -0.507551   -4.306131   -0.524834
   H    -1.072559   -3.192400    0.784608
   H    -1.909858   -3.198055   -0.799235
   H     0.680722   -3.331643   -2.863155
   H    -0.594142   -2.096181   -3.185382
   H     1.113514   -1.587013   -3.073322
43
Structure: P30 Stoichiometry: C14H26PtPN+
   C    -0.672875    4.064802   -0.091472
   C     0.601568    3.490949   -0.196829
   C     0.768699    2.098343   -0.315269
   C    -0.359613    1.232408   -0.355344
   C    -1.640017    1.841035   -0.200970
   C    -1.798143    3.233275   -0.072489
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   C     2.170564    1.517316   -0.331803
   C     2.417443    0.606311    0.888217
   N     3.434717   -0.420001    0.658017
   Pt   -0.321469   -0.920875   -0.469437
   C     1.616430   -1.424308   -2.070030
   C    -2.844650    0.918154   -0.096975
   P    -2.162505   -0.632351    0.646696
   H     1.489648    4.135283   -0.172859
   H    -2.799387    3.665304    0.047556
   H    -0.784772    5.150661    0.001255
   H    -3.249664    0.640969   -1.089464
   H    -3.670763    1.340829    0.504401
   H     2.310244    0.909820   -1.242149
   H     2.914745    2.332207   -0.371928
   H     2.642148    1.230796    1.788283
   C    -3.450223   -1.932820    0.551625
   C    -1.964290   -0.269848    2.435365
   H     1.470192    0.069983    1.100794
   C     4.763853    0.121644    0.411056
   C     3.436442   -1.419372    1.718336
   H     0.570845   -1.037513   -2.260522
   H     2.265128   -0.792937   -2.697330
   H     1.643251   -2.475707   -2.382120
   H     1.985052   -1.331435   -1.024612
   H     5.462396   -0.701973    0.181894
   H     4.741836    0.801280   -0.456802
   H     5.174070    0.688957    1.282569
   H     4.154796   -2.221154    1.472937
   H     3.715240   -1.001972    2.716805
   H     2.430007   -1.865870    1.800942
   H    -2.943564   -0.057309    2.899127
   H    -1.492889   -1.131548    2.934630
   H    -1.304813    0.607857    2.528365
   H    -4.374159   -1.599503    1.056475
   H    -3.657043   -2.148263   -0.508571
   H    -3.070438   -2.850327    1.028805
   H    -0.424085   -2.572224   -0.469475
43
Structure: P31 Stoichiometry: C14H26NPtP+
   C     0.285172    4.039721   -0.052633
   C     1.460400    3.276489   -0.044370
   C     1.417374    1.887613   -0.278915
   C     0.187731    1.233079   -0.529636
   C    -0.996257    2.019794   -0.494957
   C    -0.947658    3.407335   -0.267079
   C     2.688522    1.065301   -0.259717
   C     2.799069   -0.038327    0.818347
   N     1.536255   -0.763675    1.204919
   Pt    0.016624   -0.905390   -0.512559
   C     1.547760   -1.430896   -1.878612
   C    -2.318825    1.282685   -0.607875
   P    -2.086213   -0.266809    0.400693
   H     2.425027    3.763833    0.147439
   H    -1.874901    3.993421   -0.244465
   H     0.327151    5.120028    0.124702
   H    -2.508326    0.948152   -1.645995
   H    -3.184490    1.880803   -0.271079
   H     2.794349    0.583188   -1.243030
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   H     3.567047    1.722128   -0.128941
   H     3.508078   -0.799227    0.455684
   C    -3.511835   -1.360900   -0.004011
   C    -2.496557    0.321413    2.107833
   H     3.225964    0.379447    1.751375
   C     1.888830   -2.139897    1.636114
   C     0.911681   -0.053431    2.347299
   H     1.765918   -0.593921   -2.562918
   H     2.472356   -1.717529   -1.345174
   H     1.221087   -2.297679   -2.473962
   H    -0.883811   -0.998554   -1.789553
   H     0.977146   -2.648378    1.981642
   H     2.293858   -2.693809    0.777141
   H     2.637958   -2.114006    2.454491
   H     0.017630   -0.607767    2.664372
   H     1.623143    0.009483    3.196197
   H     0.627991    0.960554    2.031043
   H    -3.540799    0.678647    2.147360
   H    -2.365586   -0.493713    2.838941
   H    -1.822310    1.153015    2.368407
   H    -4.476172   -0.844380    0.145551
   H    -3.417371   -1.681633   -1.053953
   H    -3.471505   -2.258630    0.635206
   H    -0.189119   -2.535075   -0.376439
19
Structure: P32 Stoichiometry: C5H11PtP2+
   C     0.149746   -1.887020    1.143438
   C    -1.251022   -1.859662    0.697859
   C    -1.251022   -1.859662   -0.697859
   C     0.149746   -1.887020   -1.143438
   C     0.995779   -2.040330    0.000000
   Pt    0.036344    0.077871    0.000000
   H    -2.122556   -1.811328   -1.352463
   H    -2.122556   -1.811328    1.352463
   H     0.473469   -1.948597    2.184936
   H     0.473469   -1.948597   -2.184936
   H     2.078513   -2.168201    0.000000
   P     0.149746    1.615698    1.664688
   P     0.149746    1.615698   -1.664688
   H     0.330556    2.966751   -1.283340
   H     1.197797    1.468872   -2.606562
   H    -0.961793    1.737051   -2.535682
   H     0.330556    2.966751    1.283340
   H    -0.961793    1.737051    2.535682
   H     1.197797    1.468872    2.606562
15
Structure: P33 Stoichiometry: CH11N2Pt+
   H    -2.958216    0.506864   -0.002214
   Pt    0.032491   -0.179999   -0.030249
   C    -2.319822   -0.378159    0.131627
   N    -0.132329    2.075817    0.007085
   H     0.126154   -1.739254   -0.070012
   N     2.089609   -0.224651    0.118399
   H    -1.931655   -0.419249    1.166020
   H    -2.856667   -1.314470   -0.076082
   H     2.555928    0.692873    0.121613
   H    -1.589847   -0.341867   -0.784865
   H     0.374349    2.531002    0.778990
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   H    -1.107039    2.391496    0.106573
   H     0.207766    2.515333   -0.859847
   H     2.485556   -0.759099   -0.668799
   H     2.377339   -0.712908    0.979865
33
Structure: P34/R35 Stoichiometry: C10H15PtBN6+
   C     0.041792    3.035668    0.289077
   N     0.084647    1.686988    0.269764
   N     1.189197    1.283426    0.955281
   C     1.842895    2.382225    1.407527
   C     1.146014    3.522667    1.006266
   B     1.660932   -0.212171    1.090087
   N     0.480822   -1.051882    1.639519
   N    -0.765348   -0.972821    1.112512
   C    -1.545490   -1.834108    1.791695
   C    -0.787449   -2.494203    2.777361
   C     0.495134   -1.962354    2.646320
   Pt   -1.157506    0.355073   -0.535745
   N     2.160897   -0.768768   -0.254195
   N     1.322173   -1.228594   -1.221312
   C     2.105230   -1.549474   -2.259666
   C     3.470593   -1.301833   -1.976841
   C     3.459497   -0.802395   -0.679131
   H     1.657885   -1.953840   -3.170720
   H     4.268611   -0.474672   -0.026007
   H     4.336560   -1.471799   -2.616410
   H     2.568516   -0.216549    1.894462
   H     1.415930   -2.160924    3.193284
   H     2.762446    2.267013    1.979338
   H    -1.126814   -3.242875    3.491523
   H     1.400234    4.562037    1.206858
   H    -2.604489   -1.922708    1.547373
   H    -0.775703    3.557408   -0.205068
   H    -1.208783   -1.503057   -1.823870
   H    -1.434734    1.363252   -1.718756
   C    -2.296877   -1.361625   -1.683960
   H    -2.709671   -2.234864   -1.158001
   H    -2.678483   -0.466590   -1.028564
   H    -2.785452   -1.182548   -2.650644
28
Structure: P35 Stoichiometry: C9H11N6PtB+
   C     0.000006    2.901879   -0.958893
   N     0.000001    1.649289   -0.474676
   N     0.000001    1.734266    0.878055
   C     0.000005    3.036141    1.262711
   C     0.000009    3.823101    0.109704
   B    -0.000004    0.396245    1.655952
   N    -1.347537   -0.356341    1.296744
   N    -1.777535   -0.571070    0.002785
   C    -2.973427   -1.177286    0.069221
   C    -3.352614   -1.346912    1.416319
   C    -2.298450   -0.811536    2.154635
   Pt    0.000002   -0.426073   -1.096789
   N     1.347530   -0.356343    1.296749
   N     1.777535   -0.571062    0.002791
   C     2.973422   -1.177290    0.069231
   C     3.352597   -1.346931    1.416330
   C     2.298434   -0.811552    2.154643
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   H     3.493274   -1.451085   -0.848608
   H     2.156638   -0.713375    3.230376
   H     4.272371   -1.787493    1.798792
   H    -0.000007    0.587603    2.851981
   H    -2.156661   -0.713351    3.230368
   H     0.000006    3.303973    2.318703
   H    -4.272394   -1.787465    1.798778
   H     0.000013    4.910725    0.051126
   H    -3.493275   -1.451085   -0.848619
   H     0.000007    3.073575   -2.035484
   H     0.000017   -1.958420   -1.458150
65
Structure: R1 Stoichiometry: C24H37N3Sc+
   N    -0.427229   -2.172998    0.457295
   N    -1.519880    1.919034   -0.560946
   C    -0.062200   -0.700311   -1.927744
   H    -1.054905   -1.158708   -2.036744
   H     0.219501   -0.158926   -2.842899
   C     1.020302   -1.537386   -1.415243
   C     0.894680   -2.217120   -0.153834
   C     1.982626   -2.904939    0.425891
   H     1.853694   -3.436529    1.372053
   C     3.220321   -2.932724   -0.218636
   H     4.058435   -3.473454    0.230418
   C     3.372177   -2.280030   -1.459867
   H     4.334486   -2.317952   -1.980301
   C     2.305177   -1.593674   -2.031945
   H     2.430912   -1.097787   -2.999925
   C    -0.478985   -2.549297    1.887289
   H    -0.232825   -3.618027    2.029581
   H    -1.502184   -2.372806    2.246896
   H     0.216843   -1.934465    2.475529
   C    -1.419204   -3.008392   -0.281792
   H    -1.315793   -2.854392   -1.362511
   H    -2.431989   -2.724121    0.036003
   H    -1.233183   -4.074167   -0.056957
   C    -1.533826    0.559240    1.934683
   H    -1.641312   -0.018338    2.863730
   H    -1.325500    1.615421    2.165756
   C    -2.577283    0.288426    0.945818
   C    -2.524488    0.874940   -0.364362
   C    -3.425864    0.487471   -1.378213
   H    -3.378841    0.958476   -2.362446
   C    -4.388599   -0.489503   -1.130693
   H    -5.085105   -0.782338   -1.921617
   C    -4.473266   -1.073411    0.149499
   H    -5.248211   -1.817767    0.359553
   C    -3.585146   -0.699079    1.153324
   H    -3.672755   -1.140942    2.151946
   C    -1.882143    3.159151    0.190798
   H    -1.031109    3.856990    0.182208
   H    -2.156059    2.920769    1.225681
   H    -2.747983    3.640505   -0.298291
   C    -1.302793    2.311176   -1.975710
   H    -1.109291    1.423193   -2.587348
   H    -0.428564    2.979726   -2.022472
   H    -2.177734    2.859977   -2.370940
   Sc   -0.129333    0.125300    0.213047
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   C     1.692491    2.468469    1.480189
   C     1.711272    3.297520    0.195681
   N     1.806204    0.999729    1.204928
   C     2.948919    3.005833   -0.659793
   C     3.034889    1.497401   -0.915689
   C     3.041592    0.727422    0.402691
   C     1.910144    0.276123    2.499027
   H     0.763231    2.632318    2.051775
   H     2.540050    2.762008    2.133666
   H     0.807969    3.059842   -0.394555
   H     1.645890    4.365629    0.465076
   H     2.900477    3.564970   -1.609666
   H     3.859972    3.345555   -0.132052
   H     2.170504    1.169327   -1.528615
   H     3.940069    1.230778   -1.486626
   H     3.099368   -0.359553    0.239274
   H     3.922556    1.023821    1.009728
   H     2.060959   -0.796736    2.299392
   H     0.989575    0.425917    3.083926
   H     2.776413    0.646311    3.080623
60
Structure: R2 Stoichiometry: C21H36ScN2+
   N     1.250047    0.964798    1.327356
   C     1.963028    1.505703   -1.414569
   H     2.857585    1.082237   -0.927105
   H     2.173073    1.805985   -2.449920
   C     1.189640    2.478849   -0.637444
   C     0.757160    2.200502    0.707829
   C    -0.138968    3.057934    1.381298
   H    -0.430942    2.844638    2.412454
   C    -0.655759    4.183887    0.742134
   H    -1.349840    4.842964    1.271506
   C    -0.267060    4.468786   -0.582389
   H    -0.665289    5.353291   -1.089346
   C     0.628295    3.638346   -1.247821
   H     0.929454    3.870940   -2.274507
   C     0.399092    0.442973    2.421625
   H     0.416087    1.094830    3.314406
   H     0.772410   -0.550937    2.712718
   H    -0.647697    0.354509    2.079294
   C     2.662479    1.080937    1.778642
   H     3.278578    1.487047    0.964782
   H     3.040149    0.087555    2.064214
   H     2.724088    1.762071    2.646859
   Sc    0.433481    0.099179   -0.649468
   C     1.115507   -2.863022    0.403327
   C     2.278933   -2.811104    1.394081
   N     1.305464   -1.937074   -0.744235
   C     3.626296   -3.032892    0.692929
   C     3.786390   -2.045785   -0.471677
   C     2.608576   -2.149273   -1.438852
   C     0.124674   -1.852896   -1.610388
   H     0.158473   -2.599816    0.891777
   H     0.998742   -3.890953    0.002613
   H     2.286547   -1.826415    1.896167
   H     2.109029   -3.568514    2.178517
   H     4.455327   -2.924700    1.412896
   H     3.673408   -4.068394    0.305675
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   H     3.849762   -1.011303   -0.084115
   H     4.720477   -2.237418   -1.026738
   H     2.682910   -1.396839   -2.242067
   H     2.585320   -3.149194   -1.918030
   H     0.419427   -1.761879   -2.671495
   H    -0.586813   -2.680290   -1.469154
   C    -2.185133   -0.205469   -1.296479
   H    -2.207198   -0.699795   -2.275222
   C    -1.755562    1.090361   -1.217466
   H    -1.876473    1.681524   -0.298960
   H    -1.438512    1.640272   -2.112758
   C    -2.849735   -0.942843   -0.164363
   H    -2.477785   -1.982318   -0.115358
   H    -2.612016   -0.457541    0.803187
   C    -4.387275   -0.977017   -0.341594
   H    -4.626563   -1.440759   -1.317503
   H    -4.766697    0.060821   -0.387470
   C    -5.094329   -1.745898    0.784185
   H    -4.696848   -2.778748    0.822265
   H    -4.838802   -1.280722    1.756411
   C    -6.617025   -1.782572    0.613046
   H    -7.094975   -2.339636    1.436480
   H    -7.041936   -0.762978    0.603487
   H    -6.899482   -2.273415   -0.335316
23
Structure: R3 Stoichiometry: C8H12N2Ti+
   C    -0.847181   -1.737876    0.449746
   C    -0.741009   -1.485729   -0.945439
   C    -1.684829   -0.474279   -1.293359
   C    -2.364838   -0.091307   -0.105009
   C    -1.843249   -0.865470    0.975123
   Ti   -0.068164    0.509504    0.271915
   C     1.727178    0.591470   -1.402683
   C     2.268785   -0.216904   -0.483233
   C     2.977311   -1.087948    0.206030
   N     0.862945    0.587390    1.703604
   N    -0.529972    2.330459   -0.131771
   H    -1.845331   -0.057770   -2.289967
   H    -0.054076   -1.988982   -1.629993
   H    -3.134396    0.677888   -0.022635
   H    -2.146158   -0.795449    2.020885
   H    -0.247795   -2.445861    1.023562
   H     1.153748    0.187147   -2.245931
   H     1.404116    0.448670    2.565818
   H    -1.252472    2.662497   -0.777914
   H    -0.157757    3.132901    0.383586
   H     1.917194    1.670480   -1.390693
   H     3.920546   -1.464764   -0.214377
   H     2.658172   -1.452534    1.185652
22
Structure: R4 Stoichiometry: C7H12N2Ti+
   C    -1.403363   -1.222040    0.823481
   C    -1.313454   -1.379412   -0.587693
   C    -1.703182   -0.153561   -1.200172
   C    -2.030543    0.764953   -0.164442
   C    -1.841069    0.108485    1.087295
   Ti    0.301763    0.301704    0.136320
   N     0.687534    1.883026   -0.876693
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   N     1.186214    0.511696    1.599272
   C     2.563557   -0.748660    0.030078
   C     1.780840   -1.175279   -1.017002
   H    -1.730941    0.047073   -2.273076
   H    -1.020635   -2.289210   -1.114478
   H    -2.343338    1.801328   -0.299467
   H    -1.993632    0.549849    2.072979
   H    -1.156053   -1.973819    1.575004
   H     1.339863   -2.176401   -1.012349
   H     2.766714   -1.395836    0.887906
   H     1.648148    0.464366    2.515525
   H     0.161790    2.252188   -1.674033
   H     1.354062    2.594868   -0.566112
   H     1.740821   -0.604827   -1.951407
   H     3.161457    0.162953   -0.046847
62
Structure: R5 Stoichiometry: C18H38NMnO2P2+
   Mn   -0.000001   -0.049787   -0.115828
   P     2.242482    0.191186   -0.257069
   P    -2.242484    0.191184   -0.257068
   N    -0.000001    1.960508   -0.651655
   C     2.430797    1.958835   -0.802346
   H     3.379519    2.414177   -0.467901
   H     2.411921    1.960354   -1.907203
   C     1.195227    2.694770   -0.276940
   H     1.297858    2.843177    0.830716
   H     1.169226    3.720148   -0.711960
   C    -1.195230    2.694769   -0.276942
   H    -1.169230    3.720146   -0.711962
   H    -1.297861    2.843177    0.830714
   C    -2.430799    1.958832   -0.802347
   H    -2.411922    1.960350   -1.907205
   H    -3.379521    2.414174   -0.467904
   C    -3.193393    0.115106    1.359864
   C    -2.915888   -1.173502    2.152958
   H    -3.325226   -1.073955    3.174508
   H    -1.838269   -1.380045    2.235295
   H    -3.394819   -2.048771    1.683313
   C    -3.140188   -0.802818   -1.580902
   C    -3.276071   -2.285710   -1.196491
   H    -3.577942   -2.877850   -2.079498
   H    -4.053991   -2.424303   -0.425521
   H    -2.331887   -2.701771   -0.809070
   C     3.140180   -0.802818   -1.580904
   C     3.276063   -2.285709   -1.196490
   H     3.577926   -2.877852   -2.079498
   H     2.331882   -2.701767   -0.809060
   H     4.053989   -2.424301   -0.425527
   C     3.193394    0.115107    1.359861
   C     2.915893   -1.173502    2.152954
   H     3.325229   -1.073953    3.174506
   H     3.394832   -2.048769    1.683310
   H     1.838276   -1.380052    2.235288
   C     0.000003    0.412020    1.582080
   O     0.000008    0.765180    2.702339
   C     0.000006   -1.796209    0.230483
   C    -4.470307   -0.220246   -2.087560
   H    -5.271513   -0.316825   -1.337726
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   H    -4.382747    0.844332   -2.361172
   H    -4.792912   -0.771650   -2.990218
   C     4.470298   -0.220248   -2.087568
   H     4.792901   -0.771655   -2.990225
   H     4.382736    0.844329   -2.361184
   H     5.271505   -0.316823   -1.337736
   C     4.699622    0.402253    1.265171
   H     5.110903    0.565999    2.278015
   H     5.242140   -0.451741    0.824602
   H     4.923104    1.299956    0.664144
   C    -4.699622    0.402248    1.265178
   H    -5.242139   -0.451747    0.824611
   H    -5.110900    0.565995    2.278023
   H    -4.923107    1.299951    0.664151
   H    -2.714293    0.951186    1.907326
   H     2.714294    0.951185    1.907325
   H    -2.407486   -0.734463   -2.409420
   H     2.407475   -0.734464   -2.409420
   O     0.000016   -2.938342    0.523238
   H    -0.000018   -0.613460   -1.840593
   H     0.000014    0.189364   -1.871464
37
Structure: R6 Stoichiometry: C10H20O2FeN2P2+
   Fe   -0.468475    0.310456   -0.185058
   P    -1.637832   -0.758430   -1.737619
   P     0.619081    1.973257   -1.190546
   N    -1.058948   -1.136877    1.008538
   N     0.544051    0.832463    1.389514
   H    -1.029439   -1.607467    3.092928
   H     0.413884    0.571602    3.505325
   H    -1.790185   -0.038714    2.675620
   C    -0.965444   -0.733878    2.412834
   H     1.190213   -0.775679    2.625262
   C     0.379750   -0.012515    2.564141
   H    -2.479486   -2.677654    1.310756
   H     1.945202    2.141470    2.244832
   C    -2.040068   -1.984970    0.572608
   C     1.396791    1.868316    1.326312
   C    -2.441013   -2.022727   -0.742281
   C     1.607972    2.590320    0.156480
   H    -3.136417   -2.776641   -1.121559
   H     2.259025    3.467192    0.120186
   H     1.456483    1.750694   -2.328386
   H    -0.118696    3.054422   -1.762299
   H    -0.965111   -1.418692   -2.810995
   H    -2.655124   -0.137012   -2.517662
   C    -1.781898    1.365680    0.134766
   O    -2.669764    2.091753    0.358054
   H     2.524620   -0.415953    0.633511
   C     2.404117   -1.165369   -0.170226
   C     3.190131   -0.721815   -1.396125
   C     2.816720   -2.545902    0.339136
   O     0.997757   -1.213382   -0.536137
   H     4.269283   -0.710900   -1.166441
   H     3.013058   -1.411799   -2.239593
   H     2.899420    0.295507   -1.699259
   H     2.210728   -2.838300    1.215624
   H     2.680547   -3.307184   -0.449046
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   H     3.876807   -2.542416    0.646529
   H     0.474788   -1.635660    0.211080
67
Structure: R8 Stoichiometry: C29H33ON3Fe+
   Fe   -0.730822    0.521675    0.030762
   O     0.707087    1.530512   -2.278575
   N    -2.176305   -0.420728   -0.990913
   N    -0.702285   -2.342604    0.538095
   C     0.023318    1.490044    1.723369
   C    -1.092913    0.662238    2.131599
   C    -2.255581    1.111150    1.433761
   C    -3.650598    0.586750    1.595967
   H    -3.648310   -0.451031    1.961763
   H    -4.202854    0.607815    0.642600
   H    -4.203395    1.214377    2.321275
   C    -1.882079    2.204828    0.569241
   C    -2.819534    3.038096   -0.255143
   H    -3.243351    3.864398    0.348799
   H    -3.660888    2.438478   -0.638480
   H    -2.304300    3.488264   -1.119955
   C    -0.475712    2.447370    0.770667
   C     0.317161    3.589549    0.199573
   H    -0.069733    3.906869   -0.781552
   H     1.378207    3.321287    0.073891
   H     0.264483    4.458263    0.882937
   C    -1.048776   -0.436422    3.153434
   H    -1.295938   -0.048220    4.159805
   H    -0.047225   -0.893970    3.204461
   H    -1.769636   -1.231798    2.900798
   C     1.387293    1.528000    2.343214
   H     2.181246    1.641173    1.587867
   H     1.587853    0.611111    2.913828
   H     1.464647    2.379209    3.047969
   C     0.163270    1.038851   -1.362650
   C    -2.797158    0.255927   -1.991857
   H    -2.234591    1.102707   -2.396279
   C    -4.062459   -0.046402   -2.470895
   H    -4.501435    0.545416   -3.277872
   C    -4.756602   -1.129243   -1.861006
   H    -5.773304   -1.385879   -2.179127
   C    -4.130506   -1.870483   -0.884847
   H    -4.626941   -2.729167   -0.421031
   C    -2.781636   -1.566696   -0.471546
   C    -2.109997   -2.390304    0.428142
   H    -2.567081   -3.307721    0.799236
   C     0.070847   -1.238146    0.279157
   C     0.087213   -3.464624    0.792240
   H    -0.353410   -4.434333    1.012998
   C     1.389729   -3.076949    0.655816
   H     2.320473   -3.632940    0.741481
   N     1.371922   -1.723983    0.329517
   C     2.539399   -1.015517   -0.113017
   C     3.539099   -0.651521    0.811472
   C     4.638226    0.086607    0.335170
   H     5.413965    0.394776    1.046636
   C     4.768032    0.435491   -1.018267
   C     5.923141    1.283837   -1.499433
   H     5.593212    2.323174   -1.686843
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   H     6.336692    0.898943   -2.447940
   H     6.736049    1.319602   -0.755183
   C     3.795333   -0.030101   -1.922324
   H     3.905626    0.185148   -2.991405
   C     2.687921   -0.778785   -1.499793
   C     1.741666   -1.396734   -2.503242
   H     1.969038   -2.474298   -2.612816
   H     1.851352   -0.919021   -3.488723
   H     0.688389   -1.316971   -2.190549
   C     3.494687   -1.098770    2.254655
   H     4.091571   -2.021509    2.385742
   H     2.469481   -1.324891    2.584732
   H     3.924760   -0.333964    2.922109
59
Structure: R10 Stoichiometry: C16H36ONbN4Na+
   N    -0.156705   -0.088026    1.680580
   C    -0.756207    0.014171    2.870781
   O    -1.007653   -0.954037    3.641028
   Na   -0.656690   -2.387537    1.966899
   Nb    0.009620    0.017049   -0.188604
   N    -1.610113   -0.958501   -0.936037
   N     1.599828   -1.033122   -0.825495
   N     0.292184    1.980932   -0.607813
   C    -3.013265   -0.547874   -0.637865
   C     2.814590   -1.650045   -0.233895
   C     0.712049    3.077974    0.317265
   C    -3.641377   -1.531725    0.376440
   C    -3.859633   -0.502375   -1.928119
   C    -2.989155    0.859170   -0.012768
   C     3.302759   -2.820576   -1.115992
   C     3.933161   -0.592586   -0.092718
   C     2.470489   -2.198847    1.159790
   C    -0.493320    3.472714    1.199248
   C     1.232235    4.309472   -0.455226
   C     1.855515    2.553351    1.204579
   H    -3.562044   -2.576645    0.024562
   H    -4.712413   -1.313585    0.533568
   H    -3.139113   -1.435264    1.356521
   H    -3.372762    0.141188   -2.682113
   H    -4.857500   -0.084338   -1.709647
   H    -4.005504   -1.504318   -2.366557
   H    -2.353859    0.887467    0.892314
   H    -4.005406    1.160525    0.294314
   H    -2.616125    1.603212   -0.736096
   H     2.484064   -3.542480   -1.287411
   H     4.133108   -3.349117   -0.616860
   H     3.671337   -2.472882   -2.095980
   H     4.164104   -0.125939   -1.066025
   H     4.862223   -1.050654    0.290150
   H     3.618369    0.200966    0.603708
   H     2.036187   -1.408074    1.793834
   H     3.374051   -2.598659    1.650998
   H     1.743389   -3.030780    1.066069
   H    -1.354880    3.763922    0.570982
   H    -0.244656    4.330410    1.851048
   H    -0.787815    2.619760    1.836353
   H     0.439249    4.802414   -1.043240
   H     2.054454    4.030031   -1.138164
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   H     1.622623    5.052022    0.262131
   H     2.136634    3.309607    1.958598
   H     2.743141    2.327161    0.588366
   H     1.540513    1.640217    1.736075
   C     1.679645   -0.720880   -2.254878
   H     0.794759   -0.112764   -2.549966
   H     2.572243   -0.121046   -2.524558
   H     1.647120   -1.623870   -2.895913
   C    -0.276794    2.411664   -1.883237
   H    -0.696502    1.533891   -2.414231
   H    -1.117520    3.128067   -1.755995
   H     0.467050    2.882122   -2.557933
   C    -1.469635   -2.112232   -1.826983
   H    -1.710989   -1.872207   -2.883119
   H    -0.430711   -2.478337   -1.789177
   H    -2.129140   -2.953053   -1.525141
54
Structure: R11 Stoichiometry: C24H25NbN3F+
   C    -1.480751    3.821105   -1.641722
   H    -1.054483    4.454020   -2.435819
   H    -1.653620    4.463378   -0.758311
   H    -2.463388    3.440119   -1.968625
   C    -0.547608    2.679672   -1.312387
   C     0.814041    2.747894   -1.620821
   H     1.149798    3.621805   -2.185251
   C     1.836082    1.861394   -1.181704
   C     3.260046    2.249038   -1.539968
   H     3.867129    2.394381   -0.629496
   H     3.273220    3.177648   -2.129644
   H     3.755841    1.452548   -2.121489
   C     2.789582    0.123688    0.129667
   C     3.529547   -0.825763   -0.601279
   C     4.639224   -1.455683   -0.019968
   H     5.201574   -2.196532   -0.598516
   C     5.028395   -1.143122    1.290033
   H     5.893416   -1.639096    1.742051
   C     4.301074   -0.185828    2.015792
   H     4.600907    0.073313    3.037068
   C     3.191343    0.444272    1.441418
   C    -2.211117    1.320366   -0.029852
   C    -2.776363    0.017876   -0.218363
   C    -3.791147   -0.436897    0.659225
   H    -4.197795   -1.441764    0.515206
   C    -4.280436    0.393584    1.661715
   H    -5.068677    0.042450    2.334662
   C    -3.768659    1.710026    1.799766
   H    -4.171234    2.365006    2.580495
   C    -2.746462    2.173681    0.985580
   C     0.229082    0.109611    3.406153
   C     0.420140   -1.860988   -2.016492
   H     1.296953   -1.500545   -2.564896
   C    -0.750932   -2.105064   -2.708994
   H    -0.797225   -1.890399   -3.782100
   C    -1.892353   -2.713596   -2.074572
   H    -2.771287   -3.029334   -2.641253
   C    -1.821239   -2.898799   -0.716154
   C    -0.727934   -2.440348    0.089831
   H    -0.697067   -2.809718    1.119886
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   C     0.529832   -2.078458   -0.586579
   H     1.502616   -2.339504   -0.151120
   N     1.630827    0.764496   -0.425152
   N    -1.030419    1.561855   -0.740687
   N     0.041226   -0.092608    2.007962
   Nb   -0.266225   -0.126696    0.250481
   H    -0.273629   -0.686567    3.991774
   H     1.307063    0.078447    3.668431
   H    -0.176204    1.084957    3.745639
   H     2.615222    1.189330    1.996576
   H     3.231952   -1.067226   -1.625495
   H    -2.556616   -0.544810   -1.134478
   H    -2.318475    3.169215    1.131844
   F    -2.856945   -3.483193   -0.062630
57
Structure: R12 Stoichiometry: C16H35NSiMoOP2+
   Mo   -0.261509    0.035017   -0.370790
   Si   -0.349600    0.250597    2.194103
   P    -0.432971   -2.425903   -0.180876
   P    -0.412439    2.497564   -0.482557
   N     1.500581   -0.006132   -0.377514
   H    -0.933380    0.090743   -2.025485
   C    -0.618477   -3.545885   -1.658297
   H    -0.587470   -4.615443   -1.380955
   H     0.205441   -3.321865   -2.356418
   H    -1.566145   -3.329328   -2.177876
   C    -1.706523   -3.113176    0.980118
   H    -1.671415   -4.216805    1.008851
   H    -2.718688   -2.793710    0.682774
   H    -1.501089   -2.709713    1.985169
   C     1.122208   -3.094657    0.561221
   H     1.058761   -4.187398    0.707886
   H     1.289677   -2.590160    1.526651
   H     1.965720   -2.857973   -0.107384
   C    -0.641471    3.316011   -2.131967
   H    -0.622659    4.419257   -2.064180
   H    -1.603844    2.984977   -2.557268
   H     0.160290    2.968974   -2.804772
   C    -1.724412    3.325990    0.526637
   H    -1.702943    4.422099    0.393820
   H    -1.559039    3.076966    1.587509
   H    -2.712308    2.938956    0.228252
   C     1.131807    3.297661    0.136969
   H     1.066307    4.398880    0.086746
   H     1.980796    2.947227   -0.472620
   H     1.293105    2.974374    1.178408
   C    -2.077478    0.300277    3.043828
   H    -2.670204   -0.599435    2.794382
   H    -2.658273    1.176431    2.701879
   H    -1.989071    0.357334    4.144328
   H     0.374594   -0.862222    2.937451
   H     0.351970    1.466942    2.782049
   C     2.862117   -0.041376   -0.216752
   C     5.100770   -0.316133   -1.146699
   C     3.714213   -0.277492   -1.324929
   C     3.432647    0.156308    1.066747
   C     4.820012    0.120325    1.228202
   C     5.659811   -0.116650    0.126377
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   H     5.752755   -0.500548   -2.007631
   H     3.260278   -0.426152   -2.309269
   H     2.761246    0.333337    1.912351
   H     5.252615    0.275309    2.222644
   H     6.746303   -0.145740    0.259732
   C    -3.538876   -0.209735   -0.520275
   O    -2.466518    0.156904   -0.005623
   C    -3.552039   -1.121272   -1.710675
   H    -4.471200   -1.007937   -2.308978
   H    -3.493995   -2.174111   -1.377889
   H    -2.632075   -0.905708   -2.294237
   C    -4.837266    0.299515    0.050225
   H    -5.353959    0.923413   -0.704177
   H    -4.652795    0.888446    0.960127
   H    -5.514558   -0.543991    0.278558
50
Structure: R13 Stoichiometry: C20H25P2RuON+
   C    -4.056788   -0.340323   -0.361332
   C    -2.751814   -0.231625   -0.815448
   C    -2.026449    0.985079   -0.550115
   C    -2.646732    2.042960    0.222340
   C    -3.999034    1.877991    0.659338
   C    -4.684380    0.717203    0.363142
   C    -1.863507    3.174653    0.513342
   C    -0.525106    3.245536    0.085806
   C    -0.017787    2.136920   -0.697265
   C     1.354286    2.133655   -1.138245
   C     2.162309    3.208853   -0.803218
   C     1.660319    4.310504   -0.047293
   C     0.351243    4.334533    0.390070
   H    -4.619489   -1.261097   -0.551957
   H    -4.472259    2.678075    1.238961
   H    -5.718807    0.590282    0.699143
   H    -2.293812    3.999188    1.093982
   H     3.210757    3.215567   -1.122081
   H     2.332828    5.140919    0.191916
   H    -0.028466    5.173866    0.982762
   N    -0.770160    1.071480   -1.014745
   Ru    0.811511   -1.366009    0.979028
   C    -2.019889   -1.352398   -1.494641
   H    -1.334356   -0.951860   -2.258724
   H    -2.724592   -2.065522   -1.957556
   C     1.842458    0.923729   -1.873330
   H     1.056604    0.554550   -2.552192
   H     2.758849    1.143627   -2.448880
   P    -0.949736   -2.340151   -0.293751
   P     2.238476   -0.524113   -0.718464
   C     3.871771    0.066513   -0.062322
   H     4.333745   -0.742077    0.528363
   H     4.560207    0.375051   -0.869695
   H     3.689752    0.918255    0.613933
   C     2.818404   -1.733341   -2.013346
   H     3.608376   -1.303994   -2.655402
   H     3.208206   -2.639201   -1.518331
   H     1.962006   -2.024845   -2.644501
   C    -2.264343   -3.116628    0.749639
   H    -3.057812   -3.582775    0.137625
   H    -1.791225   -3.874180    1.394979
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   H    -2.696818   -2.338807    1.398938
   C    -0.494247   -3.767588   -1.397253
   H     0.081656   -4.505883   -0.813606
   H    -1.389777   -4.259140   -1.817460
   H     0.141679   -3.405483   -2.221474
   C     1.796512   -0.633032    2.382709
   O     2.327975   -0.139588    3.300358
   H    -0.029193   -0.061651    1.080038
   H    -0.101699   -1.987342    2.202121
39
Structure: R14 Stoichiometry: C12H21RuO2N2P+
   C     2.328175   -1.311506    0.438590
   C     2.354441    0.169237    0.128930
   N     1.117219    0.721770    0.029603
   C     0.929407    2.103474   -0.125985
   C     2.126079    2.908635   -0.190316
   C     3.375012    2.328266   -0.115197
   C     3.519072    0.919601    0.048477
   C    -0.379874    2.585717   -0.195463
   P    -1.684314    1.378971   -0.115349
   H     4.500918    0.446006    0.127427
   H     2.018069    3.990537   -0.312508
   H     4.269486    2.958195   -0.180302
   C     1.501933   -2.188015   -1.675108
   C     0.912226   -3.296535    0.407631
   H    -0.570338    3.658999   -0.302478
   H     2.177451   -1.448590    1.524146
   H     3.285784   -1.798993    0.168371
   C    -2.832298    1.636728   -1.542368
   C    -2.802934    1.853747    1.298530
   H    -3.667841    0.918044   -1.481093
   H    -3.230738    2.666776   -1.546549
   H    -2.268647    1.453667   -2.470233
   H    -3.664744    1.165273    1.350753
   H    -2.236317    1.798324    2.244254
   H    -3.171940    2.888063    1.177630
   H     1.807611   -3.952028    0.374095
   H     0.623806   -3.122075    1.455211
   H     0.080766   -3.789330   -0.117365
   H     2.375515   -2.864414   -1.787046
   H     0.626702   -2.617076   -2.182787
   H     1.730642   -1.210441   -2.123411
   C    -2.023063   -1.650145   -0.158965
   O    -2.999149   -2.301314   -0.247193
   Ru   -0.526372   -0.571196   -0.050393
   H    -0.604388   -0.442404   -1.626830
   O    -0.129120   -0.631117    2.282764
   H    -1.033021   -0.510719    2.627358
   H     0.261227    0.266633    2.300561
   N     1.181664   -1.993505   -0.239429
19
Structure: R15 Stoichiometry: C5H11RhP2+
   C    -0.575022   -1.298366    0.750071
   C    -1.929301   -1.343708    1.084751
   C    -2.947226   -0.631299    0.422964
   C    -2.707813    0.197797   -0.694307
   C    -1.422072    0.390567   -1.180413
   Rh    0.313092    0.020216   -0.384828
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   P     0.491010    1.972555    0.734347
   P     2.429124   -0.981842   -0.022854
   H     0.088956   -1.895383    1.402534
   H    -2.236218   -2.011134    1.904159
   H    -3.983312   -0.777661    0.754721
   H    -1.311627    0.891140   -2.167411
   H    -3.578365    0.599940   -1.232589
   H     3.116567   -1.464614   -1.175117
   H     2.467546   -2.200724    0.718047
   H     3.595041   -0.418134    0.589009
   H     1.298535    3.135885    0.502882
   H     0.867637    1.808673    2.095798
   H    -0.727304    2.671659    0.954448
21
Structure: R16 Stoichiometry: C10H10Pd+
   C     2.110750    1.099630    0.529522
   C     2.116595   -0.165610    1.207219
   C     2.117258   -1.196938    0.213317
   C     2.119785   -0.574734   -1.072627
   C     2.114267    0.849427   -0.875332
   Pd    0.122975   -0.002849    0.000864
   H     2.124507   -2.271033    0.406477
   H     2.124479   -0.314380    2.288104
   H     2.113909    2.080318    1.008226
   H     2.132935   -1.087096   -2.035901
   H     2.123117    1.603638   -1.663858
   C    -1.270222    1.357224   -0.004235
   C    -1.275247   -1.358697   -0.004272
   C    -2.650451    1.241145   -0.000212
   C    -2.655052   -1.236559   -0.000193
   C    -3.324214    0.003559    0.003194
   H    -0.864596    2.383775   -0.011748
   H    -3.263286    2.153781   -0.001566
   H    -4.421506    0.005614    0.005553
   H    -3.271672   -2.146656   -0.001470
   H    -0.875577   -2.387597   -0.011839
92
Structure: R17 Stoichiometry: C31H55NPdP3Br+
   N    -4.147597   -4.350554   -0.961927
   C    -3.902594   -3.429599   -1.912698
   C    -2.767556   -2.615051   -1.943072
   C    -1.794794   -2.711077   -0.917083
   C    -2.041430   -3.706974    0.058273
   C    -3.206219   -4.476432   -0.009085
   C    -0.585937   -1.878048   -0.939849
   Pd   -0.692364    0.064060    0.162685
   P     1.081757    1.656836    0.456559
   C     0.400777   -1.895732    0.081478
   C     1.841047   -1.733424   -0.165532
   C     2.774414   -2.159498    0.809137
   C     4.153380   -1.992366    0.635833
   C     4.625654   -1.392358   -0.538975
   C     3.732666   -1.003170   -1.552543
   C     2.361234   -1.181741   -1.362731
   Br    6.498188   -1.092032   -0.768925
   P    -2.074526    1.234579   -1.333747
   H    -0.271844   -1.588852   -1.950656
   H     0.174149   -2.464139    0.990707
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H	-2.630235	-1.901888	-2.763041
H	-1.314604	-3.897438	0.853467
H	-4.659630	-3.339614	-2.705115
H	-3.390675	-5.248268	0.751920
H	2.406704	-2.622195	1.731450
H	1.672950	-0.869318	-2.153920
H	4.855082	-2.313841	1.410494
H	4.112674	-0.559563	-2.477066
P	-1.918549	-0.098867	2.269659
C	1.727934	2.255202	-1.205510
C	3.155026	2.803019	-1.327937
H	0.986810	2.995498	-1.562652
H	1.613111	1.379922	-1.866144
H	3.377983	3.046744	-2.383022
H	3.307508	3.719058	-0.734934
H	3.896470	2.054258	-1.001298
C	2.621691	1.124332	1.378212
C	3.511554	2.162349	2.072229
H	3.212044	0.539745	0.653754
H	2.263242	0.391979	2.121532
H	4.342042	1.648753	2.590014
H	3.957433	2.875303	1.360638
H	2.956633	2.738952	2.832627
C	0.573875	3.232503	1.342441
C	1.276858	4.560121	1.032966
H	0.643965	2.990597	2.419878
H	-0.503475	3.334521	1.139206
H	0.815779	5.378445	1.616056
H	2.349763	4.537398	1.279593
H	1.180089	4.825180	-0.034385
C	-3.202533	1.171217	2.787164
C	-2.736263	2.625630	2.728706
H	-3.552385	0.909681	3.805226
H	-4.065762	1.033427	2.111524
H	-3.554291	3.314504	3.005384
H	-1.892356	2.815825	3.413885
H	-2.401642	2.881507	1.709879
C	-0.801919	-0.016528	3.772531
C	0.291425	-1.089033	3.764754
H	-1.416828	-0.079225	4.691953
H	-0.337873	0.987090	3.755060
H	0.982772	-0.960950	4.616600
H	-0.135780	-2.105347	3.829659
H	0.874790	-1.027896	2.830396
C	-2.909048	-1.634356	2.689266
C	-4.167430	-1.794086	1.827957
H	-3.166509	-1.614209	3.766915
H	-2.236093	-2.494514	2.529843
H	-4.632940	-2.781129	1.988951
H	-4.923056	-1.025821	2.068331
H	-3.922689	-1.713675	0.755603
C	-3.869162	0.743335	-1.140502
C	-5.002182	1.597834	-1.722493
H	-3.988471	0.670241	-0.045805
H	-3.924816	-0.299919	-1.500781
H	-5.978188	1.145158	-1.469292
H	-4.995723	2.617473	-1.299822
H	-4.950721	1.683459	-2.819308

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   C    -2.114218    3.110121   -1.243416
   C    -2.531418    3.933134   -2.469631
   H    -1.092969    3.402127   -0.944600
   H    -2.758125    3.347611   -0.376273
   H    -2.469545    5.012370   -2.238828
   H    -1.862389    3.743440   -3.326404
   H    -3.562985    3.718799   -2.790168
   C    -1.621575    0.903301   -3.126924
   C    -2.695978    0.934737   -4.221385
   H    -1.143484   -0.090420   -3.111971
   H    -0.805130    1.616188   -3.350014
   H    -2.249591    0.672719   -5.197996
   H    -3.494163    0.200266   -4.017546
   H    -3.165558    1.925840   -4.323670
92
Structure: R18 Stoichiometry: C31H55P3NIPd+
   N     4.616577   -4.030420   -1.079785
   C     4.043086   -4.177653    0.128346
   C     2.817606   -3.609135    0.491827
   C     2.103479   -2.813118   -0.434826
   C     2.696029   -2.688087   -1.716743
   C     3.923561   -3.299706   -1.977065
   C     0.829617   -2.190887   -0.059941
   Pd    1.002207    0.049786   -0.038293
   P    -0.045870    1.729379   -1.288093
   C    -0.083141   -1.657757   -1.007152
   C    -1.528170   -1.518214   -0.790322
   C    -2.396004   -1.321819   -1.891750
   C    -3.766416   -1.087316   -1.723552
   C    -4.304022   -1.073122   -0.429376
   C    -3.484765   -1.333155    0.683628
   C    -2.119027   -1.552336    0.495407
   I    -6.364591   -0.638328   -0.141647
   P     0.238919    0.760742    2.224229
   H     0.435165   -2.519751    0.907758
   H     0.206074   -1.683845   -2.064487
   H     2.415033   -3.773561    1.497328
   H     2.204418   -2.107028   -2.502659
   H     4.599210   -4.785090    0.856526
   H     4.384166   -3.192917   -2.969440
   H    -1.984710   -1.353433   -2.906984
   H    -1.480692   -1.717954    1.367485
   H    -4.405722   -0.917405   -2.594603
   H    -3.909002   -1.350614    1.691368
   P     3.356866    0.510773   -0.157237
   C     0.785110    3.405338   -1.348197
   C     0.071239    4.576346   -2.032921
   H     1.764375    3.212935   -1.825510
   H     1.010657    3.655161   -0.296541
   H     0.724567    5.467474   -2.053563
   H    -0.200547    4.341632   -3.076720
   H    -0.851263    4.855102   -1.496235
   C    -1.782094    2.078885   -0.669560
   C    -2.851083    2.597744   -1.640579
   H    -1.658958    2.769134    0.186342
   H    -2.114814    1.116957   -0.242120
   H    -3.804053    2.744731   -1.101530
   H    -2.574318    3.556739   -2.108400
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   H    -3.043844    1.867638   -2.443335
   C    -0.349047    1.375369   -3.094890
   C     0.900372    0.928700   -3.855292
   H    -0.811697    2.257071   -3.574048
   H    -1.107968    0.575046   -3.107026
   H     0.652249    0.660077   -4.897439
   H     1.667560    1.721792   -3.887072
   H     1.351778    0.050160   -3.364138
   C     0.652248    2.589382    2.383236
   C     0.712800    3.203634    3.786378
   H    -0.110024    3.104293    1.769180
   H     1.610658    2.731040    1.859551
   H     0.862979    4.296754    3.724060
   H    -0.217193    3.030800    4.356969
   H     1.548874    2.787267    4.373466
   C    -1.537168    0.857436    2.888300
   C    -2.012652   -0.255216    3.828146
   H    -2.184932    0.895118    1.996164
   H    -1.648396    1.829641    3.402937
   H    -3.074837   -0.101053    4.090317
   H    -1.928461   -1.256325    3.372542
   H    -1.438658   -0.267347    4.770488
   C     1.181430    0.069721    3.690765
   C     1.206621   -1.462592    3.732325
   H     0.795667    0.487044    4.639212
   H     2.211417    0.451271    3.565426
   H     1.898659   -1.825220    4.512897
   H     0.211003   -1.885641    3.942845
   H     1.541938   -1.863128    2.761396
   C     3.969016    0.674887   -1.929968
   C     5.435610    0.366645   -2.260445
   H     3.697622    1.702022   -2.240741
   H     3.321517    0.003350   -2.514942
   H     5.620627    0.534160   -3.337415
   H     6.142866    0.997951   -1.698553
   H     5.676823   -0.687341   -2.044150
   C     3.876302    2.147387    0.603425
   C     5.305578    2.660063    0.393499
   H     3.665878    2.037079    1.683579
   H     3.148027    2.888659    0.230301
   H     5.467278    3.594347    0.961737
   H     6.060481    1.930937    0.735167
   H     5.503358    2.881867   -0.668836
   C     4.643934   -0.634007    0.566104
   C     4.453886   -0.903079    2.058467
   H     5.649215   -0.221235    0.369640
   H     4.574809   -1.577492    0.001247
   H     5.191614   -1.642696    2.416498
   H     4.578845    0.014046    2.662320
   H     3.448097   -1.305524    2.251829
90
Structure: R19 Stoichiometry: C31H53NPdP3Br+
   C     1.748118   -0.901275   -3.612454
   C     1.202358   -1.595634   -2.498262
   C     1.667360   -2.925121   -2.301279
   C     2.626514   -3.451169   -3.169809
   N     3.159946   -2.784482   -4.210938
   C     2.700115   -1.534111   -4.413917
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C	0.289193	-0.982904	-1.597637
C	-0.771540	-0.601295	-0.990971
C	-2.210413	-0.575785	-0.932662
C	-2.874024	0.050418	0.147836
C	-4.269656	0.086160	0.226446
C	-5.022989	-0.513316	-0.792987
C	-4.396031	-1.144455	-1.881381
C	-3.001253	-1.173438	-1.946526
Pd	0.802601	0.184378	0.231129
P	0.121358	2.465024	0.056949
P	3.148327	0.216587	0.192336
H	1.278636	-3.521288	-1.469663
H	1.430549	0.124376	-3.823990
H	2.993552	-4.475854	-3.014093
H	3.126800	-0.997696	-5.273648
H	-2.504654	-1.662497	-2.790396
H	-2.256975	0.509136	0.926189
H	-4.999545	-1.606907	-2.667488
H	-4.769979	0.573519	1.067984
C	4.023442	1.085393	1.606334
C	5.461576	0.692128	1.967540
H	3.360408	0.932745	2.477300
H	3.956984	2.165337	1.374383
H	5.807959	1.268738	2.844714
H	5.529556	-0.377670	2.230098
H	6.165934	0.882740	1.142314
C	3.873999	-1.511253	0.163862
C	5.200912	-1.784212	-0.554355
H	3.079509	-2.120037	-0.301635
H	3.922961	-1.829941	1.220937
H	5.433778	-2.863660	-0.509722
H	5.141218	-1.512475	-1.621551
H	6.046872	-1.240523	-0.102700
C	3.804778	1.028944	-1.360311
C	5.241143	1.563432	-1.415050
H	3.094830	1.849641	-1.557788
H	3.623063	0.287050	-2.159494
H	5.433105	2.027814	-2.399608
H	5.412585	2.339159	-0.648333
H	5.991198	0.769973	-1.271188
C	-0.907600	3.151481	1.475028
C	-1.915412	4.281605	1.229531
H	-0.174493	3.428366	2.256596
H	-1.439720	2.272823	1.878592
H	-2.455645	4.521282	2.164028
H	-1.433412	5.206976	0.876399
H	-2.670571	3.984239	0.481730
C	-0.948763	2.714516	-1.463487
C	-1.030590	4.084206	-2.148103
H	-1.954512	2.357410	-1.174726
H	-0.571874	1.959778	-2.177649
H	-1.665448	4.017583	-3.050618
H	-1.464198	4.857445	-1.493535
H	-0.035694	4.433994	-2.474730
C	1.499940	3.728450	-0.129231
C	1.265484	5.207126	0.206104
H	1.853879	3.618183	-1.171669
H	2.314782	3.333953	0.503827

H	2.201636	5.780039	0.072192
H	0.498751	5.666233	-0.437716
H	0.950863	5.336090	1.255923
Br	-6.929351	-0.471762	-0.703309
P	0.226972	-1.095848	2.174855
C	1.674853	-1.823585	3.126099
C	1.513856	-2.287288	4.579818
H	2.451737	-1.039299	3.078624
H	2.047039	-2.647737	2.489072
H	2.482344	-2.647641	4.973265
H	1.184528	-1.459396	5.231016
H	0.786887	-3.108606	4.680097
C	-0.788678	-0.240660	3.508484
C	-1.724557	-1.050265	4.415432
H	-1.379669	0.514901	2.962114
H	-0.056785	0.339949	4.102179
H	-2.270923	-0.375449	5.100094
H	-2.478681	-1.594958	3.821785
H	-1.183227	-1.784449	5.032967
C	-0.806511	-2.582087	1.683250
C	-0.805401	-3.855642	2.536907
H	-0.460920	-2.816913	0.660022
H	-1.833730	-2.193649	1.554164
H	-1.429506	-4.631955	2.057374
H	0.211602	-4.272617	2.639882
H	-1.206560	-3.685233	3.548951

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Structure: R20 Stoichiometry: C31H53PdINP3+

C	1.882644	-1.309121	-3.520950
C	1.354859	-1.850885	-2.316946
C	1.765014	-3.174158	-1.994857
C	2.658908	-3.838633	-2.838200
N	3.175139	-3.316442	-3.966467
C	2.765544	-2.072907	-4.286428
C	0.516474	-1.096116	-1.451242
C	-0.506859	-0.607793	-0.852763
C	-1.943341	-0.560826	-0.748942
C	-2.574548	0.288573	0.188567
C	-3.968134	0.346760	0.299526
C	-4.753112	-0.460089	-0.537414
C	-4.157131	-1.317791	-1.479594
C	-2.764750	-1.363710	-1.581234
Pd	1.149232	0.278090	0.173299
P	0.531107	2.544622	-0.152447
P	3.486202	0.207427	0.042742
H	1.386775	-3.657882	-1.089236
H	1.605134	-0.296639	-3.829814
H	2.984103	-4.858249	-2.585797
H	3.177068	-1.654690	-5.216305
H	-2.293453	-2.027617	-2.312991
H	-1.939157	0.903917	0.831579
H	-4.776545	-1.943788	-2.128337
H	-4.435987	1.011957	1.030983
C	4.458366	1.207891	1.298231
C	5.859532	0.744081	1.715915
H	3.798722	1.264723	2.182058
H	4.492793	2.235390	0.888998
H	6.273098	1.420026	2.486515

H	5.832916	-0.270645	2.149508
H	6.563925	0.730965	0.868735
C	4.095036	-1.555658	0.219484
C	5.403498	-2.005058	-0.441440
H	3.261762	-2.153313	-0.189457
H	4.108478	-1.760385	1.306664
H	5.560562	-3.084131	-0.261658
H	5.364636	-1.863453	-1.534505
H	6.283435	-1.468459	-0.050862
C	4.135459	0.772064	-1.616921
C	5.606068	1.177751	-1.776238
H	3.481729	1.619071	-1.887938
H	3.865507	-0.042002	-2.314488
H	5.797441	1.503965	-2.814822
H	5.865684	2.022791	-1.114799
H	6.296982	0.348719	-1.556340
C	-0.379262	3.379175	1.268262
C	-1.375135	4.513007	0.992881
H	0.415112	3.704315	1.967139
H	-0.897728	2.552941	1.785943
H	-1.845747	4.847313	1.935898
H	-0.895253	5.390184	0.530340
H	-2.185344	4.176309	0.323391
C	-0.614678	2.716130	-1.628292
C	-0.696626	4.032605	-2.410227
H	-1.612841	2.412024	-1.263218
H	-0.296036	1.898807	-2.300888
H	-1.381728	3.918434	-3.270187
H	-1.072651	4.865563	-1.794429
H	0.287992	4.325622	-2.814409
C	1.943335	3.728906	-0.519156
C	1.778905	5.238449	-0.298592
H	2.234084	3.515692	-1.565349
H	2.776893	3.356475	0.102387
H	2.724727	5.762239	-0.530051
H	0.992696	5.672510	-0.936211
H	1.528502	5.465293	0.752071
P	0.718578	-0.863272	2.253176
C	2.108631	-0.898449	3.517249
C	2.261769	-2.091154	4.470079
H	2.015222	0.050210	4.079896
H	3.029998	-0.794313	2.918601
H	3.153387	-1.957054	5.110197
H	1.390349	-2.214531	5.132107
H	2.398327	-3.032368	3.910176
C	-0.776093	-0.324424	3.258454
C	-0.905812	-0.705124	4.739161
H	-1.650276	-0.679483	2.682251
H	-0.784363	0.776515	3.161941
H	-1.831631	-0.273494	5.162274
H	-0.948509	-1.795479	4.889041
H	-0.061678	-0.312411	5.332027
C	0.383194	-2.664390	1.853502
C	-0.437624	-3.550243	2.798976
H	1.380618	-3.103635	1.659648
H	-0.114711	-2.617343	0.867561
H	-0.563951	-4.557073	2.359968
H	0.037897	-3.673824	3.785391

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   H    -1.448135   -3.135508    2.955764
   I    -6.871785   -0.389171   -0.378691
45
Structure: R21 Stoichiometry: C11H29N4Ta+
   Ta    0.025488    0.072926   -0.091869
   N     0.264319    2.078376   -0.135247
   N    -2.016989    0.263629   -0.328478
   N     2.079164   -0.299616   -0.179255
   N    -0.139742   -0.700283    1.763679
   C     0.000913   -1.000564   -2.086500
   H    -0.948873   -0.784011   -2.601678
   H     0.851468   -0.793179   -2.753688
   C     0.040813   -2.327363   -1.445080
   H     1.037381   -2.771978   -1.304147
   C    -1.013835   -2.981099   -0.888943
   H    -2.040642   -2.617088   -1.001361
   H    -0.875141   -3.918087   -0.339073
   H    -2.996714    0.343341   -2.223797
   C    -2.571529    1.016829   -1.446059
   H    -1.791079    1.634456   -1.922119
   H    -3.391562    1.688010   -1.111862
   H    -3.818481    0.212851    0.793831
   C    -3.062872   -0.478474    0.360304
   H    -3.610978   -1.158950   -0.328625
   H    -2.631646   -1.086583    1.169706
   H     3.810100   -0.133201   -1.403239
   C     3.029146   -0.872197   -1.114188
   H     2.536546   -1.213901   -2.035799
   H     3.565209   -1.739884   -0.668709
   H     3.292930   -0.709261    1.532372
   C     2.800528    0.144209    1.016891
   H     3.594721    0.877861    0.758457
   H     2.117520    0.626281    1.735596
   H     2.154144    2.040388   -1.079521
   C     1.443544    2.766915   -0.660761
   H     1.955218    3.350072    0.134838
   H     1.155585    3.481637   -1.460196
   H    -0.998257    3.778648   -0.363309
   C    -0.694847    3.038160    0.407002
   H    -1.597238    2.517811    0.761971
   H    -0.253552    3.605908    1.254087
   C    -0.698298    0.103706    2.841369
   H    -0.955745    1.112643    2.476312
   H     0.024064    0.215193    3.678517
   H    -1.624825   -0.348203    3.257720
   H    -0.625783   -2.682316    2.383308
   C     0.255731   -2.034043    2.184260
   H     0.862027   -1.990993    3.114080
   H     0.859948   -2.512284    1.398132
60
Structure: R22 Stoichiometry: C16H38TaN5+
   Ta   -0.623968    0.002693   -0.093396
   N    -0.942635   -0.470725    1.882675
   N    -2.067564   -1.186280   -0.876689
   N    -1.541328    1.774836   -0.361607
   N     1.293242   -1.165548    0.147865
   N     1.302455    1.029149    0.430025
   C     0.019070   -0.505835    2.973848
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   H     0.152230   -1.535414    3.370107
   H     0.994246   -0.125669    2.639510
   H    -0.329497    0.127817    3.817318
   C    -2.241388   -0.961065    2.341306
   H    -2.967291   -0.973422    1.512732
   H    -2.162507   -1.993135    2.749454
   H    -2.645588   -0.319583    3.154195
   H    -3.188455    0.307486   -1.843548
   C    -3.099525   -0.789821   -1.824041
   H    -4.083455   -1.224980   -1.547524
   H    -2.858552   -1.138471   -2.851549
   H    -1.664050   -3.092870   -1.748007
   C    -1.946589   -2.636454   -0.775552
   H    -2.903954   -3.096895   -0.451695
   H    -1.175110   -2.906376   -0.035247
   C    -1.142888    2.857232   -1.251172
   H    -0.854120    3.763234   -0.678171
   H    -0.290543    2.553737   -1.874971
   H    -1.981692    3.140913   -1.920884
   H    -2.353422    3.030750    1.161758
   C    -2.642011    2.177074    0.512865
   H    -3.520876    2.491786   -0.088054
   H    -2.950534    1.343543    1.162386
   C     1.804414   -2.524830    0.011103
   H     1.356440   -2.937068   -0.916865
   C     1.326090   -3.389639    1.193122
   H     0.237520   -3.291077    1.339976
   H     1.563977   -4.455209    1.025233
   H     1.818659   -3.061937    2.125288
   C     3.330890   -2.610257   -0.130655
   H     3.628353   -3.655987   -0.319335
   H     3.692741   -1.988109   -0.965167
   H     3.835905   -2.282107    0.796081
   H     3.716531    3.463973    0.790735
   C     3.377544    2.417205    0.706459
   H     3.721658    1.877145    1.607817
   H     3.863034    1.970265   -0.178169
   C     1.848994    2.373842    0.581478
   H     1.582576    2.943126   -0.332598
   C     1.161566    3.063944    1.771112
   H     0.066028    2.996884    1.664927
   H     1.440391    2.567858    2.717937
   H     1.448132    4.129053    1.833797
   H     3.134623   -0.105784    0.412879
   C     2.036697   -0.084139    0.342271
   C     0.307462   -0.029656   -2.251333
   H     0.329061   -1.090296   -2.565600
   H    -0.544911    0.461689   -2.769110
   C     1.573041    0.654762   -2.528816
   H     1.542265    1.757133   -2.507750
   C     2.786617    0.086562   -2.731053
   H     2.900229   -1.002758   -2.800081
   H     3.690518    0.690588   -2.871428
53
Structure: R23 Stoichiometry: C21H29ONW+
   C     2.341936   -0.974774    0.099668
   C     1.246642   -1.904596    0.248381
   C     0.478100   -1.499391    1.390024
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   C     1.079620   -0.314226    1.950345
   C     2.240095   -0.004558    1.164429
   W     0.380414    0.181847   -0.362403
   C    -0.854207    2.495917   -0.324829
   C     0.133338    2.334775   -1.303052
   H    -0.196345    2.246614   -2.344982
   C     1.504309    2.042884   -0.971741
   H     1.942591    2.567467   -0.113589
   H     2.200577    1.920650   -1.810208
   C    -2.288804    2.686310   -0.756551
   H    -2.479435    2.217609   -1.734921
   H    -2.989989    2.248529   -0.027215
   H    -2.512417    3.769683   -0.831402
   N     0.325982   -0.385656   -2.067725
   O     0.447309   -0.932221   -3.136046
   C    -0.535687    2.974572    1.077786
   H     0.515994    2.813531    1.361976
   H    -0.741893    4.062954    1.142867
   H    -1.178912    2.485290    1.828269
   C     1.002251   -3.134732   -0.581124
   H     1.316402   -2.985496   -1.626017
   H     1.563036   -3.996883   -0.172981
   H    -0.067967   -3.396554   -0.588039
   C    -0.627738   -2.307947    2.004358
   H    -1.298631   -2.728663    1.239335
   H    -0.185277   -3.145275    2.577573
   H    -1.241869   -1.708937    2.691804
   C     0.684770    0.347377    3.241565
   H    -0.405751    0.317389    3.398491
   H     1.155025   -0.166233    4.102277
   H     1.002469    1.401889    3.273760
   C     3.269035    1.034276    1.508134
   H     2.813197    1.939093    1.944275
   H     3.973876    0.627336    2.257953
   H     3.855160    1.336294    0.626340
   C     3.443896   -1.074578   -0.919729
   H     3.905995   -0.091713   -1.105997
   H     4.238799   -1.762994   -0.574149
   H     3.062381   -1.452768   -1.881873
   C    -1.756303   -0.272233   -0.063182
   C    -2.474869   -0.995003   -1.047590
   C    -2.469008    0.039314    1.120091
   C    -3.813515   -1.379592   -0.859905
   H    -1.983154   -1.265367   -1.988409
   C    -3.805129   -0.337388    1.319940
   H    -1.967057    0.593452    1.923406
   C    -4.487325   -1.053643    0.325192
   H    -4.331897   -1.936784   -1.649386
   H    -4.313463   -0.073063    2.255004
   H    -5.530896   -1.352980    0.472826
86
Structure: R24 Stoichiometry: C32H47N2P2O2Re+
   C     1.179271   -0.035808    2.302620
   C    -1.044584   -0.952285    2.430388
   C     1.319675   -0.022323    3.686849
   C    -0.882364   -1.022418    3.862134
   C     0.261223   -0.556917    4.471290
   H     2.236397    0.359483    4.143320
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H	-1.711424	-1.423412	4.452823
H	0.355657	-0.594534	5.562502
N	0.059640	-0.512901	1.678792
P	2.344024	-0.683235	-0.090130
P	-2.461013	-0.715290	0.113553
C	2.308353	0.434743	1.405952
H	2.098908	1.448824	1.024660
H	3.260258	0.475240	1.958554
C	-0.240066	-0.504570	-2.446439
O	-0.350673	-0.373163	-3.610540
C	-2.249469	-1.266179	1.790515
H	-3.105957	-1.535715	2.418193
C	-3.334540	1.016015	0.222938
C	-3.674592	-1.921909	-0.740709
C	3.520408	0.113515	-1.370882
C	3.125320	-2.284865	0.642877
C	-3.157808	1.772593	-1.110745
H	-3.835338	1.384197	-1.887331
H	-3.393979	2.844734	-0.966907
H	-2.130559	1.690360	-1.496196
C	-4.829330	0.978376	0.591971
H	-5.456845	0.553596	-0.208108
H	-5.002739	0.409500	1.521629
H	-5.177663	2.014803	0.767828
C	-2.614788	1.748059	1.381146
H	-2.833174	2.831492	1.321460
H	-2.969490	1.371973	2.354171
H	-1.525137	1.608299	1.361914
C	-4.183115	-1.317543	-2.063355
H	-3.342637	-0.982715	-2.696235
H	-4.742515	-2.090175	-2.623417
H	-4.864537	-0.466366	-1.904960
C	-2.915324	-3.218957	-1.065239
H	-2.175594	-3.061796	-1.863567
H	-2.402414	-3.620008	-0.175883
H	-3.640025	-3.976889	-1.417986
C	-4.845853	-2.298573	0.191282
H	-5.461384	-1.439024	0.489418
H	-5.502243	-3.015038	-0.338011
H	-4.473792	-2.797239	1.101947
C	3.475037	-3.256127	-0.503190
H	3.761136	-4.230843	-0.066685
H	2.620730	-3.429196	-1.175946
H	4.331727	-2.896431	-1.096778
C	2.108132	-2.958015	1.597545
H	1.965609	-2.369728	2.516813
H	1.125075	-3.123643	1.140772
H	2.521531	-3.942688	1.885015
C	4.387953	-2.004438	1.487308
H	4.751110	-2.969003	1.888255
H	5.209818	-1.554200	0.913838
H	4.163587	-1.360459	2.353819
C	2.999793	1.542263	-1.634056
H	3.057110	2.188087	-0.741228
H	3.626897	2.002539	-2.419693
H	1.959915	1.520092	-1.994220
C	3.388122	-0.671003	-2.695327
H	2.333585	-0.741796	-3.006819

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   H     3.946565   -0.133815   -3.484463
   H     3.799425   -1.688703   -2.626197
   C     4.994610    0.190538   -0.936547
   H     5.115056    0.681028    0.045013
   H     5.465570   -0.804221   -0.893844
   H     5.555094    0.787624   -1.680267
   Re   -0.073866   -0.638471   -0.531784
   C     0.004887   -2.557055   -0.785508
   O     0.145524   -3.696228   -1.032137
   N     0.020247    1.433203   -0.413133
   C     0.113140    2.602328   -0.325862
   C     0.220126    4.006146   -0.161919
   C     0.193913    4.870218   -1.285361
   C     0.354100    4.546270    1.143397
   C     0.299898    6.250267   -1.096864
   H     0.088243    4.446657   -2.287989
   C     0.459999    5.928767    1.310242
   H     0.367279    3.872147    2.004766
   C     0.433429    6.783302    0.195670
   H     0.277646    6.916553   -1.965113
   H     0.561485    6.344134    2.317952
   H     0.515494    7.865989    0.334719
88
Structure: R25 Stoichiometry: C30H51P2O2ReN2+
   C     1.125717   -0.643968    2.393831
   C    -1.157401   -1.376791    2.222313
   C     1.233149   -1.077064    3.711583
   C    -1.049280   -1.874669    3.571301
   C     0.110935   -1.721746    4.296502
   H     2.165083   -0.932802    4.264177
   H    -1.925950   -2.362582    4.007776
   H     0.168891   -2.094434    5.325526
   N    -0.010248   -0.794960    1.652143
   P     2.365630   -0.460092   -0.094742
   P    -2.474438   -0.477478    0.009633
   C     2.294489    0.033945    1.711848
   H     2.119073    1.123557    1.710139
   H     3.233709   -0.153273    2.259393
   C    -0.214730    0.096551   -2.390833
   O    -0.343243    0.377065   -3.526549
   C    -2.354331   -1.437855    1.497361
   H    -3.241534   -1.826712    2.008700
   C    -3.312546    1.191487    0.535054
   C    -3.701180   -1.377625   -1.160134
   C     3.550615    0.821611   -0.951972
   C     3.194244   -2.187781   -0.029738
   C    -3.148175    2.243759   -0.578719
   H    -3.800525    2.033264   -1.439091
   H    -3.426928    3.242375   -0.191257
   H    -2.112410    2.283480   -0.949396
   C    -4.798860    1.073324    0.918405
   H    -5.447250    0.867155    0.051578
   H    -4.957502    0.287692    1.677213
   H    -5.133269    2.033154    1.358616
   C    -2.557145    1.623571    1.812097
   H    -2.849073    2.659024    2.075298
   H    -2.817723    0.966362    2.656948
   H    -1.464831    1.581663    1.691215
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   C    -4.191618   -0.430514   -2.271818
   H    -3.344347    0.051480   -2.789792
   H    -4.753955   -1.018725   -3.021133
   H    -4.868624    0.352188   -1.893888
   C    -2.969495   -2.551925   -1.830442
   H    -2.165745   -2.202542   -2.496425
   H    -2.542383   -3.239811   -1.084809
   H    -3.698124   -3.116675   -2.442589
   C    -4.889317   -1.973992   -0.375870
   H    -5.494222   -1.218110    0.143715
   H    -5.551426   -2.504395   -1.086383
   H    -4.535299   -2.710386    0.364676
   C     3.224116   -2.758849   -1.462699
   H     3.659980   -3.775006   -1.438285
   H     2.215306   -2.834790   -1.892431
   H     3.844289   -2.145412   -2.138033
   C     2.324769   -3.080505    0.889573
   H     2.493580   -2.837794    1.950896
   H     1.248754   -2.995438    0.694059
   H     2.620273   -4.133215    0.726401
   C     4.614837   -2.200949    0.579406
   H     4.859265   -3.243101    0.855815
   H     5.389111   -1.859361   -0.119415
   H     4.678445   -1.597755    1.502155
   C     3.663930    2.085161   -0.077791
   H     4.199995    1.888657    0.865986
   H     4.233361    2.853774   -0.633969
   H     2.676950    2.503388    0.162323
   C     2.883864    1.187738   -2.293907
   H     1.895989    1.647728   -2.138752
   H     3.527962    1.903804   -2.838715
   H     2.736369    0.300030   -2.931525
   C     4.988386    0.345309   -1.232976
   H     5.558838    0.176613   -0.306949
   H     5.024157   -0.567773   -1.846709
   H     5.504967    1.142840   -1.799692
   Re   -0.063661   -0.345349   -0.521653
   C    -0.100737   -2.203769   -1.018968
   O    -0.056839   -3.326301   -1.362099
   N     0.124439    1.716284   -0.064845
   C     0.249195    2.865062    0.134209
   C     0.403175    4.308316    0.400172
   C    -0.995508    4.970610    0.480676
   C     1.141597    4.475201    1.753978
   C     1.216920    4.947548   -0.754839
   H    -1.537415    4.866497   -0.472198
   H    -1.601846    4.518145    1.280504
   H    -0.864894    6.044814    0.697633
   H     2.146589    4.023982    1.720042
   H     1.249248    5.551190    1.973655
   H     0.571185    4.004058    2.571331
   H     1.320522    6.029238   -0.562575
   H     2.222862    4.506028   -0.829404
   H     0.700841    4.810110   -1.719261
33
Structure: R26 Stoichiometry: C7H22P2OOs+
   Os   -0.000267   -0.004691   -0.186064
   H    -0.454476    0.000882   -1.927739
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   H     0.436890   -0.004142   -1.931177
   P    -2.316333   -0.311353    0.099088
   P     2.316011   -0.313409    0.097900
   C     3.304438    1.162056    0.607750
   H     4.368408    0.910373    0.764542
   H     3.217578    1.938228   -0.170571
   H     2.876508    1.563875    1.541041
   C     2.733284   -1.539387    1.411478
   H     2.260950   -2.500574    1.152659
   H     3.825615   -1.667268    1.512476
   H     2.305581   -1.190868    2.365300
   C     3.278248   -0.951521   -1.345707
   H     3.219713   -0.218825   -2.168080
   H     4.337297   -1.127783   -1.085610
   H     2.817281   -1.894203   -1.684057
   C    -2.738373   -1.401706    1.525874
   H    -3.829533   -1.548359    1.613400
   H    -2.235585   -2.371534    1.382138
   H    -2.345771   -0.942570    2.447432
   C    -3.341775    1.189454    0.432325
   H    -3.254884    1.879783   -0.423122
   H    -4.403668    0.933872    0.596729
   H    -2.940133    1.698056    1.324346
   C    -3.237701   -1.115896   -1.286638
   H    -2.751865   -2.078580   -1.515826
   H    -4.298168   -1.285178   -1.027751
   H    -3.176828   -0.472502   -2.180501
   C     0.003805    1.906324    0.007157
   O     0.004608    3.068059    0.162050
   H    -0.008858   -1.730524   -0.269503
   H     0.010657   -0.204657    1.460062
39
Structure: R27 Stoichiometry: C7H26NBOOsP2+
   Os   -0.022037   -0.106704    0.075935
   H    -0.229586    1.023048   -1.423128
   H     0.051665    2.561886    0.408690
   P     2.318267   -0.106126    0.308901
   P    -2.356317   -0.093919    0.256674
   C    -3.002585   -0.384055    1.963579
   H    -4.105601   -0.337171    2.001739
   H    -2.658110   -1.375096    2.301042
   H    -2.568560    0.375220    2.634592
   C    -3.249708    1.467555   -0.208237
   H    -2.989147    1.734523   -1.246865
   H    -4.345717    1.357958   -0.124177
   H    -2.921741    2.276713    0.467336
   C    -3.287563   -1.348814   -0.731806
   H    -2.915855   -2.351969   -0.465313
   H    -4.375677   -1.294867   -0.549942
   H    -3.081142   -1.182162   -1.802138
   C     3.121419    1.432129    0.953210
   H     4.212444    1.304107    1.068683
   H     2.926563    2.255100    0.245845
   H     2.670324    1.681685    1.927780
   C     2.955156   -1.380005    1.487748
   H     2.618235   -2.371734    1.143823
   H     4.057667   -1.362384    1.556405
   H     2.513893   -1.193716    2.480432
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   C     3.315283   -0.462150   -1.206892
   H     3.086279    0.301559   -1.967622
   H     4.399178   -0.466919   -0.994274
   H     3.010680   -1.446469   -1.600075
   C     0.043625   -1.649722   -1.029650
   O     0.087467   -2.633780   -1.669577
   H    -0.995361    3.448555   -0.550551
   H     0.575546    3.973386   -0.428738
   H     1.610179    2.050001   -1.687205
   H    -0.093549    2.491640   -2.708153
   B     0.397889    2.110209   -1.658079
   N    -0.020025    3.138464   -0.473088
   H    -0.083089    1.217869    1.241833
   H    -0.046719   -1.060287    1.406251
51
Structure: R28 Stoichiometry: C17H28IrP2O2N+
   C    -3.048370    0.724819   -1.076065
   C    -2.219473    0.021488   -0.160913
   C    -2.901101   -0.770729    0.802742
   C    -4.301786   -0.843233    0.863027
   C    -5.088241   -0.135699   -0.058805
   C    -4.449151    0.645418   -1.034389
   Ir   -0.175950    0.133454   -0.235168
   P     0.195003   -2.051856   -0.784229
   C     1.947042   -2.243360   -0.181289
   C     2.696774   -0.940249   -0.270069
   N     1.954037    0.217781   -0.275877
   C     2.609569    1.425125   -0.267708
   C     4.006064    1.499573   -0.234932
   C     4.767807    0.324608   -0.250515
   C     4.096851   -0.903188   -0.278600
   C     1.758374    2.670374   -0.352959
   P     0.017322    2.342527    0.253680
   H     4.651493   -1.846283   -0.282817
   H     4.487873    2.481829   -0.218334
   H     5.861312    0.365745   -0.239620
   H     2.249156    3.525694    0.144914
   H     1.636510    2.938255   -1.421132
   H     1.805191   -2.507118    0.893258
   H     2.505838   -3.065289   -0.663395
   H    -2.579799    1.346220   -1.850485
   H    -5.047768    1.200829   -1.767520
   H    -6.181840   -0.194412   -0.019804
   H    -4.782114   -1.463605    1.630189
   H    -2.314554   -1.351652    1.527306
   H     0.023418   -0.209630    1.835234
   O     0.041690   -0.377483    2.853933
   H    -0.903663   -0.293422    3.081913
   H     0.565948   -2.001249    2.868106
   O     0.898901   -2.939456    2.756114
   H     1.646006   -2.989477    3.376876
   C     0.015128    2.887875    2.019214
   H     0.445044    3.897979    2.140355
   H    -1.030853    2.891592    2.371535
   H     0.570144    2.148640    2.618940
   C    -0.968721    3.666620   -0.571857
   H    -2.022095    3.548464   -0.267679
   H    -0.614416    4.677032   -0.301057
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   H    -0.909605    3.529270   -1.663919
   C     0.248302   -2.443944   -2.589261
   H     0.641251   -3.459730   -2.774073
   H    -0.773177   -2.362948   -2.997645
   H     0.884094   -1.698511   -3.094294
   C    -0.682236   -3.490373   -0.046552
   H    -1.764898   -3.361746   -0.209810
   H    -0.344857   -4.438641   -0.500841
   H    -0.464357   -3.503550    1.034310
53
Structure: R29 Stoichiometry: C17H30O2IrNP2+
   C     4.000075   -1.001520   -0.690878
   C     2.580991   -1.074153   -0.509245
   N     1.867281    0.118615   -0.504222
   C     2.482848    1.311310   -0.725368
   C     3.865621    1.410598   -0.876427
   C     4.627217    0.220850   -0.851256
   C     1.892322   -2.296756   -0.275792
   P     0.114758   -2.270441   -0.319642
   Ir   -0.273223    0.016585   -0.138760
   P    -0.090327    2.316112   -0.154979
   C     1.597172    2.529492   -0.916161
   C    -2.341118   -0.058349    0.013687
   C    -3.154962   -0.376724   -1.103886
   C    -4.555791   -0.411145   -1.022761
   C    -5.206847   -0.123672    0.185929
   C    -4.432124    0.198509    1.309169
   C    -3.031299    0.228775    1.218815
   O     2.208530   -1.735441    2.580998
   O     1.847625    0.933815    2.897401
   H     4.573897   -1.933205   -0.693358
   H     4.333116    2.384777   -1.040434
   H     5.714705    0.265776   -0.977965
   C    -0.531800   -3.121988   -1.825770
   C    -0.512525   -3.344711    1.043805
   H     2.097538    3.448210   -0.564152
   H     1.417302    2.652589   -2.002273
   H     2.104465   -1.975105    1.604254
   H     2.446640   -3.233853   -0.417587
   C    -1.219299    3.326603   -1.193930
   C    -0.002988    3.202435    1.451034
   H    -2.678777   -0.602017   -2.065093
   H    -5.143059   -0.663771   -1.914205
   H    -6.300188   -0.150293    0.251387
   H    -4.918996    0.426768    2.265260
   H    -2.460266    0.487979    2.121048
   H    -0.457666   -0.299291    1.655730
   H     1.332510    0.851793    3.720207
   H     2.105081   -0.016031    2.724632
   H     3.093636   -2.076181    2.802706
   H    -0.456601    0.091201   -1.721341
   H     0.245592    0.136472    1.683135
   H    -0.182236   -4.168511   -1.866425
   H    -1.635257   -3.100118   -1.811239
   H    -0.171417   -2.577285   -2.712707
   H    -0.220030   -4.397449    0.881420
   H    -0.071674   -2.989685    1.989656
   H    -1.612054   -3.270583    1.093923
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   H     0.259806    4.265912    1.313686
   H    -0.983777    3.125900    1.950891
   H     0.759148    2.685189    2.060026
   H    -0.914063    4.386831   -1.228090
   H    -1.236098    2.903226   -2.211211
   H    -2.234741    3.244032   -0.771496
43
Structure: R30/R31 Stoichiometry: C14H26NPtP+
   C    -0.371670    3.965513   -0.080246
   C     0.851265    3.296350   -0.201203
   C     0.925395    1.896895   -0.355788
   C    -0.277572    1.138646   -0.408500
   C    -1.512699    1.825285   -0.208760
   C    -1.556070    3.222209   -0.058509
   C     2.300038    1.254372   -0.373498
   C     2.512249    0.296882    0.812070
   N     3.668792   -0.580332    0.644359
   Pt   -0.394688   -0.907016   -0.580189
   C     0.948826   -0.995664   -2.197953
   C    -2.775537    1.000216   -0.031812
   P    -2.193452   -0.513832    0.878704
   H     1.786624    3.867899   -0.165266
   H    -2.520759    3.721548    0.090890
   H    -0.397878    5.054838    0.031002
   H    -3.184355    0.645145   -0.997077
   H    -3.569986    1.552910    0.501825
   H     2.446954    0.672460   -1.295276
   H     3.060515    2.054641   -0.364766
   H     2.556514    0.878793    1.767908
   C    -3.658920   -1.626458    1.016721
   C    -1.925307    0.088595    2.600569
   H     1.617267   -0.354039    0.874678
   C     4.942342    0.124235    0.662149
   C     3.646741   -1.684548    1.591049
   H     1.051966   -0.023366   -2.707329
   H     1.944918   -1.336996   -1.857245
   H     0.559862   -1.728398   -2.930865
   H    -0.803535   -2.614745   -1.007624
   H     5.762803   -0.589894    0.472558
   H     4.968115    0.887101   -0.133221
   H     5.149542    0.634888    1.636193
   H     4.482167   -2.375242    1.378960
   H     3.736506   -1.359002    2.657952
   H     2.699442   -2.241538    1.484813
   H    -2.852929    0.497059    3.038955
   H    -1.553950   -0.740144    3.226284
   H    -1.154347    0.875828    2.562751
   H    -4.508428   -1.112682    1.500414
   H    -3.956779   -1.952241    0.006183
   H    -3.391806   -2.518386    1.608624
   H    -0.217047   -2.694536   -0.415359
19
Structure: R32 Stoichiometry: C5H11P2Pt+
   C     1.296029   -1.408425   -0.116276
   C     2.652688   -1.257211    0.085979
   C     3.291795    0.000000    0.198525
   C     2.652689    1.257211    0.085978
   C     1.296029    1.408425   -0.116277
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   Pt   -0.150201    0.000000   -0.058773
   P    -1.823412    1.734801    0.098651
   P    -1.823413   -1.734800    0.098651
   H     0.978351   -2.450633   -0.285488
   H     3.293173   -2.147749    0.107913
   H     4.382515    0.000000    0.320252
   H     0.978352    2.450632   -0.285490
   H     3.293173    2.147748    0.107911
   H    -2.721288   -1.715301    1.194801
   H    -1.351131   -3.067269    0.187378
   H    -2.749040   -1.871269   -0.966131
   H    -2.721291    1.715299    1.194799
   H    -2.749036    1.871274   -0.966133
   H    -1.351129    3.067269    0.187384
15
Structure: R33 Stoichiometry: CH11N2Pt+
   C    -2.048474   -0.414344   -0.081640
   Pt   -0.012689   -0.191301   -0.000763
   N     2.256113   -0.059289   -0.060911
   N    -0.299445    2.054899    0.012490
   H     0.106910   -1.741889   -0.084422
   H     2.644832   -0.206304   -1.003339
   H    -0.135301   -0.630550    1.456068
   H    -2.381457   -1.411665    0.240615
   H    -2.303988   -0.272068   -1.151777
   H    -2.557705    0.352273    0.529503
   H     0.101490    2.575181   -0.780999
   H     0.086559    2.493876    0.859818
   H    -1.304358    2.280642    0.016764
   H     2.676602    0.811941    0.288439
   H     2.650321   -0.813153    0.517660
33
Structure: R34 Stoichiometry: C10H15N6BPt+
   H    -3.296353    1.591009    0.000000
   N    -1.208504    1.296987    0.000000
   B     1.310932    1.557237    0.000000
   N    -0.134761    2.128454    0.000000
   C    -0.557629    3.419371    0.000000
   Pt   -0.853151   -0.847841    0.000000
   H     0.164750    4.234951    0.000000
   C    -1.952394    3.423153    0.000000
   H    -2.613453    4.288575    0.000000
   C    -2.312933    2.060895    0.000000
   H     2.116813    2.458954    0.000000
   C    -0.466082   -2.877424    0.000000
   H    -1.388300   -3.480060    0.000000
   H     0.127896   -3.132326    0.896226
   H     0.127896   -3.132326   -0.896226
   N     1.494032    0.672003   -1.263237
   N     1.494032    0.672003    1.263237
   N     0.687550   -0.398925   -1.477011
   N     0.687550   -0.398925    1.477011
   C     2.374377    0.793408   -2.290434
   C     2.374377    0.793408    2.290434
   H     3.105994    1.600706   -2.296034
   H     3.105994    1.600706    2.296034
   C     2.129254   -0.235077   -3.200279
   C     2.129254   -0.235077    3.200279
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   C     1.055538   -0.956926   -2.641816
   C     1.055538   -0.956926    2.641816
   H     2.651398   -0.432130   -4.135407
   H     2.651398   -0.432130    4.135407
   H     0.530725   -1.837384   -3.012826
   H     0.530725   -1.837384    3.012826
   H    -1.969728   -1.159884   -1.053791
   H    -1.969728   -1.159884    1.053791
65
Structure: TS1 Stoichiometry: C24H37N3Sc+
   N     0.659374    2.204150    0.385901
   N     1.317632   -2.050054   -0.508971
   C    -0.078437    0.721676   -1.933975
   H     0.929988    1.095334   -2.168443
   H    -0.506225    0.191173   -2.797634
   C    -1.020942    1.660651   -1.326003
   C    -0.705726    2.355401   -0.107214
   C    -1.666977    3.147779    0.555895
   H    -1.399258    3.683581    1.469709
   C    -2.958806    3.266023    0.043842
   H    -3.696825    3.885674    0.561352
   C    -3.295558    2.601121   -1.153827
   H    -4.301265    2.708080   -1.572681
   C    -2.354590    1.814730   -1.810034
   H    -2.620744    1.307783   -2.743216
   C     0.874266    2.623110    1.790058
   H     0.768241    3.718243    1.900648
   H     1.899304    2.344833    2.074662
   H     0.160722    2.118614    2.455788
   C     1.647334    2.926160   -0.468216
   H     1.437225    2.744292   -1.529110
   H     2.659754    2.572627   -0.226408
   H     1.571680    4.011575   -0.274631
   C     1.650555   -0.671134    2.026807
   H     1.980736   -0.116244    2.917912
   H     1.486338   -1.721016    2.314244
   C     2.591556   -0.468471    0.894914
   C     2.411429   -1.097197   -0.383325
   C     3.269070   -0.787892   -1.461732
   H     3.125508   -1.275459   -2.427763
   C     4.313235    0.121478   -1.302550
   H     4.973647    0.343877   -2.145711
   C     4.526123    0.727822   -0.050205
   H     5.362824    1.419352    0.089889
   C     3.677263    0.442487    1.015587
   H     3.858406    0.901368    1.993374
   C     1.578853   -3.318581    0.229706
   H     0.661771   -3.926135    0.239676
   H     1.898770   -3.118812    1.259263
   H     2.380355   -3.883834   -0.279756
   C     0.975237   -2.411618   -1.908578
   H     0.814862   -1.503356   -2.501017
   H     0.045179   -2.998949   -1.894998
   H     1.771163   -3.030759   -2.363091
   Sc    0.161284   -0.074684    0.187159
   C    -1.738831   -2.415621    1.382212
   C    -2.153818   -3.314014    0.216026
   N    -1.745087   -0.978230    0.994722
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   C    -3.510515   -2.896620   -0.368897
   C    -3.497510   -1.401033   -0.714249
   C    -3.092778   -0.573962    0.502859
   C    -1.212066   -0.102821    2.055592
   H    -0.729723   -2.670259    1.746545
   H    -2.436925   -2.546533    2.235598
   H    -1.384756   -3.250346   -0.574503
   H    -2.175333   -4.361413    0.563889
   H    -3.745487   -3.504225   -1.259365
   H    -4.307706   -3.093959    0.372767
   H    -2.781617   -1.203337   -1.535395
   H    -4.489339   -1.065281   -1.062383
   H    -3.055456    0.499310    0.267415
   H    -3.820065   -0.716494    1.328791
   H    -1.729141    0.868548    2.038027
   H     0.303963   -0.237352    2.085062
   H    -1.291182   -0.550045    3.061442
60
Structure: TS2 Stoichiometry: C21H36N2Sc+
   N     1.226750    1.356420    1.448937
   C     2.118727    1.083277   -1.290791
   H     2.982888    0.794886   -0.667992
   H     2.384359    1.084273   -2.356479
   C     1.371323    2.272635   -0.855430
   C     0.866478    2.408603    0.485688
   C    -0.007574    3.457509    0.840706
   H    -0.359786    3.552380    1.870846
   C    -0.419114    4.386457   -0.112838
   H    -1.091747    5.200654    0.171550
   C     0.040990    4.266751   -1.438787
   H    -0.278571    4.991140   -2.194494
   C     0.905173    3.237030   -1.795085
   H     1.259390    3.154007   -2.827680
   C     0.272004    1.182914    2.569376
   H     0.287531    2.038186    3.269095
   H     0.549961    0.274909    3.128663
   H    -0.755328    1.075559    2.176619
   C     2.622281    1.449978    1.951323
   H     3.307362    1.609747    1.107489
   H     2.887672    0.515761    2.471710
   H     2.714463    2.299836    2.651507
   Sc    0.473187    0.046697   -0.215424
   C     1.917803   -2.574590    1.179324
   C     3.402193   -2.408418    0.853214
   N     1.061414   -2.051209    0.077471
   C     3.747253   -3.097761   -0.474168
   C     2.862580   -2.546127   -1.600133
   C     1.377445   -2.656253   -1.249409
   C    -0.379645   -2.051504    0.333504
   H     1.639582   -2.032434    2.100280
   H     1.674091   -3.644434    1.340643
   H     3.643445   -1.330376    0.788173
   H     3.996214   -2.825424    1.684499
   H     4.812361   -2.950506   -0.719538
   H     3.589958   -4.188665   -0.372957
   H     3.111108   -1.486139   -1.785734
   H     3.036833   -3.090308   -2.543970
   H     0.754308   -2.140181   -2.006197
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   H     1.048730   -3.716179   -1.235143
   H    -0.868863   -2.996943    0.057390
   H    -0.564159   -1.829772    1.401703
   C    -1.827943   -0.963722   -0.726932
   H    -1.809472   -1.683031   -1.557425
   C    -1.520578    0.396933   -1.076837
   H    -2.029313    1.202835   -0.527047
   H    -1.315286    0.627341   -2.133350
   C    -2.942466   -1.224246    0.274888
   H    -2.886835   -2.251902    0.678385
   H    -2.829176   -0.535758    1.135894
   C    -4.329784   -1.014019   -0.362613
   H    -4.433930   -1.690149   -1.233255
   H    -4.393527    0.015446   -0.761628
   C    -5.480599   -1.263269    0.623669
   H    -5.403287   -2.294045    1.020782
   H    -5.362697   -0.589171    1.494664
   C    -6.861831   -1.054935   -0.007247
   H    -7.665708   -1.238116    0.725665
   H    -6.976448   -0.022562   -0.383671
   H    -7.018492   -1.741450   -0.858476
23
Structure: TS3 Stoichiometry: C8H12TiN2+
   C     0.830237   -1.741814   -0.434738
   C     0.812253   -1.467994    0.960236
   C     1.773294   -0.449829    1.231777
   C     2.376734   -0.085419   -0.003050
   C     1.789389   -0.877013   -1.035563
   Ti    0.060952    0.505504   -0.239996
   C    -1.669878    0.541847    1.424472
   C    -2.236259   -0.191675    0.446220
   C    -3.015231   -1.047793   -0.189496
   N    -0.978701    0.568969   -1.605210
   N     0.553506    2.329364    0.097228
   H     1.993275   -0.016107    2.209381
   H     0.172356   -1.961983    1.694978
   H     3.138137    0.682940   -0.146173
   H     2.024591   -0.821965   -2.099537
   H     0.195706   -2.458306   -0.957962
   H    -1.164599    0.056189    2.267718
   H    -1.622564    0.429957   -2.393085
   H     1.327271    2.672466    0.674127
   H     0.138968    3.121765   -0.401076
   H    -1.812897    1.626997    1.473540
   H    -3.942436   -1.384002    0.295829
   H    -2.775624   -1.439243   -1.181111
22
Structure: TS4 Stoichiometry: C7H12N2Ti+
   C    -1.768316   -0.174036    1.169694
   C    -1.355487   -1.393375    0.558018
   C    -1.365623   -1.200551   -0.851879
   C    -1.791077    0.132328   -1.115206
   C    -2.041599    0.766102    0.134176
   Ti    0.300895    0.267541    0.134375
   C     1.729944   -0.886617   -1.205332
   C     2.518029   -0.713387   -0.058731
   N     0.624316    2.040367   -0.508991
   N     1.335805    0.128457    1.529043
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H	-1.888040	0.590677	-2.101431
H	-1.105135	-1.946275	-1.604548
H	-2.356720	1.800500	0.278571
H	-1.846503	0.011948	2.241803
H	-1.056170	-2.302096	1.083445
H	1.314510	-1.874446	-1.427225
H	2.737734	-1.570981	0.584198
H	1.879930	-0.137864	2.357130
H	0.045290	2.585590	-1.153319
H	1.333168	2.656430	-0.101979
H	1.816429	-0.178855	-2.036111
H	3.229743	0.114917	-0.001583

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Structure: TS5 Stoichiometry: C18H38MnO2NP2+

P	-2.223709	-0.162779	-0.113668
N	-0.015778	-1.597345	-1.260111
C	1.197968	-2.321891	-1.595807
C	-1.265033	-2.250566	-1.605692
C	-2.387825	-1.205101	-1.647966
H	-3.388354	-1.657898	-1.765766
H	-2.205153	-0.526496	-2.497908
C	2.398133	-1.363445	-1.579449
H	2.357741	-0.716528	-2.474622
P	2.228269	-0.187977	-0.138230
C	0.030872	1.176580	1.433152
O	0.050772	1.891817	2.366588
Mn	0.007277	0.064440	0.057104
C	0.024198	1.348855	-1.166737
O	0.054237	2.191691	-1.986065
C	-3.365096	1.317244	-0.332830
H	-4.349511	0.993029	0.054956
C	-2.868693	2.504421	0.511131
H	-3.615217	3.319230	0.483280
H	-2.695898	2.230858	1.564020
H	-1.918521	2.895381	0.110966
C	-3.535310	1.723083	-1.806359
H	-4.022076	0.933301	-2.402396
H	-4.168064	2.627391	-1.866213
H	-2.563379	1.964743	-2.269332
C	3.236386	1.286164	-0.721946
H	2.697770	1.553369	-1.651358
C	3.141622	2.488818	0.229609
H	3.563877	3.385216	-0.259400
H	2.097838	2.707720	0.505444
H	3.715542	2.316581	1.156896
C	4.692009	0.952023	-1.081646
H	5.173099	1.829543	-1.550942
H	5.283130	0.696501	-0.184002
H	4.764524	0.110785	-1.791903
H	1.402541	-3.185894	-0.914357
H	1.102095	-2.761491	-2.612182
H	3.364165	-1.899439	-1.583362
H	-1.550616	-3.077274	-0.901590
H	-1.177323	-2.729383	-2.604503
C	3.228340	-0.942769	1.266633
H	4.290794	-0.759774	1.016735
C	3.011832	-2.459079	1.386330
H	3.592442	-2.850060	2.241878

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   H     1.948382   -2.692844    1.569834
   H     3.334885   -3.003759    0.483604
   C     2.890939   -0.245564    2.595762
   H     3.558938   -0.614713    3.395508
   H     2.994354    0.849446    2.539704
   H     1.849668   -0.462491    2.888153
   C    -3.059816   -1.201276    1.215478
   H    -2.418548   -2.103672    1.236650
   C    -4.498814   -1.630891    0.895677
   H    -4.877006   -2.298806    1.691271
   H    -5.180750   -0.762901    0.846575
   H    -4.570552   -2.177012   -0.059912
   C    -2.959159   -0.517417    2.588482
   H    -3.292610   -1.209085    3.383332
   H    -1.924995   -0.206732    2.809152
   H    -3.604605    0.377753    2.636756
   H    -0.013843   -1.609992    0.249153
   H    -0.010036   -1.276048    1.150418
37
Structure: TS6 Stoichiometry: C10H20N2FeO2P2+
   Fe   -0.677217   -0.057983   -0.204173
   P    -0.676522   -1.702235   -1.686974
   P    -0.667784    1.860602   -1.318093
   N    -0.348365   -1.495870    1.090224
   N    -0.285503    1.043747    1.356864
   H    -0.066979   -1.782245    3.184726
   H    -0.301876    0.851876    3.483094
   H    -1.621543   -1.032369    2.675891
   C    -0.535664   -1.078237    2.470843
   H     1.172881    0.232744    2.680334
   C     0.069428    0.334649    2.575207
   H     0.663648   -3.300480    1.398951
   H     0.095015    2.964577    2.113680
   C     0.269564   -2.565717    0.675309
   C    -0.152838    2.372801    1.215258
   H     0.959431   -3.621403   -1.123494
   C     0.567253   -2.669313   -0.742465
   H     1.325648   -1.512671   -0.761778
   H     0.277387    2.005212   -2.377564
   H    -1.811418    2.321798   -2.037583
   H    -0.128428   -1.643302   -2.997120
   H    -1.804324   -2.527891   -1.972208
   C    -2.392459    0.012268    0.011681
   O    -3.551586    0.074329    0.142821
   O     1.329195   -0.224920   -0.670212
   C     2.430195    0.408215   -0.017628
   C     3.402708   -0.651683    0.514468
   C     3.104873    1.381079   -0.989289
   H     2.041947    0.991238    0.838631
   H     2.899830   -1.319728    1.235596
   H     3.796912   -1.269632   -0.313105
   H     4.258757   -0.177627    1.026531
   H     2.390741    2.162698   -1.296992
   H     3.971694    1.877194   -0.515456
   H     3.453657    0.843775   -1.889492
   C    -0.314814    3.012331   -0.008103
   H    -0.274021    4.099504   -0.110301
37
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Structure: TS7 Stoichiometry: C10H20FeN2O2P2+

Fe	0.521958	0.392868	-0.046166
P	-0.746930	2.053251	-0.701352
P	1.805084	-0.197486	-1.755845
N	-0.679780	0.356910	1.486475
N	1.374006	-1.111788	0.868753
H	-1.069488	-0.891574	3.171397
H	1.195453	-2.184584	2.698675
H	0.444431	0.065202	3.225111
C	-0.223755	-0.519472	2.560855
H	-0.149391	-2.420751	1.532969
C	0.566495	-1.676259	1.938247
H	-2.675115	0.502812	2.129219
H	2.690372	-2.733977	0.737110
C	-1.987908	0.646520	1.273683
C	2.295667	-1.840453	0.220737
H	-2.174153	2.809253	1.168935
C	-2.207062	1.943843	0.483745
H	-3.171583	1.961525	-0.050018
H	1.120823	-0.659684	-2.924135
H	2.674578	0.720335	-2.417281
H	-1.382671	2.268007	-1.960164
H	-0.309381	3.394942	-0.521359
C	1.714706	1.484548	0.537901
O	2.508213	2.235233	0.952510
O	-0.809140	-1.100346	-0.637331
C	-2.102694	-1.132244	-0.665115
C	-2.837926	-0.487359	-1.842982
C	-2.735927	-2.423221	-0.143006
H	-2.453881	-0.240731	0.423140
H	-2.364470	0.459429	-2.141306
H	-2.769746	-1.171769	-2.711078
H	-3.906538	-0.314100	-1.628943
H	-2.294435	-2.693614	0.829970
H	-3.831165	-2.336882	-0.039501
H	-2.516060	-3.244088	-0.852168
C	2.763193	-1.510580	-1.044823
H	3.578293	-2.047674	-1.535770

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Structure: TS8 Stoichiometry: C29H33OFeN3+

Fe	-0.692773	0.623479	-0.188021
O	0.279297	-0.490187	-2.693573
N	-2.117614	-1.793335	-0.594406
N	-0.715860	-1.189511	1.857881
C	0.131283	2.451889	0.150126
C	-0.864909	2.228432	1.182229
C	-2.130131	2.051720	0.540994
C	-3.465399	1.882596	1.202320
H	-3.363071	1.658365	2.273993
H	-4.049740	1.072214	0.735437
H	-4.047816	2.819287	1.096763
C	-1.945595	2.134865	-0.888913
C	-3.035666	2.023975	-1.916240
H	-3.593461	2.976012	-2.016220
H	-3.758315	1.237153	-1.642732
H	-2.624398	1.768149	-2.906071
C	-0.554247	2.437114	-1.124844
C	0.070747	2.773460	-2.448744

H	-0.443089	2.271093	-3.283412
H	1.132264	2.480075	-2.479500
H	0.014966	3.865058	-2.621270
C	-0.622740	2.204443	2.663179
H	-0.863256	3.180115	3.126734
H	0.431231	1.976269	2.890136
H	-1.244618	1.434292	3.149124
C	1.570374	2.823804	0.349435
H	2.222265	2.324696	-0.385646
H	1.918245	2.539923	1.352861
H	1.709708	3.917794	0.243942
C	-0.102057	-0.111981	-1.652490
C	-2.760365	-2.247815	-1.668337
H	-2.129874	-2.460178	-2.544336
C	-4.155428	-2.410881	-1.737775
H	-4.639512	-2.743624	-2.660258
C	-4.888556	-2.104719	-0.577056
H	-5.978576	-2.224182	-0.563623
C	-4.227994	-1.665943	0.569572
H	-4.781440	-1.470591	1.494538
C	-2.809249	-1.485344	0.542934
C	-2.108279	-0.929294	1.663598
H	-2.668385	-0.782082	2.593450
C	0.176118	-0.583011	1.026639
C	-0.080282	-2.092859	2.712503
H	-0.628160	-2.678327	3.448065
C	1.249115	-2.055214	2.393952
H	2.104564	-2.593035	2.797710
N	1.392323	-1.139110	1.345372
C	2.589674	-0.940192	0.578731
C	3.581087	-0.056964	1.047315
C	4.700156	0.168210	0.226452
H	5.475847	0.863919	0.568449
C	4.845062	-0.468397	-1.017493
C	6.027641	-0.170307	-1.911604
H	6.431829	-1.092654	-2.363886
H	6.838995	0.328078	-1.355549
H	5.731399	0.496836	-2.743060
C	3.857658	-1.386670	-1.419720
H	3.971007	-1.916032	-2.373111
C	2.726397	-1.653401	-0.633014
C	1.732856	-2.721465	-1.028499
H	1.979964	-3.668695	-0.511763
H	1.769749	-2.904885	-2.113269
H	0.697766	-2.459449	-0.755835
C	3.474659	0.588392	2.409185
H	3.911414	-0.068452	3.185375
H	2.425074	0.766207	2.691850
H	4.021625	1.544704	2.439700

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Structure: TS9 Stoichiometry: C29H33FeON3+

Fe	-0.762217	0.903257	-0.162727
O	-0.515419	-0.466432	-2.706539
N	-2.228957	-2.081512	-0.592162
N	-1.054064	-0.799987	1.995372
C	0.435250	2.398627	0.780622
C	-0.961770	2.649809	1.018271
C	-1.599496	2.827969	-0.262778

C	-3.036996	3.195457	-0.497842
H	-3.693444	2.784118	0.286637
H	-3.394100	2.814692	-1.468290
H	-3.166448	4.294970	-0.496209
C	-0.594011	2.664823	-1.280810
C	-0.794008	2.865779	-2.756796
H	-0.585017	3.917046	-3.032162
H	-1.828941	2.636637	-3.057810
H	-0.124326	2.221623	-3.348255
C	0.675122	2.394748	-0.630976
C	2.001440	2.205877	-1.312204
H	1.875939	1.741084	-2.303607
H	2.659769	1.546895	-0.722817
H	2.521599	3.173195	-1.455508
C	-1.601315	2.733730	2.374719
H	-1.240442	3.617716	2.933397
H	-1.374037	1.832263	2.970977
H	-2.697547	2.818415	2.297183
C	1.471660	2.281661	1.854128
H	2.383506	1.801342	1.472666
H	1.099769	1.702059	2.713442
H	1.746370	3.289512	2.220668
C	-0.621602	-0.025193	-1.627172
C	-2.836518	-3.181690	-1.036241
H	-2.195514	-3.915597	-1.544909
C	-4.214715	-3.423654	-0.890668
H	-4.663318	-4.339828	-1.287737
C	-4.983120	-2.462223	-0.224205
H	-6.059454	-2.606421	-0.079898
C	-4.347447	-1.316536	0.268091
H	-4.911688	-0.551301	0.811284
C	-2.959857	-1.143869	0.055943
C	-2.293549	0.093394	0.503349
H	-2.946306	0.676213	1.175552
C	-0.109025	-0.437479	1.096294
C	-0.604014	-1.881511	2.727733
H	-1.201535	-2.354008	3.508113
C	0.674289	-2.180302	2.314793
H	1.404698	-2.913416	2.654804
N	0.981212	-1.274097	1.293498
C	2.216277	-1.239509	0.564949
C	3.367909	-0.685253	1.168225
C	4.523619	-0.539929	0.380441
H	5.416875	-0.091357	0.832269
C	4.564000	-0.954979	-0.961322
C	5.789721	-0.715950	-1.813508
H	5.690264	0.227148	-2.384335
H	5.935774	-1.527609	-2.546618
H	6.701189	-0.634515	-1.197438
C	3.433217	-1.601728	-1.488883
H	3.466681	-1.994426	-2.512296
C	2.257774	-1.781133	-0.739960
C	1.133668	-2.636626	-1.272796
H	1.340594	-3.693972	-1.015324
H	1.066568	-2.562924	-2.369126
H	0.154067	-2.371911	-0.845360
C	3.409421	-0.339303	2.640242
H	3.845842	-1.182653	3.208621

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   H     2.407126   -0.152527    3.051148
   H     4.043632    0.543424    2.827362
59
Structure: TS10 Stoichiometry: C16H36NaN4NbO+
   N     0.190059   -0.153267    1.622436
   C    -0.391602   -0.357383    3.230049
   O    -0.539957   -1.549162    3.437526
   Na   -0.249710   -2.503738    1.414104
   Nb    0.119614    0.102431   -0.132259
   N    -1.031647   -1.536946   -0.819780
   N     1.983073   -0.253510   -0.835923
   N    -0.545957    1.976170   -0.519854
   C    -2.507024   -1.666162   -0.625191
   C     3.239180   -0.644926   -0.132347
   C    -0.744328    3.180213    0.335950
   C    -2.888751   -3.116990   -0.239528
   C    -3.277305   -1.272895   -1.908003
   C    -2.941496   -0.717597    0.506910
   C     4.283973   -1.203831   -1.123742
   C     3.809850    0.588433    0.602379
   C     2.922929   -1.749055    0.895699
   C    -2.208587    3.230287    0.827339
   C    -0.408813    4.465980   -0.452833
   C     0.194756    3.092168    1.551157
   H    -2.509807   -3.847696   -0.975147
   H    -3.984343   -3.238543   -0.180756
   H    -2.491635   -3.389177    0.759254
   H    -2.996835   -0.252909   -2.222056
   H    -4.365464   -1.289814   -1.722449
   H    -3.069928   -1.963112   -2.743129
   H    -2.472381   -0.972621    1.472288
   H    -4.035941   -0.754902    0.643946
   H    -2.662431    0.325557    0.268356
   H     3.867143   -2.048088   -1.701781
   H     5.161420   -1.571655   -0.564944
   H     4.640225   -0.437312   -1.832053
   H     4.001768    1.410673   -0.109733
   H     4.760733    0.349205    1.111795
   H     3.080338    0.938698    1.352119
   H     2.212199   -1.367559    1.647059
   H     3.843422   -2.073318    1.411204
   H     2.490981   -2.629560    0.379357
   H    -2.917424    3.210107   -0.020346
   H    -2.400081    4.153207    1.403415
   H    -2.414346    2.365812    1.480575
   H    -1.118243    4.650409   -1.278368
   H     0.610975    4.406327   -0.873230
   H    -0.452290    5.338011    0.222143
   H     0.059418    3.979573    2.194486
   H     1.247987    3.060783    1.218998
   H    -0.007879    2.186695    2.145030
   C     2.167766    0.337477   -2.163943
   H     1.199530    0.718288   -2.540350
   H     2.866843    1.199310   -2.157973
   H     2.529199   -0.396594   -2.911154
   C    -1.054174    2.080524   -1.887609
   H    -0.993832    1.088651   -2.383181
   H    -2.124899    2.373355   -1.923841
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H	-0.484166	2.793808	-2.516869
C	-0.523669	-2.191649	-2.035545
H	-0.800267	-1.668987	-2.976974
H	0.577350	-2.230633	-1.989363
H	-0.889988	-3.235947	-2.131668

54

Structure: TS11 Stoichiometry: C24H25FN3Nb+

C	2.603904	-0.976192	2.880151
H	3.456602	-1.319044	2.271737
H	2.339020	-1.753401	3.614851
H	2.930492	-0.082541	3.440311
C	1.406766	-0.667685	2.002358
C	0.116187	-0.873087	2.540047
H	0.069768	-1.352352	3.521582
C	-1.062479	-0.200522	2.109910
C	-2.171936	-0.014126	3.124591
H	-2.541040	1.025086	3.114357
H	-1.817481	-0.260986	4.136350
H	-3.029503	-0.668053	2.886214
C	-2.156273	1.282167	0.530500
C	-3.530800	0.983273	0.501963
C	-4.455339	1.959081	0.104249
H	-5.522505	1.712691	0.083560
C	-4.021994	3.238915	-0.269817
H	-4.747084	3.997340	-0.582483
C	-2.650889	3.539035	-0.241512
H	-2.300669	4.536796	-0.527416
C	-1.722510	2.568460	0.153163
C	2.806956	0.441372	0.380261
C	3.537945	-0.028693	-0.730049
C	4.695470	0.644587	-1.140690
H	5.258120	0.268893	-2.002179
C	5.141507	1.784333	-0.453726
H	6.048479	2.304818	-0.778492
C	4.414001	2.255021	0.649885
H	4.746617	3.150507	1.186257
C	3.250935	1.593349	1.062371
C	0.218667	1.816488	-2.842965
C	-2.797909	-2.189125	-0.552914
H	-3.862003	-1.975801	-0.384690
C	-2.181246	-3.173980	0.189379
H	-2.719459	-3.806648	0.901531
C	-0.722779	-3.230568	0.055683
H	-0.051406	-3.438466	0.898701
C	-0.287181	-2.851949	-1.175144
C	-0.901807	-2.056394	-2.151134
H	-0.673335	-2.119753	-3.221661
C	-2.059448	-1.388868	-1.522990
H	-2.596392	-0.625393	-2.096490
N	-1.163351	0.315821	0.877815
N	1.589523	-0.185210	0.761261
N	0.177508	0.800591	-1.845826
Nb	0.025488	-0.551260	-0.715611
H	-0.503783	2.623852	-2.605410
H	1.230118	2.264429	-2.907531
H	-0.040525	1.410153	-3.840896
H	-0.649849	2.782209	0.168176
H	-3.869996	-0.017279	0.778299

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   H     3.189693   -0.928369   -1.245672
   H     2.659543    1.975478    1.901079
   F     1.434146   -2.261141   -1.016021
57
Structure: TS12 Stoichiometry: C16H35SiP2ONMo+
   Mo    0.565778    0.056033   -0.215742
   Si    0.788342   -0.313147    2.255605
   P    -0.340175    2.434815    0.000808
   P     0.967626   -2.409319   -0.483099
   N    -1.189088   -0.360326   -0.287505
   H     1.655073    1.084630    0.705276
   C    -0.963779    3.341219   -1.497154
   H    -1.420862    4.310340   -1.228326
   H    -1.720337    2.705447   -1.987185
   H    -0.140609    3.512136   -2.210498
   C     0.681045    3.717371    0.860761
   H     0.094945    4.639771    1.017268
   H     1.583393    3.955565    0.279139
   H     0.988983    3.308312    1.837675
   C    -1.851075    2.477381    1.066116
   H    -2.155751    3.521934    1.254012
   H    -1.626872    1.975171    2.021126
   H    -2.674433    1.938996    0.573135
   C     0.858939   -2.884456   -2.266179
   H     1.046605   -3.962041   -2.419662
   H     1.598605   -2.288835   -2.825658
   H    -0.148890   -2.629256   -2.633823
   C     2.581219   -3.154715    0.020982
   H     2.618722   -4.232900   -0.214823
   H     2.723695   -3.011922    1.104947
   H     3.391463   -2.634666   -0.515472
   C    -0.274663   -3.508217    0.316808
   H    -0.101622   -4.567840    0.060223
   H    -1.278440   -3.201091   -0.019812
   H    -0.221894   -3.371847    1.409201
   C     2.535508   -0.383923    3.043974
   H     3.079654    0.567073    2.903042
   H     3.156869   -1.189689    2.612324
   H     2.450323   -0.572866    4.129984
   H     0.067462    0.743759    3.061385
   H     0.130763   -1.587015    2.746138
   C    -2.543490   -0.463120   -0.174800
   C    -4.784641   -0.268876   -1.136846
   C    -3.396941   -0.167979   -1.273393
   C    -3.132045   -0.886280    1.049689
   C    -4.518993   -1.005527    1.160654
   C    -5.355856   -0.691573    0.075219
   H    -5.429271   -0.025565   -1.988980
   H    -2.941559    0.144804   -2.218419
   H    -2.469998   -1.109797    1.891757
   H    -4.956259   -1.336715    2.109283
   H    -6.442829   -0.777889    0.172751
   C     2.674969    0.936817   -0.848918
   O     2.091073   -0.012972   -1.596387
   C     2.772349    2.304941   -1.503996
   H     3.565021    2.262742   -2.278626
   H     3.056263    3.091394   -0.786162
   H     1.829641    2.579828   -2.000436
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   C     3.933250    0.508973   -0.105777
   H     3.782880   -0.453313    0.404159
   H     4.233965    1.259203    0.644378
   H     4.764312    0.394193   -0.831477
50
Structure: TS13 Stoichiometry: C20H25OP2NRu+
   C    -3.945632    0.816431   -0.926819
   C    -2.612687    0.429938   -1.142957
   C    -1.577556    1.240553   -0.612811
   C    -1.897842    2.281260    0.306204
   C    -3.243689    2.638888    0.520474
   C    -4.261448    1.939900   -0.138371
   C    -0.757978    2.710358    1.095586
   C     0.484673    2.868341    0.389695
   C     0.723161    1.823565   -0.557792
   C     2.033563    1.613714   -1.079692
   C     3.033617    2.531683   -0.757709
   C     2.780757    3.617452    0.116091
   C     1.533970    3.758609    0.719927
   H    -4.751438    0.210786   -1.357838
   H    -3.485229    3.447764    1.218736
   H    -5.307936    2.228552    0.003304
   H    -0.934055    3.298723    2.004346
   H     4.040836    2.392610   -1.167807
   H     3.585237    4.323864    0.344960
   H     1.356135    4.552747    1.453126
   N    -0.249751    0.864471   -0.769379
   Ru    0.334534   -0.639923    0.718187
   C    -2.222734   -0.916218   -1.682713
   H    -1.407692   -0.843762   -2.424691
   H    -3.078027   -1.463052   -2.116380
   C     2.297244    0.313240   -1.784995
   H     1.536274    0.119476   -2.561386
   H     3.303247    0.278751   -2.238183
   P    -1.497821   -1.866880   -0.219695
   P     2.114470   -1.113633   -0.561570
   C     3.745319   -1.163325    0.292733
   H     3.727344   -1.954072    1.060902
   H     4.568864   -1.351275   -0.418372
   H     3.891244   -0.193046    0.794403
   C     2.201161   -2.582566   -1.684387
   H     3.142587   -2.587536   -2.262570
   H     2.133057   -3.504947   -1.084550
   H     1.347999   -2.548619   -2.381471
   C    -2.970078   -2.059375    0.885143
   H    -3.822847   -2.528053    0.361645
   H    -2.681347   -2.678442    1.751326
   H    -3.264330   -1.062054    1.249673
   C    -1.313792   -3.585947   -0.884421
   H    -0.922871   -4.237183   -0.084563
   H    -2.279603   -3.984810   -1.241744
   H    -0.591012   -3.586440   -1.715663
   C     0.744662   -1.870635    2.020555
   O     0.988431   -2.666480    2.848900
   H    -0.320423    1.008414    1.593242
   H     1.437410    0.371257    1.370308
39
Structure: TS14 Stoichiometry: C12H21PO2N2Ru+
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   C    -2.227181    1.312218   -0.848319
   C    -2.310200   -0.144410   -0.465694
   N    -1.101931   -0.679080   -0.198515
   C    -0.943813   -1.972798    0.229447
   C    -2.093539   -2.797484    0.294143
   C    -3.344820   -2.264512   -0.018309
   C    -3.475524   -0.910328   -0.386174
   C     0.401119   -2.287107    0.702608
   P     1.677895   -1.340138   -0.217824
   H    -4.451493   -0.467408   -0.601946
   H    -1.990277   -3.839070    0.611245
   H    -4.235092   -2.900053    0.040051
   C    -0.895438    3.333809   -0.620798
   C    -1.650421    2.161843    1.372508
   H     0.592249   -3.337934    0.968036
   H    -3.208826    1.817136   -0.745531
   H    -1.895905    1.386030   -1.899111
   C     2.051577   -2.165374   -1.826980
   C     3.223086   -1.607469    0.752346
   H     2.823782   -1.585827   -2.361785
   H     2.398188   -3.203522   -1.679539
   H     1.131139   -2.161660   -2.432600
   H     4.049117   -1.049511    0.280638
   H     3.066432   -1.213548    1.769243
   H     3.486441   -2.678278    0.809866
   H    -2.603697    2.729092    1.406233
   H    -1.769820    1.167833    1.826472
   H    -0.878157    2.701873    1.939219
   H    -1.807585    3.966347   -0.642469
   H    -0.122527    3.831660   -0.017398
   H    -0.511792    3.189274   -1.641137
   C     2.010105    1.740750   -0.081016
   O     2.948076    2.449527   -0.071301
   Ru    0.550459    0.613142   -0.125828
   H     0.532911    0.845427   -1.725800
   O     0.305356   -0.034161    2.026605
   H     1.103509    0.186815    2.539802
   H     0.408827   -1.286900    1.674120
   N    -1.184244    2.008835   -0.027029
19
Structure: TS15 Stoichiometry: C5H11P2Rh+
   C    -1.329395   -0.436375   -1.085218
   C    -2.653197    0.018657   -0.902920
   C    -3.157293   -0.110014    0.390965
   C    -2.276406   -0.810406    1.262305
   C    -1.031182   -1.140189    0.754207
   Rh    0.468506   -0.192942   -0.318824
   P     2.711684   -0.488577    0.241439
   P     0.134513    1.865313    0.321508
   H     0.797202    2.395204    1.467965
   H     0.351564    2.990575   -0.531306
   H    -1.212924    2.140958    0.690452
   H     3.758770   -0.258424   -0.705676
   H     3.279313    0.328363    1.264400
   H     3.267035   -1.712745    0.734777
   H    -4.146452    0.247795    0.695235
   H    -2.572593   -1.100495    2.277777
   H    -3.247387    0.395701   -1.742963
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   H    -0.988948   -0.722699   -2.107542
   H    -0.376474   -1.802912    1.343720
21
Structure: TS16 Stoichiometry: C10H10Pd+
   Pd   -0.142441   -0.098738   -0.084795
   C     1.496898    1.172074   -0.450009
   C     2.770242    1.203267    0.027931
   C     3.359952   -0.036111    0.525583
   C     2.656659   -1.140143    0.156006
   C     1.458688   -0.930162   -0.651077
   H     1.450763   -1.385856   -1.662774
   H     2.929203   -2.168183    0.426535
   H     4.282695   -0.066573    1.112078
   H     3.360202    2.128510   -0.011275
   H     1.107483    2.006835   -1.048532
   C    -2.142905    1.269991    0.262983
   C    -2.534032    0.471925   -0.888690
   C    -2.432049   -0.875884   -0.532006
   C    -1.978207   -0.933614    0.855435
   C    -1.907196    0.411452    1.361375
   H    -2.803477    0.866620   -1.870229
   H    -2.104097    2.361462    0.288410
   H    -1.644327    0.706442    2.377757
   H    -1.879607   -1.844174    1.450559
   H    -2.634830   -1.739893   -1.167142
92
Structure: TS17 Stoichiometry: C31H55PdP3NBr+
   C     7.527451   -0.426880   -1.340856
   C     6.988783   -0.000163   -0.101875
   C     7.911379    0.573911    0.805097
   C     9.259306    0.691933    0.449887
   N     9.763686    0.287641   -0.728188
   C     8.890879   -0.261712   -1.594315
   C     5.581623   -0.117483    0.267801
   C     4.585827   -0.632237   -0.507953
   C     3.176044   -0.746902   -0.167566
   C     2.272136   -1.264563   -1.120544
   C     0.898451   -1.356072   -0.858501
   C     0.360738   -0.886788    0.361445
   C     1.276867   -0.464682    1.359262
   C     2.638124   -0.376334    1.096455
   Pd   -1.287536    0.187810   -0.197038
   P    -1.784887    1.946935   -1.789825
   P    -1.285429    1.421837    1.810691
   P    -2.572480   -1.695049   -0.903667
   Br   -0.550476   -3.030075    2.031000
   C    -3.630820   -2.012434    0.592139
   C    -3.825179   -1.459236   -2.269918
   C    -1.851150   -3.363579   -1.296654
   H     0.917136   -0.219984    2.360602
   H     3.305235   -0.025654    1.891126
   H     2.653741   -1.604057   -2.091406
   H     0.247659   -1.785151   -1.620113
   H     6.889987   -0.886462   -2.102894
   H     9.309602   -0.592646   -2.555158
   H     9.974140    1.138049    1.155749
   H     7.568751    0.924921    1.785304
   C    -1.535919    0.247299    3.225971
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C	0.152780	2.538909	2.256050
H	-4.349460	-2.419087	-2.435683
H	-3.260038	-1.242985	-3.193874
H	-2.626567	-4.107306	-1.039996
H	-1.036874	-3.502812	-0.560103
H	-2.889889	-2.256430	1.380290
H	-4.085329	-1.039132	0.848070
H	0.906583	1.889564	2.730711
H	0.598085	2.847873	1.295124
H	-2.596367	-0.051533	3.138816
H	-0.978095	-0.683763	2.993017
H	4.843867	-0.999833	-1.510188
H	5.334902	0.257519	1.269116
C	-3.164012	3.164033	-2.197309
C	-3.535909	4.210840	-1.145427
H	-4.047593	2.555004	-2.459235
H	-2.840100	3.665446	-3.129578
H	-4.274862	4.916376	-1.564030
H	-3.986904	3.749158	-0.254869
H	-2.661386	4.803158	-0.825191
C	-0.362306	3.141084	-1.573165
C	1.023139	2.488546	-1.475267
H	-0.584688	3.693432	-0.640717
H	-0.399912	3.877399	-2.399204
H	1.779688	3.235792	-1.179636
H	1.033297	1.671433	-0.731341
H	1.338430	2.059664	-2.439988
C	-1.562991	1.336627	-3.548038
C	-0.604211	0.164144	-3.753626
H	-1.260530	2.211690	-4.155025
H	-2.578674	1.055707	-3.884794
H	-0.600910	-0.148149	-4.812588
H	0.428267	0.414531	-3.464095
H	-0.912346	-0.695384	-3.138204
C	-2.758524	2.548367	1.973137
C	-4.075322	1.862917	1.593912
H	-2.570716	3.416203	1.317610
H	-2.800334	2.930669	3.009059
H	-4.917664	2.575473	1.640640
H	-4.018778	1.449575	0.571819
H	-4.307411	1.029966	2.279003
C	-1.229865	0.754193	4.638372
H	-1.846467	1.627045	4.919639
H	-1.432327	-0.048271	5.369055
H	-0.167978	1.035339	4.748993
C	-0.129607	3.767703	3.130594
H	-0.564925	3.493325	4.105208
H	0.812980	4.309511	3.325929
H	-0.818914	4.473190	2.636516
C	-4.825335	-0.337551	-1.975697
H	-5.443540	-0.109756	-2.861871
H	-5.504864	-0.608641	-1.150157
H	-4.296422	0.584369	-1.676741
C	-4.695928	-3.108611	0.480941
H	-4.239646	-4.098301	0.311256
H	-5.262897	-3.171910	1.426583
H	-5.421693	-2.919412	-0.330642
C	-1.387504	-3.580202	-2.742100

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   H    -0.959981   -4.592711   -2.845904
   H    -2.217322   -3.493595   -3.465225
   H    -0.604157   -2.864897   -3.046245
92
Structure: TS18 Stoichiometry: C31H55PdINP3+
   C     7.465659   -0.096133   -1.367134
   C     6.914366   -0.059898   -0.062407
   C     7.827294    0.214573    0.983917
   C     9.178284    0.432227    0.693466
   N     9.694556    0.399510   -0.546741
   C     8.831110    0.136085   -1.546172
   C     5.504146   -0.280681    0.241407
   C     4.515860   -0.534940   -0.663027
   C     3.103524   -0.743036   -0.386241
   C     2.206053   -0.932637   -1.460750
   C     0.828569   -1.085694   -1.254049
   C     0.279073   -1.009349    0.049237
   C     1.190889   -0.927965    1.137602
   C     2.555596   -0.777617    0.926847
   Pd   -1.170645    0.434495   -0.165382
   P    -1.251222    2.697345   -1.040993
   P    -1.260477    0.889608    2.157662
   P    -2.665451   -0.816782   -1.549352
   I    -0.882946   -3.608095    0.789875
   C    -3.873467   -1.533029   -0.327549
   C    -3.762806    0.125552   -2.732029
   C    -2.164957   -2.292233   -2.569731
   H     0.819895   -0.996958    2.162318
   H     3.215812   -0.692854    1.796466
   H     2.597570   -0.962361   -2.485052
   H     0.184959   -1.269999   -2.113985
   H     6.836495   -0.305812   -2.238038
   H     9.259635    0.107956   -2.557909
   H     9.885582    0.645164    1.507480
   H     7.474737    0.255706    2.020956
   C    -1.754465   -0.642926    3.080370
   C     0.244635    1.554939    3.069859
   H    -4.378406   -0.596406   -3.300805
   H    -3.092885    0.617025   -3.460050
   H    -3.057986   -2.935998   -2.658953
   H    -1.443669   -2.851624   -1.944035
   H    -3.242381   -2.148899    0.342523
   H    -4.234560   -0.674231    0.264855
   H     0.745248    0.677825    3.513930
   H     0.933505    1.926385    2.292741
   H    -2.773880   -0.868680    2.719373
   H    -1.142611   -1.476946    2.685836
   H     4.783494   -0.581827   -1.727133
   H     5.247554   -0.224615    1.306866
   C    -2.453716    4.144356   -1.105209
   C    -2.936706    4.734835    0.220111
   H    -3.314450    3.803835   -1.707642
   H    -1.939661    4.921963   -1.702415
   H    -3.554661    5.630081    0.030961
   H    -3.554378    4.017215    0.780228
   H    -2.095438    5.046423    0.863281
   C     0.221959    3.540165   -0.258000
   C     1.526640    2.737756   -0.339776
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   H    -0.057601    3.701466    0.800157
   H     0.337428    4.540591   -0.718032
   H     2.305795    3.199695    0.290742
   H     1.380332    1.696193   -0.000723
   H     1.913803    2.699593   -1.370856
   C    -0.836026    2.738160   -2.869141
   C    -0.012469    1.570747   -3.411211
   H    -0.336245    3.706813   -3.063476
   H    -1.813657    2.779573   -3.385534
   H     0.133230    1.676635   -4.500650
   H     0.977181    1.501946   -2.933758
   H    -0.528776    0.617444   -3.219323
   C    -2.614317    2.076438    2.634009
   C    -3.965985    1.704114    2.017289
   H    -2.296922    3.075263    2.290521
   H    -2.686604    2.124425    3.734932
   H    -4.727498    2.470242    2.246421
   H    -3.879197    1.611171    0.920911
   H    -4.336282    0.740911    2.407328
   C    -1.713325   -0.585728    4.610479
   H    -2.373258    0.200144    5.020110
   H    -2.045246   -1.552085    5.028748
   H    -0.691306   -0.401264    4.984940
   C     0.015106    2.627294    4.142075
   H    -0.636089    2.265870    4.955406
   H     0.981049    2.919020    4.591465
   H    -0.442088    3.539239    3.721429
   C    -4.647832    1.162250   -2.033979
   H    -5.155920    1.811717   -2.768447
   H    -5.424506    0.680511   -1.416359
   H    -4.043978    1.801939   -1.367371
   C    -5.044177   -2.353156   -0.880350
   H    -4.693947   -3.269924   -1.383557
   H    -5.701598   -2.669779   -0.051367
   H    -5.661971   -1.781332   -1.596130
   C    -1.603897   -1.991198   -3.964715
   H    -1.322751   -2.934785   -4.463837
   H    -2.339977   -1.479623   -4.608976
   H    -0.699441   -1.360477   -3.926119
90
Structure: TS19 Stoichiometry: C31H53NPdBrP3+
   C     7.865018   -0.343239   -1.424317
   C     7.198029   -0.028250   -0.213285
   C     7.994881    0.495840    0.836006
   C     9.365345    0.672367    0.625166
   N     9.998028    0.375573   -0.524128
   C     9.242174   -0.123399   -1.518548
   C     5.800395   -0.226235   -0.059390
   C     4.589231   -0.397592    0.073100
   C     3.190374   -0.581755    0.223591
   C     2.404791   -1.108666   -0.828018
   C     1.020097   -1.254604   -0.684334
   C     0.356782   -0.836472    0.494207
   C     1.158063   -0.401435    1.579226
   C     2.534394   -0.257147    1.445368
   Pd   -1.269086    0.194801   -0.201591
   P    -1.674967    1.963244   -1.807134
   P    -1.518675    1.373096    1.825012
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P	-2.413918	-1.716101	-1.062530
Br	-0.608127	-3.064051	2.001554
C	-3.585217	-2.111937	0.326438
C	-3.551569	-1.485374	-2.526338
C	-1.601266	-3.347867	-1.431996
H	0.699703	-0.190924	2.547732
H	3.130303	0.103670	2.289786
H	2.889525	-1.408642	-1.762732
H	0.454931	-1.689568	-1.508459
H	7.303899	-0.753252	-2.269199
H	9.769258	-0.364159	-2.452380
H	9.992429	1.077551	1.431618
H	7.537440	0.755382	1.795239
C	-1.834524	0.138033	3.174860
C	-0.192956	2.556206	2.416082
H	-4.026321	-2.456889	-2.759582
H	-2.916855	-1.226656	-3.392210
H	-2.370936	-4.123103	-1.267870
H	-0.853423	-3.483148	-0.627348
H	-2.906988	-2.353153	1.169843
H	-4.094716	-1.162310	0.566603
H	0.599067	1.930799	2.859810
H	0.249593	2.978482	1.497659
H	-2.877363	-0.183187	2.998383
H	-1.234592	-0.767702	2.946219
C	-3.053732	3.143975	-2.308482
C	-3.556507	4.146026	-1.267509
H	-3.887457	2.513588	-2.665853
H	-2.664903	3.682739	-3.193921
H	-4.280295	4.838156	-1.732345
H	-4.068101	3.642476	-0.434291
H	-2.736632	4.757926	-0.853272
C	-0.317507	3.198639	-1.450781
C	1.072225	2.592812	-1.214300
H	-0.649992	3.741956	-0.546322
H	-0.297375	3.934937	-2.277430
H	1.772344	3.367494	-0.856873
H	1.038183	1.783865	-0.462603
H	1.492260	2.165689	-2.138899
C	-1.283594	1.395567	-3.549929
C	-0.267271	0.262840	-3.693614
H	-0.962333	2.293238	-4.112614
H	-2.255696	1.086550	-3.978508
H	-0.148615	-0.013337	-4.755949
H	0.722149	0.538079	-3.296108
H	-0.602477	-0.627763	-3.139571
C	-3.056196	2.421289	1.884089
C	-4.294627	1.696257	1.347646
H	-2.848621	3.327082	1.288265
H	-3.216313	2.751736	2.926591
H	-5.170697	2.368434	1.336554
H	-4.117493	1.330004	0.321336
H	-4.553035	0.825186	1.973394
C	-1.644975	0.584806	4.627341
H	-2.306848	1.425017	4.904603
H	-1.872874	-0.258599	5.302266
H	-0.602559	0.888942	4.826383
C	-0.598848	3.685624	3.372602

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   H    -1.048492    3.302379    4.302392
   H     0.292658    4.275883    3.650017
   H    -1.320006    4.377708    2.905814
   C    -4.610571   -0.403938   -2.294330
   H    -5.155447   -0.170653   -3.226009
   H    -5.350995   -0.718149   -1.539466
   H    -4.140062    0.524851   -1.926809
   C    -4.596565   -3.239631    0.094801
   H    -4.092147   -4.208073   -0.060570
   H    -5.239610   -3.349435    0.985939
   H    -5.256731   -3.051357   -0.771163
   C    -0.999273   -3.507946   -2.833034
   H    -0.538973   -4.507032   -2.925802
   H    -1.759283   -3.416397   -3.628649
   H    -0.208485   -2.766751   -3.040062
90
Structure: TS20 Stoichiometry: C31H53P3NIPd+
   C     7.797524   -0.026792   -1.412892
   C     7.116273   -0.091699   -0.170833
   C     7.899479    0.094798    0.996566
   C     9.270924    0.329943    0.864171
   N     9.917013    0.393735   -0.313873
   C     9.174241    0.214561   -1.420861
   C     5.718320   -0.328929   -0.099600
   C     4.506190   -0.532398   -0.038610
   C     3.106257   -0.747868    0.033756
   C     2.330596   -0.920358   -1.137753
   C     0.942373   -1.082421   -1.063682
   C     0.263155   -1.029807    0.180942
   C     1.057160   -0.961794    1.357669
   C     2.436645   -0.804473    1.290016
   Pd   -1.142168    0.437240   -0.161635
   P    -1.108235    2.715766   -1.001587
   P    -1.486528    0.848419    2.149297
   P    -2.495467   -0.769379   -1.721006
   I    -0.974539   -3.619753    0.723781
   C    -3.823987   -1.500799   -0.641819
   C    -3.463342    0.208165   -2.985610
   C    -1.908242   -2.226428   -2.721742
   H     0.584133   -1.045957    2.338414
   H     3.022697   -0.721865    2.210832
   H     2.827675   -0.931672   -2.113133
   H     0.386723   -1.258898   -1.984434
   H     7.247530   -0.165533   -2.348334
   H     9.712234    0.266648   -2.377759
   H     9.887393    0.475729    1.762221
   H     7.430865    0.053078    1.984207
   C    -2.082661   -0.701275    2.978787
   C    -0.089950    1.487548    3.235064
   H    -4.024367   -0.496122   -3.628316
   H    -2.721387    0.708463   -3.633496
   H    -2.795823   -2.851872   -2.924355
   H    -1.266734   -2.814200   -2.037922
   H    -3.266383   -2.127744    0.080869
   H    -4.242502   -0.649198   -0.077681
   H     0.368354    0.597488    3.698517
   H     0.673035    1.887980    2.546927
   H    -3.059993   -0.910700    2.508170
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H	-1.436927	-1.530201	2.630421
C	-2.288120	4.172937	-1.165038
C	-2.912344	4.736506	0.112272
H	-3.078137	3.853679	-1.867535
H	-1.706266	4.959746	-1.682744
H	-3.497708	5.642831	-0.122286
H	-3.595089	4.012383	0.581233
H	-2.146198	5.023073	0.853511
C	0.279118	3.533298	-0.053682
C	1.574633	2.714238	0.001644
H	-0.114156	3.690521	0.968353
H	0.456319	4.535585	-0.489363
H	2.284901	3.159949	0.719082
H	1.377922	1.672154	0.312549
H	2.073518	2.678333	-0.980198
C	-0.505373	2.784809	-2.775695
C	0.368985	1.624948	-3.250100
H	0.012275	3.755428	-2.901020
H	-1.424549	2.837187	-3.389282
H	0.619474	1.745279	-4.318745
H	1.308341	1.551162	-2.680702
H	-0.161922	0.668984	-3.121864
C	-2.881124	2.031868	2.500392
C	-4.156712	1.680852	1.728986
H	-2.524655	3.036442	2.217213
H	-3.074746	2.054969	3.587451
H	-4.936493	2.446407	1.887611
H	-3.947142	1.610538	0.647681
H	-4.571441	0.711693	2.054269
C	-2.202352	-0.681519	4.505689
H	-2.894692	0.101937	4.863001
H	-2.585358	-1.653699	4.862258
H	-1.223955	-0.518245	4.990011
C	-0.436392	2.521341	4.313805
H	-1.170360	2.132094	5.038971
H	0.474996	2.795429	4.874434
H	-0.847585	3.448254	3.878897
C	-4.406288	1.237554	-2.355926
H	-4.828880	1.911901	-3.121441
H	-5.247709	0.749706	-1.835605
H	-3.868922	1.852125	-1.613107
C	-4.933012	-2.309023	-1.323839
H	-4.535784	-3.224682	-1.792689
H	-5.678331	-2.626560	-0.573284
H	-5.466041	-1.727983	-2.098001
C	-1.195940	-1.900130	-4.039961
H	-0.884324	-2.836088	-4.535306
H	-1.848503	-1.352582	-4.742051
H	-0.286901	-1.293680	-3.887769

45

Structure: TS21 Stoichiometry: C11H29TaN4+

Ta	0.032043	0.000087	0.092918
N	-0.123168	-1.672246	-1.067243
N	-2.021119	-0.000619	0.378901
N	2.111084	0.000301	-0.033028
N	-0.123733	1.673432	-1.065589
C	0.016615	-1.265593	2.262149
H	-1.056415	-1.435538	2.397125

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   H     0.654246   -2.149541    2.377192
   C     0.592042   -0.001143    2.494674
   H     1.679555   -0.000984    2.625445
   C     0.016081    1.263311    2.263274
   H    -1.056994    1.432692    2.398633
   H     0.653370    2.147391    2.379227
   H    -3.179590   -1.232334    1.674218
   C    -2.822740   -1.193476    0.620918
   H    -2.233393   -2.101363    0.425573
   H    -3.725683   -1.202259   -0.025684
   H    -3.726447    1.200535   -0.023871
   C    -2.823310    1.191549    0.622457
   H    -3.179877    1.229066    1.675903
   H    -2.234538    2.099990    0.427933
   H     4.204084   -0.000760    0.335767
   C     3.245438   -0.000823    0.887459
   H     3.250455   -0.896128    1.541415
   H     3.251130    0.893483    1.542777
   H     3.190616    0.898082   -1.648289
   C     2.574341    0.001280   -1.427048
   H     3.189732   -0.895749   -1.649843
   H     1.717338    0.002288   -2.119673
   H     1.622480   -2.554705   -0.280923
   C     0.777334   -2.812479   -0.937843
   H     1.179133   -3.117480   -1.928044
   H     0.255329   -3.694250   -0.506396
   H    -1.757136   -2.852480   -1.784741
   C    -1.175503   -1.938841   -2.037909
   H    -1.876103   -1.091097   -2.092983
   H    -0.742534   -2.097439   -3.048951
   C    -1.176251    1.940688   -2.035885
   H    -0.743483    2.100070   -3.046889
   H    -1.757867    2.854109   -1.781899
   H    -1.876818    1.092952   -2.091450
   H     0.254502    3.695072   -0.503293
   C     0.776638    2.813687   -0.935358
   H     1.178414    3.119439   -1.925335
   H     1.621796    2.555543   -0.278598
60
Structure: TS22 Stoichiometry: C16H38TaN5+
   Ta    0.509739   -0.262787   -0.081594
   N     1.316468   -0.614256    1.738745
   N     2.166686    0.643098   -0.876719
   N     0.505163   -2.205158   -0.703136
   N    -0.577685    1.566761    0.263469
   N    -1.554987   -0.391819    0.342092
   C     2.350698    0.176094    2.394264
   H     3.133922   -0.482665    2.826782
   H     2.821094    0.858996    1.671274
   H     1.930996    0.784284    3.223737
   C     0.706507   -1.570424    2.657671
   H    -0.032775   -2.193287    2.128948
   H     1.476510   -2.240334    3.096701
   H     0.191480   -1.056762    3.496584
   H     3.226676   -1.110608   -0.315978
   C     3.369756   -0.190749   -0.906764
   H     4.241710    0.350187   -0.479989
   H     3.630615   -0.489671   -1.943892
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   H     2.597714    1.668576   -2.686930
   C     2.385532    1.873290   -1.615386
   H     3.254966    2.433091   -1.208882
   H     1.503468    2.526715   -1.562012
   C    -0.460513   -2.808008   -1.612896
   H    -0.963067   -3.681228   -1.143804
   H    -1.227644   -2.074093   -1.893805
   H     0.034223   -3.170980   -2.538727
   H     0.978731   -4.078891    0.188014
   C     1.483985   -3.199170   -0.265635
   H     2.090541   -3.569819   -1.118907
   H     2.165555   -2.770727    0.485904
   C    -0.402195    3.015639    0.292916
   H    -0.252445    3.382011   -0.749319
   C     0.856451    3.351056    1.107450
   H     1.719405    2.767456    0.751502
   H     1.100550    4.425377    1.032939
   H     0.693284    3.097603    2.169767
   C    -1.616223    3.764182    0.867191
   H    -1.405877    4.847415    0.888578
   H    -2.525162    3.609997    0.262712
   H    -1.822658    3.434592    1.901470
   H    -4.460890   -2.251563    0.096948
   C    -3.763006   -1.463305   -0.237424
   H    -4.317360   -0.509610   -0.269222
   H    -3.438212   -1.705095   -1.261548
   C    -2.565621   -1.374786    0.726198
   H    -2.047209   -2.351140    0.708604
   C    -3.054465   -1.129714    2.168870
   H    -2.203164   -1.086148    2.867061
   H    -3.605123   -0.174517    2.241489
   H    -3.737506   -1.935397    2.492624
   H    -2.678271    1.416758    0.791336
   C    -1.810585    0.964911    0.286897
   C    -0.433575    0.500275   -2.504195
   H     0.065498    1.474313   -2.532668
   H     0.053700   -0.285192   -3.098382
   C    -1.822740    0.477647   -2.353814
   H    -2.331283   -0.469887   -2.585050
   C    -2.583560    1.444800   -1.676292
   H    -2.231854    2.483900   -1.668418
   H    -3.673284    1.329012   -1.634583
53
Structure: TS23 Stoichiometry: C21H29NWO+
   C    -2.476403    0.697327    0.001033
   C    -1.515215    1.764826    0.189167
   C    -0.715069    1.442207    1.323877
   C    -1.191596    0.185667    1.881536
   C    -2.293189   -0.253085    1.071497
   W    -0.404866   -0.270079   -0.353422
   C     1.624364   -1.879950   -0.184123
   C     0.459464   -2.190077   -1.046563
   H     0.647066   -2.235207   -2.124441
   C    -0.880404   -2.402853   -0.555526
   H    -1.019017   -2.858869    0.436174
   H    -1.629143   -2.726356   -1.288741
   C     2.942137   -2.303223   -0.858482
   H     2.999759   -1.932729   -1.893344
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   H     3.812348   -1.921749   -0.297563
   H     2.979596   -3.408171   -0.886017
   N    -0.503363    0.307308   -2.069228
   O    -0.838544    0.906670   -3.069761
   C     1.538930   -2.491731    1.220672
   H     1.401845   -3.581762    1.117479
   H     2.464415   -2.310474    1.789889
   H     0.692778   -2.094544    1.804167
   C    -1.420265    3.009739   -0.647467
   H    -1.460007    2.774054   -1.723890
   H    -2.258117    3.694415   -0.416228
   H    -0.478571    3.546264   -0.451164
   C     0.280178    2.373421    1.957695
   H     0.976022    2.800927    1.218726
   H    -0.256647    3.208763    2.446277
   H     0.880100    1.867566    2.727442
   C    -0.789385   -0.401192    3.207603
   H     0.276095   -0.227741    3.430197
   H    -1.373957    0.052895    4.032096
   H    -0.967562   -1.489042    3.244085
   C    -3.199843   -1.412295    1.370927
   H    -2.673982   -2.215194    1.912363
   H    -4.041049   -1.076664    2.007062
   H    -3.623311   -1.843519    0.450300
   C    -3.552396    0.675245   -1.049947
   H    -3.964118   -0.339184   -1.174561
   H    -4.385854    1.348745   -0.772307
   H    -3.157995    1.002575   -2.025806
   C     1.911041   -0.106123   -0.003250
   C     2.436284    0.559355   -1.156674
   C     2.471716    0.269346    1.249452
   C     3.367437    1.592592   -1.047300
   H     2.088484    0.254814   -2.148478
   C     3.443325    1.270701    1.353921
   H     2.122526   -0.219404    2.162966
   C     3.883780    1.954030    0.211324
   H     3.709704    2.109079   -1.950678
   H     3.845824    1.532248    2.339082
   H     4.635380    2.746027    0.294617
86
Structure: TS24 Stoichiometry: C32H47P2N2O2Re+
   C     1.177069    0.604304    2.423288
   C     0.924128    1.192718    3.661659
   C    -0.416930    1.305492    4.093997
   C    -1.441182    0.833914    3.294193
   C    -1.158256    0.214888    2.033291
   N     0.174511    0.121547    1.632335
   H    -0.642990    1.761974    5.063964
   H     1.752574    1.559120    4.273048
   H    -2.484005    0.898783    3.620377
   C    -2.181434   -0.273380    1.172178
   H    -3.198672   -0.284001    1.583666
   C     2.588311    0.499980    1.885248
   H     2.978113   -0.520982    2.062779
   H     3.255414    1.210310    2.402552
   P    -1.673205   -1.545296   -0.008877
   P     2.590130    0.673716    0.016931
   C     0.969535   -1.161933   -2.222893
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O	1.215350	-1.452511	-3.336401
C	-1.611994	1.532296	-0.462340
C	-2.978411	-1.578690	-1.428718
C	-4.377120	-1.200955	-0.902202
C	-2.596955	-0.579205	-2.543358
C	-2.997616	-2.973969	-2.085948
H	-4.742534	-1.891886	-0.126919
H	-4.374894	-0.179068	-0.486821
H	-5.098237	-1.223355	-1.741380
H	-1.542341	-0.678365	-2.844284
H	-3.232597	-0.789149	-3.423709
H	-2.782140	0.462458	-2.248572
H	-3.665275	-2.938803	-2.966616
H	-1.992950	-3.264995	-2.437985
H	-3.378158	-3.757885	-1.414447
C	-1.825558	-3.190093	0.996933
C	-1.176124	-4.372948	0.248056
C	-1.056641	-2.953698	2.317668
C	-3.281921	-3.524953	1.373173
H	-1.772421	-4.705056	-0.613509
H	-0.164533	-4.124922	-0.104102
H	-1.088655	-5.229598	0.942770
H	-1.577420	-2.227823	2.961938
H	-0.992632	-3.914728	2.860869
H	-0.032472	-2.591116	2.149171
H	-3.282177	-4.382977	2.071867
H	-3.769514	-2.678020	1.886935
H	-3.895431	-3.810161	0.503548
C	2.471767	2.565992	-0.295774
C	2.019975	2.775689	-1.757807
C	1.391640	3.128806	0.655067
C	3.767103	3.355211	-0.027177
H	2.778835	2.438412	-2.480763
H	1.082450	2.233321	-1.957440
H	1.845287	3.854945	-1.928185
H	1.741537	3.153466	1.700101
H	1.163500	4.167282	0.350217
H	0.460347	2.549294	0.618609
H	3.549387	4.432733	-0.152152
H	4.131434	3.211568	1.004738
H	4.577885	3.101307	-0.727822
C	4.327957	0.065136	-0.513320
C	4.330706	-1.475050	-0.483404
C	4.584557	0.501233	-1.970805
C	5.452642	0.555090	0.422744
H	4.126489	-1.878626	0.520973
H	3.590197	-1.893186	-1.181576
H	5.334535	-1.825639	-0.788187
H	4.719705	1.589669	-2.072229
H	5.510829	0.015697	-2.329809
H	3.759566	0.183168	-2.631264
H	6.414682	0.145080	0.062378
H	5.548303	1.648823	0.454949
H	5.306951	0.186744	1.452552
C	1.465098	-2.239199	0.243502
O	1.966398	-3.209139	0.687583
Re	0.604947	-0.652391	-0.400350
N	-0.591956	1.051064	-0.847712

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   C    -2.651038    2.522963   -0.437928
   C    -2.856902    3.303350   -1.602662
   C    -3.460254    2.735049    0.699004
   C    -3.864810    4.271885   -1.621489
   H    -2.223537    3.134277   -2.478269
   C    -4.456096    3.715599    0.670273
   H    -3.286918    2.128088    1.588992
   C    -4.665786    4.481477   -0.487832
   H    -4.026063    4.866980   -2.526332
   H    -5.077140    3.881383    1.556518
   H    -5.453814    5.241405   -0.507200
88
Structure: TS25 Stoichiometry: C30H51N2P2O2Re+
   C     1.175362    0.564593    2.366246
   C     1.118830    1.312946    3.541661
   C    -0.105710    1.923828    3.894693
   C    -1.216175    1.766075    3.084349
   C    -1.142655    0.973774    1.894352
   N     0.081510    0.393058    1.567820
   H    -0.176516    2.516808    4.813239
   H     2.010113    1.422109    4.164716
   H    -2.176317    2.217358    3.351850
   C    -2.258527    0.779430    1.024883
   H    -3.222729    1.137262    1.405473
   C     2.469352   -0.072627    1.904471
   H     2.469497   -1.146212    2.174957
   H     3.334927    0.399806    2.399463
   P    -2.187372   -0.740180    0.032498
   P     2.566206   -0.074842    0.028042
   C     0.442644   -1.400875   -2.135898
   O     0.588540   -1.839593   -3.218407
   C    -1.142672    2.131511   -0.678182
   C    -3.436644   -0.561822   -1.426794
   C    -4.577316    0.401426   -1.047917
   C    -2.695972   -0.019434   -2.666954
   C    -4.013055   -1.928846   -1.847466
   H    -5.158748    0.046434   -0.182124
   H    -4.182340    1.401451   -0.806694
   H    -5.271513    0.503713   -1.903646
   H    -1.907047   -0.713296   -2.994594
   H    -3.427299    0.088960   -3.490256
   H    -2.230936    0.957332   -2.492892
   H    -4.614589   -1.783069   -2.764021
   H    -3.210702   -2.646541   -2.086926
   H    -4.672893   -2.372983   -1.087321
   C    -2.869791   -2.083694    1.245313
   C    -2.705846   -3.508630    0.674991
   C    -2.033983   -1.974655    2.541676
   C    -4.339441   -1.820040    1.629240
   H    -3.405942   -3.719458   -0.145007
   H    -1.681734   -3.688327    0.317408
   H    -2.910010   -4.238055    1.481540
   H    -2.235123   -1.032591    3.075322
   H    -2.314815   -2.812506    3.206498
   H    -0.953380   -2.041082    2.351514
   H    -4.633724   -2.527070    2.427863
   H    -4.473318   -0.797879    2.024449
   H    -5.036263   -1.965941    0.788564
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   C     3.142258    1.700161   -0.426656
   C     2.792300    1.940588   -1.911670
   C     2.325966    2.674365    0.447635
   C     4.630823    2.006472   -0.177759
   H     3.379894    1.299706   -2.587400
   H     1.722330    1.751415   -2.093534
   H     3.013625    2.994471   -2.167368
   H     2.649988    2.649106    1.500894
   H     2.483625    3.701940    0.070824
   H     1.250809    2.453911    0.412001
   H     4.805615    3.077047   -0.396368
   H     4.917360    1.835777    0.874327
   H     5.304325    1.425750   -0.827039
   C     3.987167   -1.295601   -0.376282
   C     3.456919   -2.734566   -0.234813
   C     4.399358   -1.098404   -1.850243
   C     5.197771   -1.148532    0.569318
   H     3.112593   -2.959855    0.786765
   H     2.627362   -2.929584   -0.930739
   H     4.282266   -3.431664   -0.472400
   H     4.903655   -0.135420   -2.027547
   H     5.105048   -1.901204   -2.133295
   H     3.523668   -1.168057   -2.518329
   H     5.962653   -1.893787    0.281050
   H     5.667704   -0.156779    0.527676
   H     4.917027   -1.358375    1.615630
   C     0.514008   -2.382330    0.412301
   O     0.640748   -3.430131    0.939913
   Re    0.250990   -0.658706   -0.368301
   N    -0.310220    1.337539   -0.995708
   C    -1.701034    3.520772   -0.786819
   C    -0.500622    4.501277   -0.741162
   C    -2.418766    3.651424   -2.153747
   C    -2.677709    3.854421    0.355479
   H    -0.007171    4.470660    0.242906
   H     0.242910    4.251969   -1.515434
   H    -0.867435    5.527860   -0.916918
   H    -3.291847    2.982927   -2.213104
   H    -2.768803    4.691441   -2.275875
   H    -1.735083    3.410238   -2.984419
   H    -2.998852    4.906040    0.256847
   H    -3.568361    3.209004    0.317195
   H    -2.194626    3.723114    1.336433
33
Structure: TS26 Stoichiometry: C7H22OsOP2+
   Os    0.000171   -0.037174    0.007773
   H     0.170976   -0.118104    3.968788
   H    -0.019180    0.611252    3.890160
   P     2.326647   -0.290008   -0.055681
   P    -2.325173   -0.297197   -0.052299
   C    -3.334528    1.123573   -0.671568
   H    -4.415719    0.897491   -0.668005
   H    -3.136432    2.004878   -0.039123
   H    -3.010157    1.361729   -1.698264
   C    -2.921450   -1.689044   -1.110702
   H    -2.475094   -2.624998   -0.738374
   H    -4.023650   -1.762546   -1.103292
   H    -2.567547   -1.525274   -2.141852
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C	-3.140166	-0.672714	1.570695
H	-2.951076	0.157722	2.271839
H	-4.230084	-0.812429	1.456257
H	-2.692988	-1.590732	1.987204
C	2.923926	-1.537874	-1.280467
H	4.024090	-1.634600	-1.258299
H	2.452658	-2.506239	-1.047767
H	2.599355	-1.228602	-2.287592
C	3.357002	1.189110	-0.470512
H	3.163937	1.979173	0.274148
H	4.435618	0.951772	-0.489575
H	3.044121	1.568469	-1.457543
C	3.116321	-0.883606	1.513122
H	2.661157	-1.848531	1.791724
H	4.208041	-1.007965	1.398255
H	2.915740	-0.156267	2.318107
C	-0.011934	1.869626	-0.080329
O	-0.017606	3.045167	-0.100909
H	0.019382	-1.773651	0.171829
H	-0.002442	-0.064970	-1.583818

39

Structure: TS27 Stoichiometry: C7H26BP2OsON+

Os	-0.030493	-0.164416	-0.198429
H	0.048263	0.995253	1.151318
H	0.181894	1.555547	-0.970351
P	-2.387122	0.011175	-0.168937
P	2.334499	-0.187162	-0.180128
C	3.152679	-1.730523	-0.771898
H	4.253209	-1.655597	-0.718527
H	2.809396	-2.573621	-0.149095
H	2.838156	-1.920129	-1.811052
C	3.106241	1.142916	-1.196328
H	2.647697	2.097787	-0.882954
H	4.201702	1.174373	-1.063454
H	2.868734	0.966534	-2.258949
C	3.080791	0.066576	1.486210
H	2.764515	-0.760384	2.143882
H	4.183520	0.102121	1.440560
H	2.684044	1.005800	1.905146
C	-3.077143	1.545287	-0.928637
H	-4.177633	1.573838	-0.845251
H	-2.644014	2.412130	-0.402416
H	-2.789851	1.587945	-1.992656
C	-3.328326	-1.336199	-1.008576
H	-3.048291	-2.298401	-0.548215
H	-4.419685	-1.188745	-0.924401
H	-3.033347	-1.366290	-2.070214
C	-3.112466	0.030484	1.525421
H	-2.662131	0.870974	2.078386
H	-4.211040	0.138188	1.497060
H	-2.846202	-0.910184	2.035732
C	-0.101578	-1.713432	0.838926
O	-0.143412	-2.697480	1.473229
H	1.589771	3.667169	0.692375
H	0.154737	3.927259	-0.077121
H	-1.185468	2.595787	1.514807
H	0.608769	2.275989	2.492751
B	0.019929	2.401441	1.427984

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   N     0.729762    3.215060    0.376850
   H    -0.031436    1.054859   -1.600560
   H    -0.060402   -1.156191   -1.554655
51
Structure: TS28 Stoichiometry: C17H28IrP2O2N+
   C    -3.068806    0.593032   -1.103069
   C    -2.255840   -0.010989   -0.107826
   C    -2.944028   -0.699636    0.923912
   C    -4.344449   -0.779018    0.963940
   C    -5.118711   -0.178882   -0.041128
   C    -4.469850    0.506194   -1.079514
   Ir   -0.218461    0.112088   -0.227758
   P     0.186389   -2.127877   -0.620351
   C     1.949786   -2.210278   -0.166188
   C     2.667264   -0.949940   -0.360149
   N     1.941363    0.224114   -0.372015
   C     2.578966    1.430903   -0.396025
   C     3.973144    1.523944   -0.412862
   C     4.731484    0.340465   -0.439238
   C     4.081092   -0.888893   -0.421325
   C     1.710257    2.669504   -0.463992
   P    -0.002528    2.348582    0.217911
   H     4.647701   -1.824586   -0.428045
   H     4.453308    2.506300   -0.426176
   H     5.825231    0.386745   -0.470882
   H     2.209424    3.533740    0.008796
   H     1.549147    2.930692   -1.528801
   H     1.805634   -2.347982    1.149564
   H     2.505531   -3.097768   -0.512113
   H    -2.592673    1.147913   -1.924303
   H    -5.058580    0.982227   -1.873501
   H    -6.212194   -0.242900   -0.014564
   H    -4.835388   -1.317551    1.783982
   H    -2.365330   -1.188278    1.718347
   H     0.041606   -0.102978    1.357454
   O     0.380962   -0.272879    2.865908
   H    -0.500496   -0.515047    3.206014
   H     0.893287   -1.227535    2.740755
   O     1.462963   -2.470596    2.432357
   H     2.285304   -2.610685    2.936098
   C    -0.636819   -3.449762    0.354608
   H    -1.729535   -3.321286    0.289726
   H    -0.352876   -4.447440   -0.024136
   H    -0.287499   -3.342724    1.395854
   C    -0.013617   -2.681266   -2.374369
   H     0.389905   -3.699713   -2.513917
   H    -1.085164   -2.670549   -2.638873
   H     0.523589   -1.981698   -3.035735
   C     0.059356    2.848747    1.987281
   H     0.521127    3.843021    2.116774
   H    -0.976331    2.871238    2.367862
   H     0.606639    2.071752    2.546358
   C    -1.029850    3.662641   -0.569598
   H    -2.069888    3.536608   -0.225267
   H    -0.672932    4.675354   -0.312039
   H    -1.012181    3.530203   -1.664045
53
Structure: TS29 Stoichiometry: C17H30IrO2NP2+
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C	3.895897	-0.982996	-1.105137
C	2.580529	-1.046406	-0.598608
N	1.918395	0.111874	-0.295287
C	2.546650	1.315713	-0.360506
C	3.851319	1.421834	-0.854475
C	4.521471	0.254232	-1.252662
C	1.916691	-2.306624	-0.210778
P	0.085633	-2.240981	-0.315085
Ir	-0.251879	0.035274	-0.055574
P	-0.032874	2.329322	0.011227
C	1.807283	2.489209	0.235943
C	-2.317878	-0.025192	-0.095677
C	-3.038852	0.105188	-1.311179
C	-4.441384	0.068463	-1.354796
C	-5.186339	-0.102423	-0.178846
C	-4.503708	-0.236161	1.038367
C	-3.100683	-0.197476	1.074140
O	1.828516	-1.880111	2.458549
O	1.713965	0.611375	2.739739
H	4.412141	-1.911101	-1.365957
H	4.335334	2.400697	-0.909035
H	5.537999	0.313469	-1.655871
C	-0.472805	-2.989430	-1.898967
C	-0.489798	-3.360055	1.016953
H	1.943870	2.378386	1.333188
H	2.214305	3.458905	-0.096298
H	2.019607	-2.251572	1.008864
H	2.388202	-3.212820	-0.623178
C	-0.473104	3.286002	-1.494535
C	-0.741413	3.291163	1.407500
H	-2.486131	0.236342	-2.248463
H	-4.955085	0.172976	-2.318429
H	-6.281070	-0.132560	-0.210746
H	-5.064701	-0.373162	1.970860
H	-2.603193	-0.308218	2.046443
H	-0.552710	-0.232870	1.719184
H	1.401711	0.684884	3.659496
H	1.865119	-0.458239	2.633188
H	2.539533	-2.310753	2.967496
H	-0.292491	0.136377	-1.651013
H	0.208380	0.106880	1.851017
H	-0.169323	-4.048112	-1.972328
H	-1.572317	-2.912730	-1.954192
H	-0.038172	-2.415248	-2.732928
H	-0.276267	-4.417025	0.778870
H	0.087203	-3.039638	1.908701
H	-1.572681	-3.219301	1.169295
H	-0.442830	4.353481	1.377046
H	-1.840398	3.209859	1.367033
H	-0.384368	2.828294	2.342110
H	-0.224724	4.356535	-1.391742
H	0.069600	2.853620	-2.350717
H	-1.555138	3.167995	-1.674507

43

Structure: TS30 Stoichiometry: C14H26NPPt+

C	-0.535943	4.030865	-0.121999
C	0.713834	3.404963	-0.195648
C	0.839823	2.005427	-0.302391

C	-0.322260	1.182612	-0.353614
C	-1.583036	1.843661	-0.231958
C	-1.689629	3.241636	-0.121647
C	2.241585	1.422400	-0.320747
C	2.497106	0.444677	0.839475
N	3.615596	-0.464996	0.588418
Pt	-0.361442	-0.936549	-0.492785
C	1.344089	-1.275331	-1.947241
C	-2.833224	0.984645	-0.125824
P	-2.230198	-0.542821	0.722796
H	1.626037	4.013622	-0.161536
H	-2.678134	3.707293	-0.026643
H	-0.606877	5.120937	-0.040258
H	-3.210811	0.666449	-1.116672
H	-3.656682	1.486797	0.413815
H	2.412067	0.878030	-1.263395
H	2.970962	2.251081	-0.295503
H	2.622046	1.012491	1.795349
C	-3.601207	-1.767286	0.718024
C	-2.037599	-0.058181	2.485856
H	1.591553	-0.183237	0.957079
C	4.905902	0.205610	0.510181
C	3.630861	-1.570677	1.535360
H	1.184060	-0.419869	-2.620051
H	2.273377	-1.178782	-1.361492
H	1.418443	-2.179769	-2.580854
H	0.338216	-2.240626	-1.267750
H	5.690110	-0.529483	0.258319
H	4.890023	0.970315	-0.283571
H	5.197693	0.706733	1.466425
H	4.432764	-2.280851	1.266724
H	3.800791	-1.246344	2.591767
H	2.664164	-2.102333	1.493033
H	-3.003451	0.252060	2.921563
H	-1.627224	-0.907005	3.057119
H	-1.322032	0.779020	2.526342
H	-4.504047	-1.351796	1.198973
H	-3.828894	-2.040643	-0.325005
H	-3.281840	-2.674565	1.256947
H	-0.477858	-2.631554	-0.591357

43

Structure: TS31 Stoichiometry: C14H26PPtN+

C	-0.656087	4.022568	-0.010919
C	0.655424	3.533904	-0.001743
C	0.926952	2.158969	-0.164113
C	-0.138830	1.245838	-0.368591
C	-1.469429	1.751334	-0.292970
C	-1.724503	3.123134	-0.127962
C	2.342952	1.669365	0.059480
C	2.442657	0.843204	1.360328
N	2.018334	-0.559043	1.186597
Pt	0.081356	-0.837762	-0.649192
C	1.433900	-0.543571	-2.256554
C	-2.602706	0.741107	-0.309645
P	-1.924311	-0.745835	0.584138
H	1.491414	4.228332	0.150825
H	-2.758082	3.487797	-0.085866
H	-0.846791	5.095047	0.105941

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   H    -2.832648    0.400649   -1.337754
   H    -3.532177    1.128416    0.146872
   H     2.700399    1.054214   -0.782754
   H     3.024430    2.534099    0.142902
   H     3.482794    0.871775    1.756872
   C    -3.202003   -2.063235    0.397375
   C    -2.081246   -0.250117    2.357714
   H     1.792903    1.305157    2.122752
   C     3.116970   -1.372525    0.653578
   C     1.522310   -1.134306    2.439577
   H     1.540548    0.528725   -2.488938
   H     2.426838   -0.974551   -2.032298
   H     1.047246   -1.051973   -3.156901
   H    -0.505557   -1.973776   -1.597169
   H     2.756429   -2.392498    0.448463
   H     3.477428   -0.939945   -0.291663
   H     3.969756   -1.419118    1.368838
   H     1.159412   -2.157934    2.252387
   H     2.311404   -1.173232    3.225582
   H     0.685072   -0.526725    2.813905
   H    -3.131573   -0.024486    2.614080
   H    -1.709935   -1.056544    3.011190
   H    -1.466962    0.652295    2.512472
   H    -4.191323   -1.719667    0.747556
   H    -3.266642   -2.343752   -0.666959
   H    -2.900319   -2.953392    0.974784
   H     0.268349   -2.486678   -0.799738
19
Structure: TS32 Stoichiometry: C5H11P2Pt+
   C     1.413205   -1.025958   -0.616734
   Pt   -0.185471   -0.076552   -0.138340
   P    -1.963114   -1.528928    0.282768
   C     2.543793   -1.259791    0.272966
   C     3.228023   -0.165832    0.686644
   C     2.721344    1.125226    0.197504
   C     1.478724    1.267847   -0.322155
   P    -1.619875    1.837613    0.233832
   H    -3.108898   -1.456483   -0.547066
   H    -1.676183   -2.911638    0.210839
   H    -2.563514   -1.455441    1.563245
   H    -2.928581    1.934128   -0.304529
   H    -1.880868    2.200497    1.578484
   H    -1.060506    3.045075   -0.247896
   H     4.136774   -0.234637    1.290846
   H     3.394046    1.993369    0.215010
   H     2.822743   -2.292645    0.521129
   H     1.553036   -1.313482   -1.680180
   H     1.212994    2.183098   -0.867720
15
Structure: TS33 Stoichiometry: CH11PtN2+
   H     2.656254    0.474687    0.099531
   Pt    0.001323   -0.183674   -0.069869
   C     2.053413   -0.408054    0.365735
   N     0.201132    2.066186    0.014073
   H    -0.101647   -1.739904   -0.152662
   N    -2.158682   -0.153793    0.267656
   H     1.930288   -0.489306    1.461232
   H     2.527568   -1.319534   -0.023542
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   H    -2.627396    0.760391    0.317231
   H     1.141564   -0.364337   -1.107645
   H    -0.289206    2.534971    0.788479
   H     1.187830    2.344090    0.110210
   H    -0.129634    2.519743   -0.849287
   H    -2.615408   -0.675234   -0.493867
   H    -2.401053   -0.657431    1.133602
33
Structure: TS34 Stoichiometry: C10H15PtBN6+
   C     0.182207    2.981300    0.566468
   N     0.209002    1.641005    0.428990
   N     1.360693    1.186847    0.992134
   C     2.060434    2.240296    1.482946
   C     1.341935    3.410018    1.234251
   B     1.807262   -0.305893    0.929303
   N     0.665948   -1.192222    1.509699
   N    -0.610734   -1.117142    1.056795
   C    -1.332964   -2.025162    1.739555
   C    -0.507952   -2.712090    2.649639
   C     0.754751   -2.147398    2.470537
   Pt   -1.174421    0.361760   -0.419994
   N     2.093202   -0.690722   -0.533755
   N     1.145727   -0.490017   -1.482120
   C     1.668219   -0.929366   -2.635171
   C     2.979035   -1.426228   -2.439324
   C     3.211139   -1.252315   -1.076888
   H     1.084711   -0.864293   -3.555988
   H     4.078613   -1.480593   -0.457419
   H     3.660037   -1.844032   -3.180447
   H     2.801075   -0.450987    1.606272
   H     1.709560   -2.352208    2.953266
   H     3.021237    2.076229    1.968933
   H    -0.791453   -3.500610    3.345087
   H     1.617342    4.428698    1.502234
   H    -2.402340   -2.126498    1.553045
   H    -0.667384    3.545851    0.185565
   H    -1.793213   -1.156578   -2.210808
   H    -1.583370    1.489540   -1.439631
   C    -2.564498   -0.999897   -1.438494
   H    -2.743472   -1.937015   -0.891076
   H    -2.738053   -0.052744   -0.450100
   H    -3.485472   -0.661734   -1.939230
33
Structure: TS35 Stoichiometry: C10H15N6BPt+
   C    -1.911397   -2.194434   -1.344813
   N    -1.174378   -1.300373   -0.664698
   N    -2.035904   -0.482446    0.021193
   C    -3.311299   -0.886868   -0.217757
   C    -3.279683   -1.975630   -1.088025
   B    -1.544653    0.684273    0.960022
   N    -0.527564    0.088236    1.964992
   N     0.600488   -0.477519    1.469118
   C     1.326830   -0.914244    2.511328
   C     0.652403   -0.623567    3.715381
   C    -0.524563    0.014409    3.320984
   Pt    0.692253   -0.373993   -0.686587
   N    -0.851387    1.871174    0.200629
   N     0.390282    1.776098   -0.375113
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C	0.666616	2.969048	-0.925170
C	-0.394375	3.869262	-0.694865
C	-1.332625	3.131313	0.024060
H	1.611663	3.117791	-1.447957
H	-2.304979	3.409521	0.429415
H	-0.463284	4.913486	-0.997445
H	-2.513109	1.121665	1.540749
H	-1.354225	0.418458	3.899861
H	-4.146587	-0.371723	0.255155
H	0.975243	-0.848355	4.731005
H	-4.127505	-2.540655	-1.473052
H	2.283319	-1.409274	2.342025
H	-1.419607	-2.940434	-1.968047
H	2.739066	-0.866833	-0.841613
H	0.668585	-0.258102	-2.255990
C	3.843004	-0.952404	-0.639905
H	4.128228	-0.207800	0.118359
H	4.050869	-1.970593	-0.276766
H	4.379645	-0.764578	-1.582209