Supporting Information for

From M_6 to M_{12}, M_{19} and M_{38} molecular alloy carbonyl nanoclusters: selective growth of atomically precise heterometallic nanoclusters

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Figure S1

IR spectrum (ν_{CO} region) recorded in thf of $[NBu_4]_2[Ni_6(CO)_{12}]$.

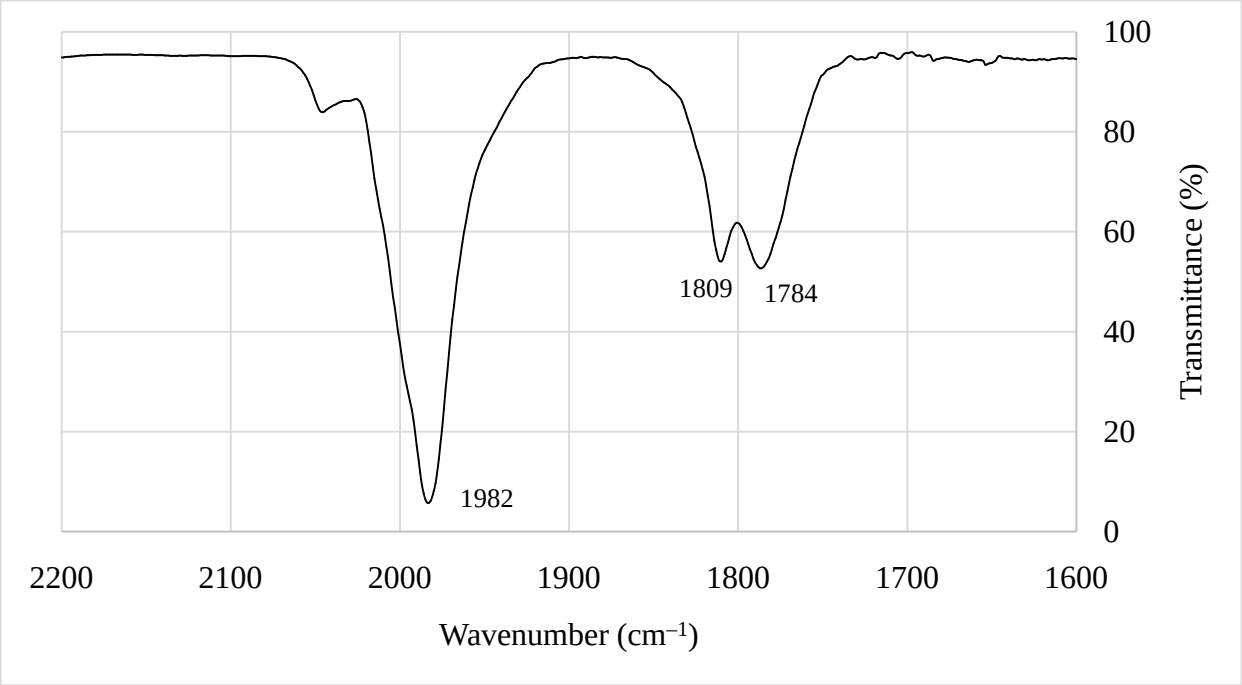


Figure S2

IR spectrum (ν_{CO} region) recorded in thf of $[NBu_4]_2[Ni_9(CO)_{18}]$.

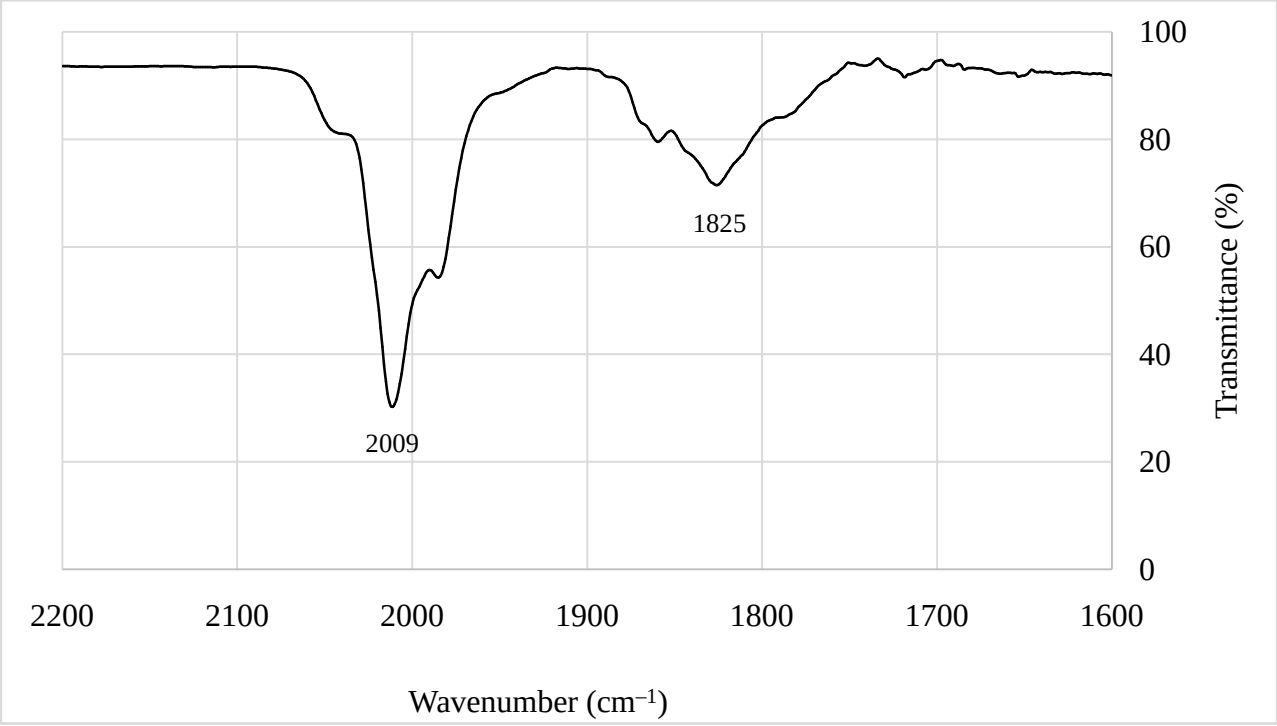


Figure S3

IR spectrum (ν_{CO} region) recorded in thf of $[NBu_4]_2[H_2Ni_{12}(CO)_{21}]$.

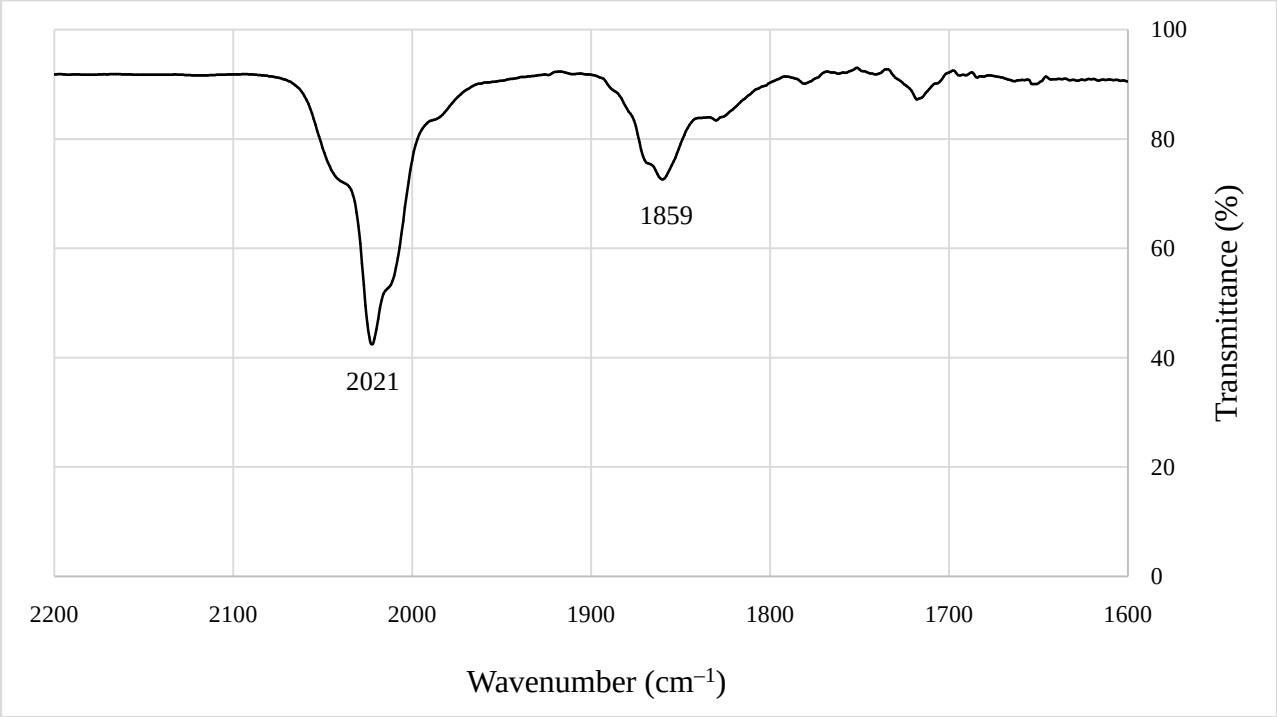


Figure S4

IR spectrum (ν_{CO} region) recorded in thf of $[NBu_4]_2[Pt_6(CO)_{12}]$.

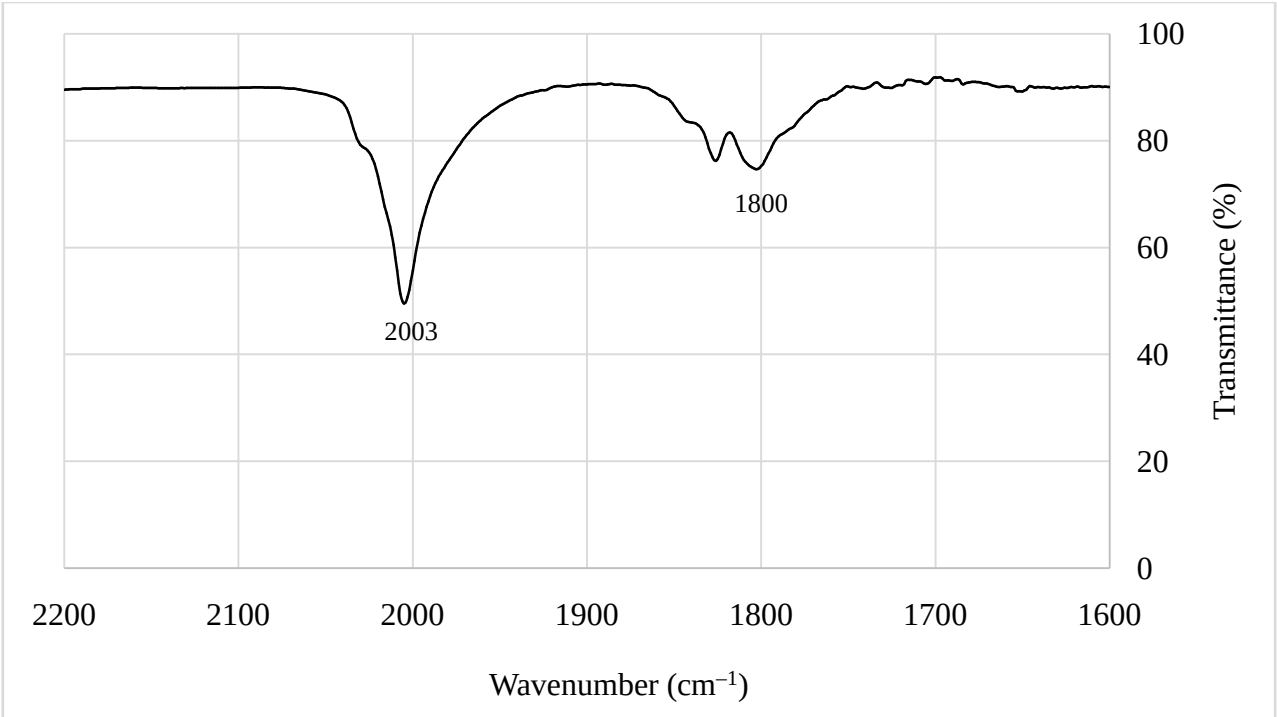


Figure S5

IR spectrum (ν_{CO} region) recorded in thf of $[NBu_4]_2[Pt_9(CO)_{18}]$.

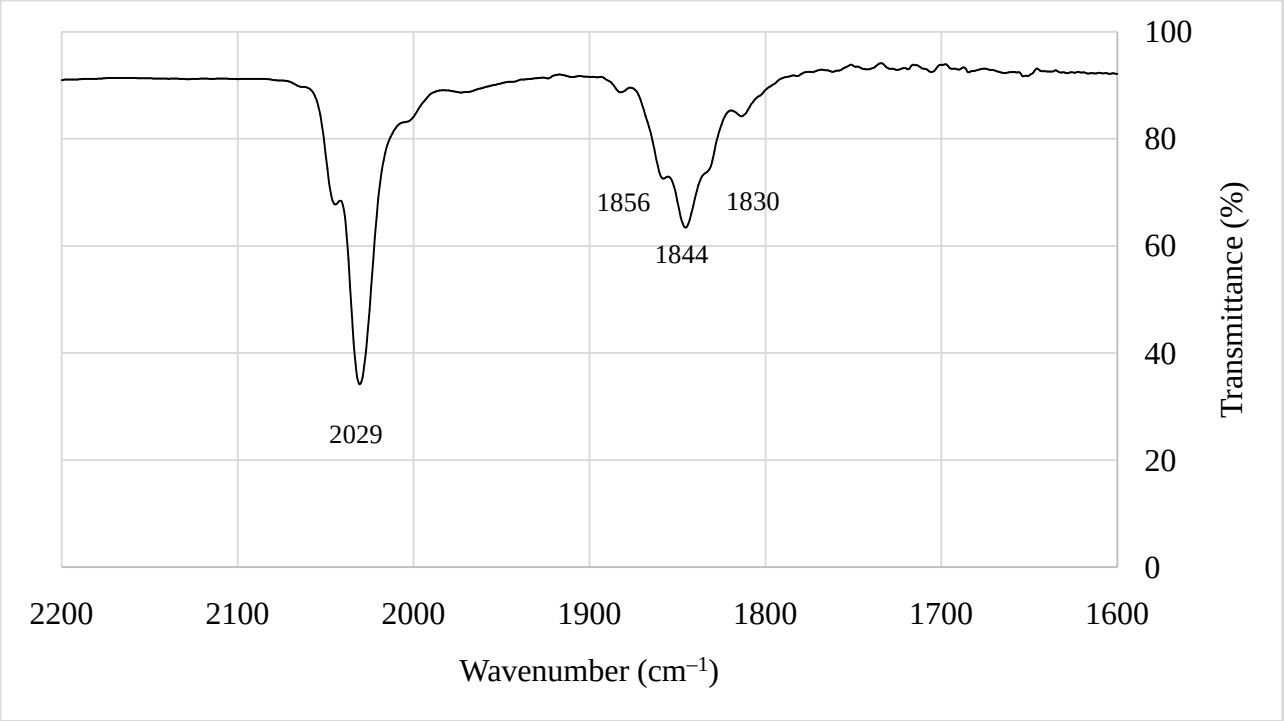


Figure S6

IR spectrum (ν_{CO} region) recorded in thf of $[NBu_4]_2[Pt_{12}(CO)_{24}]$.

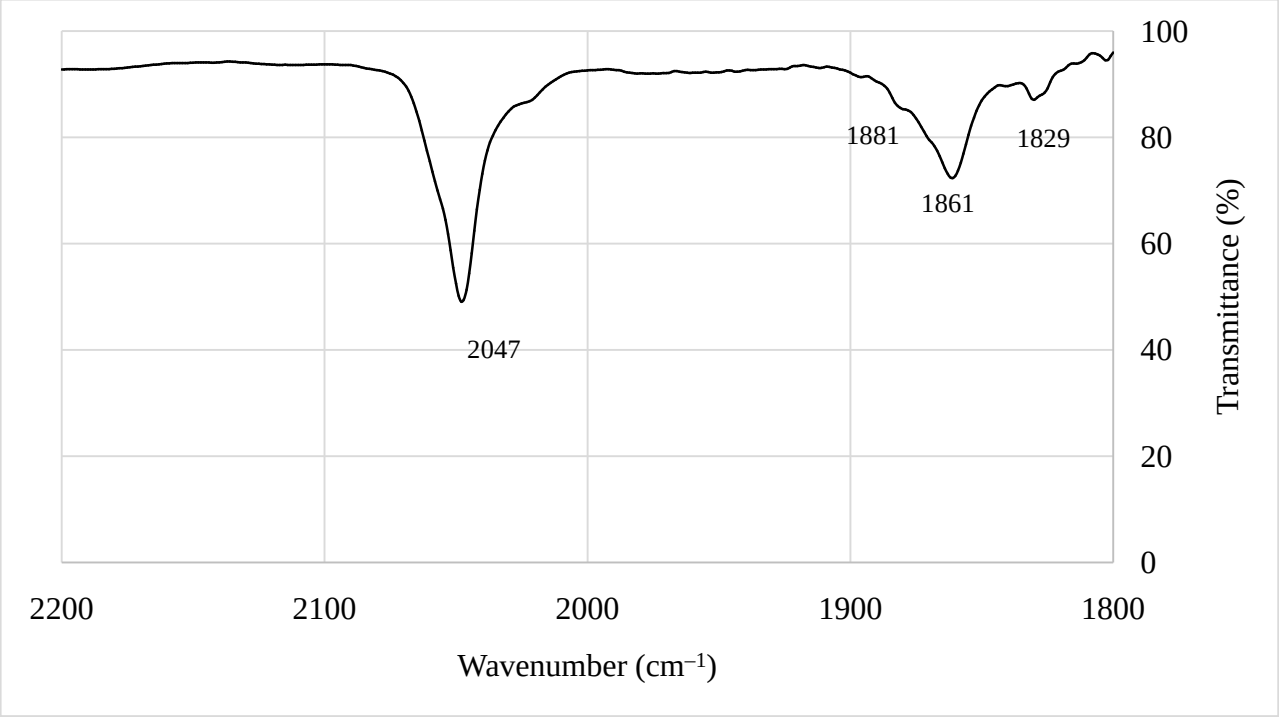


Figure S7

IR spectrum (ν_{CO} region) recorded in thf of $[NBu_4]_2[Pt_{6-x}Ni_x(CO)_{12}]$ (x = 4.20).

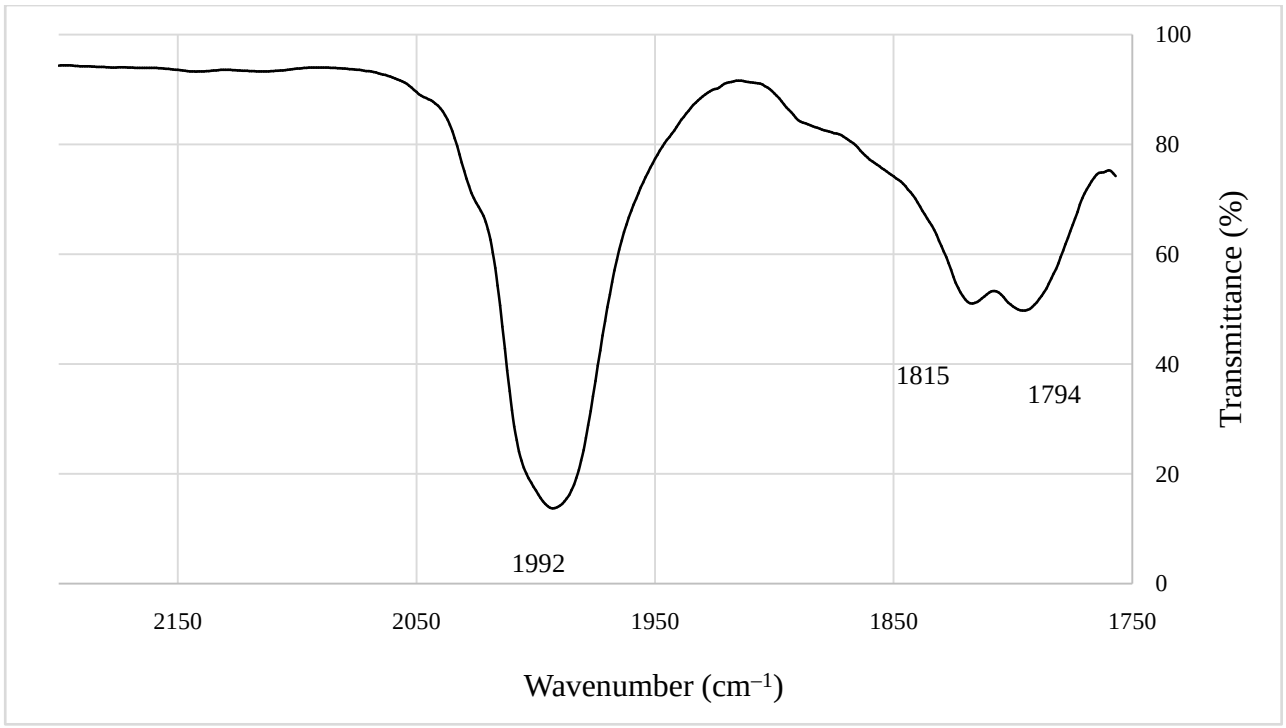


Figure S8

IR spectrum (ν_{CO} region) recorded in thf of a mixture of $[NBu_4]_2[Pt_9(CO)_{18}]$ + $[NBu_4]_2[Ni_9(CO)_{18}]$ (1:1 molar ratio).

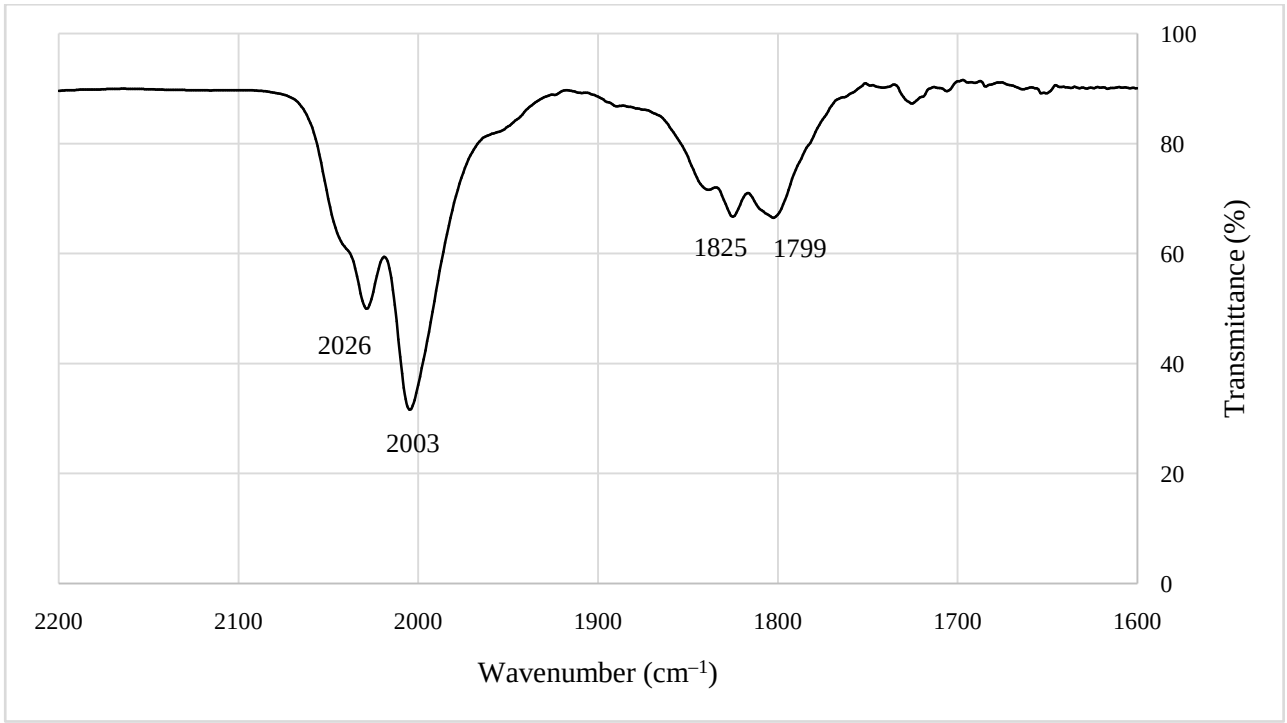


Figure S9

IR spectrum (ν_{CO} region) recorded in thf of a mixture of $[NBu_4]_2[Pt_9(CO)_{18}]$ + $[NBu_4]_2[Ni_9(CO)_{18}]$ (1:2 molar ratio).

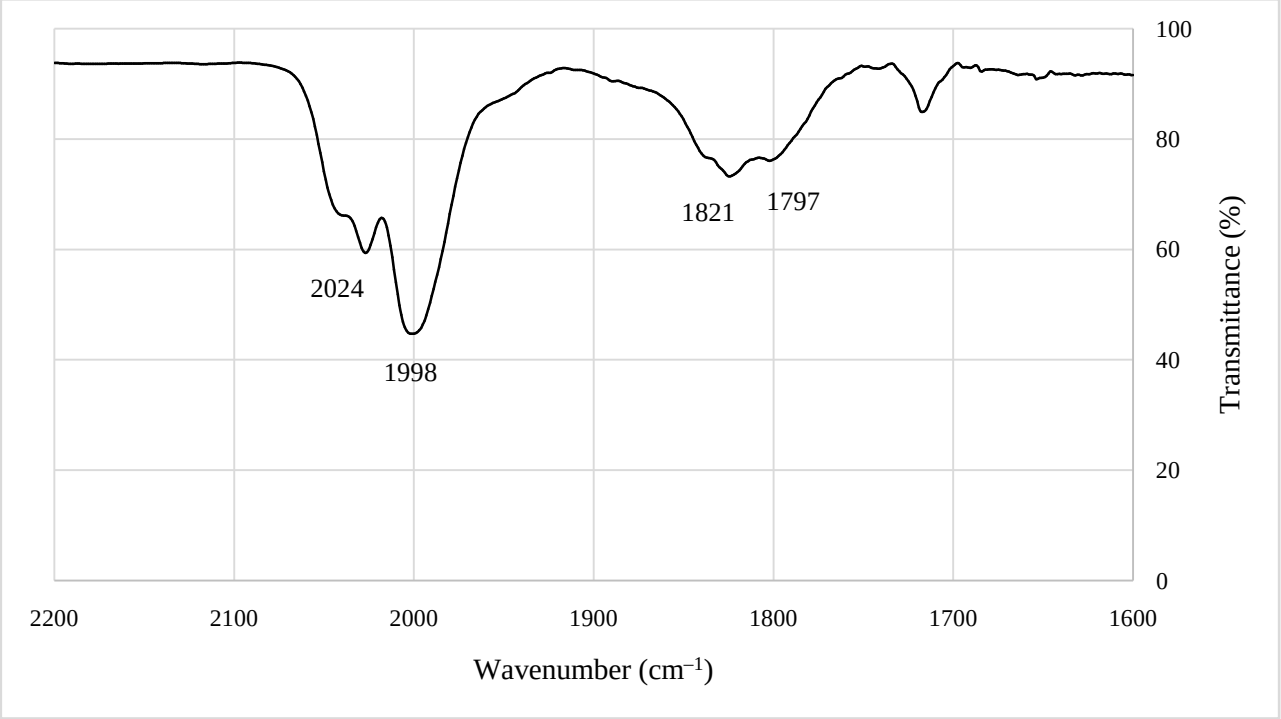


Figure S10

IR spectrum (ν_{CO} region) recorded in thf of a mixture of $[NBu_4]_2[Pt_9(CO)_{18}]$ + $[NBu_4]_2[H_2Ni_{12}(CO)_{21}]$ (1:1 molar ratio).

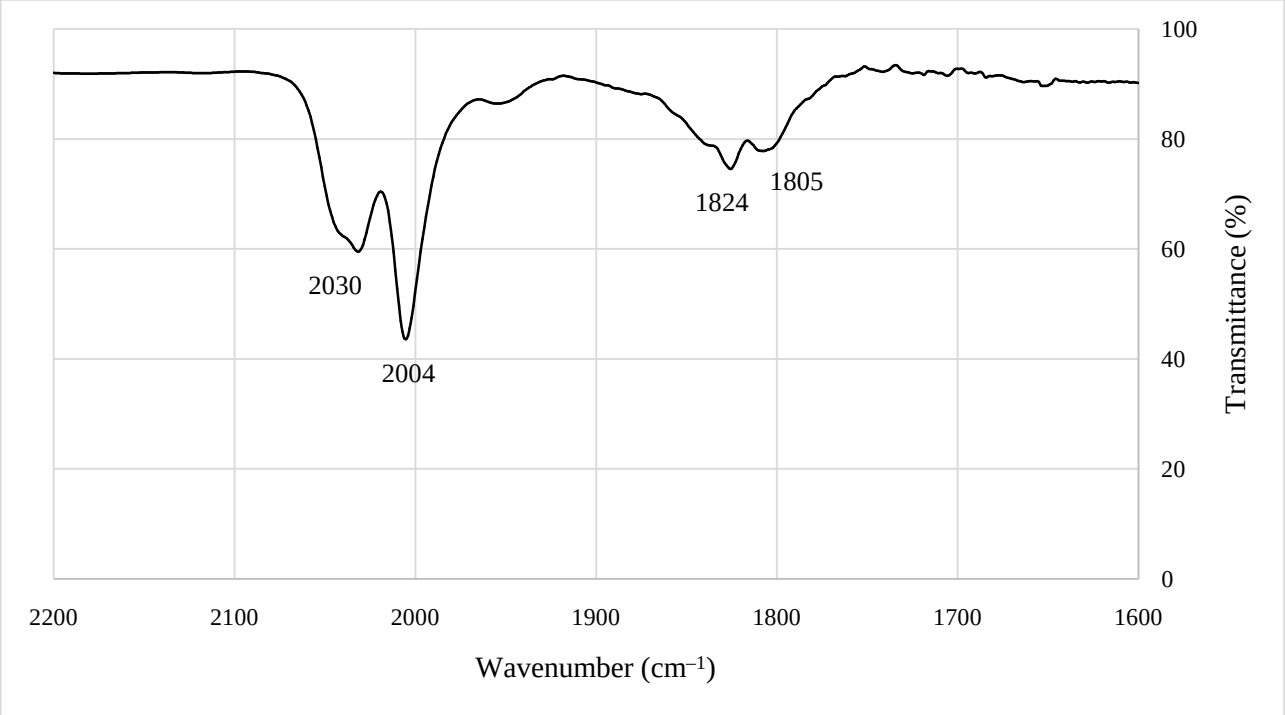


Figure S11

IR spectra (ν_{CO} region) recorded in CH_3CN of a mixture of (A) $[Pt_{6-x}Ni_x(CO)_{12}]^{2-}$ (x = 3) and (B-C) after the addition of increasing amounts of $HBF_4 \cdot Et_2O$.

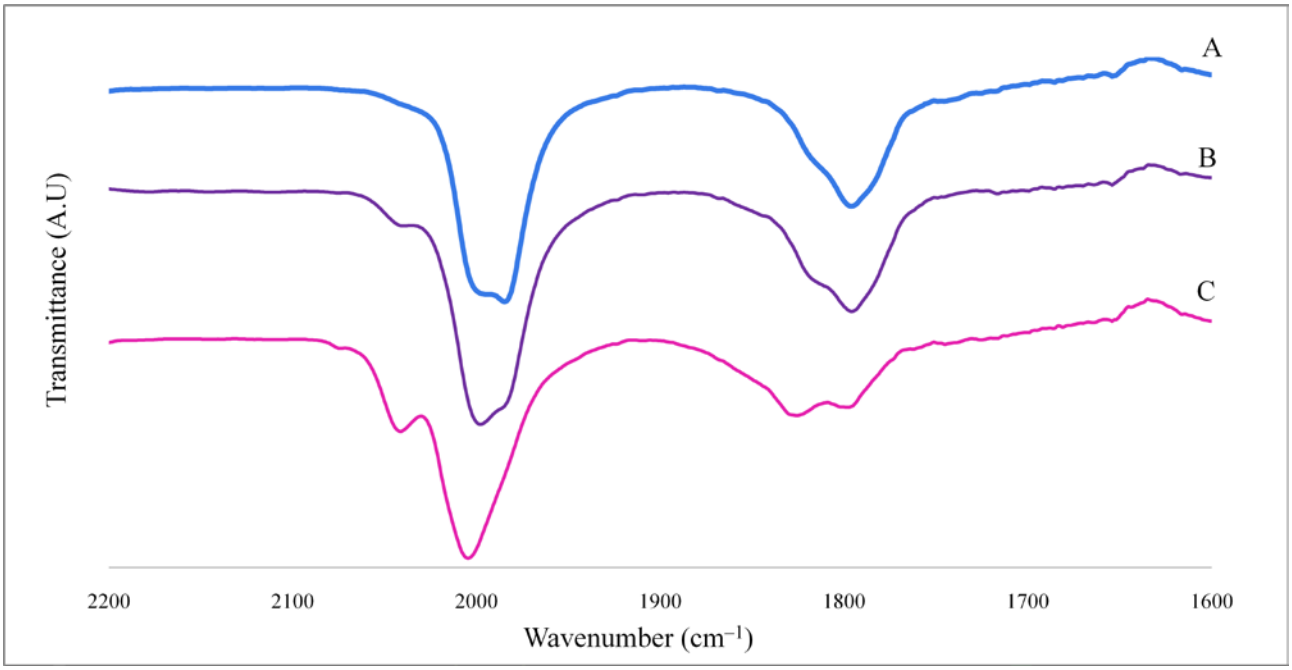


Figure S12

IR spectra (ν_{CO} region) recorded in thf of a mixture of (A) $[Pt_{6-x}Ni_x(CO)_{12}]^{2-}$ (x = 3) and (B-E) after the addition of increasing amounts of $HBF_4 \cdot Et_2O$.

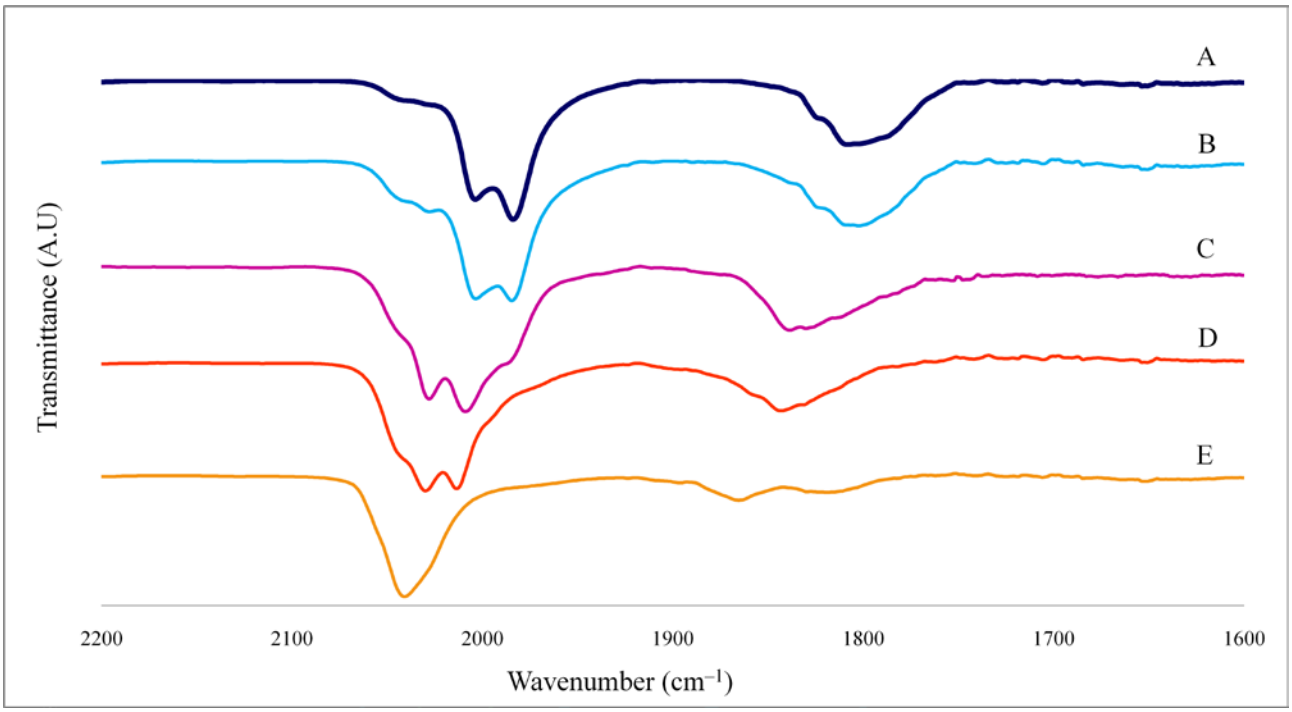


Figure S13

IR spectra (ν_{CO} region) recorded in thf of a mixture of (A) $[Pt_{6-x}Ni_x(CO)_{12}]^{2-}$ (x = 4) and (B-E) after the addition of increasing amounts of $HBF_4 \cdot Et_2O$.

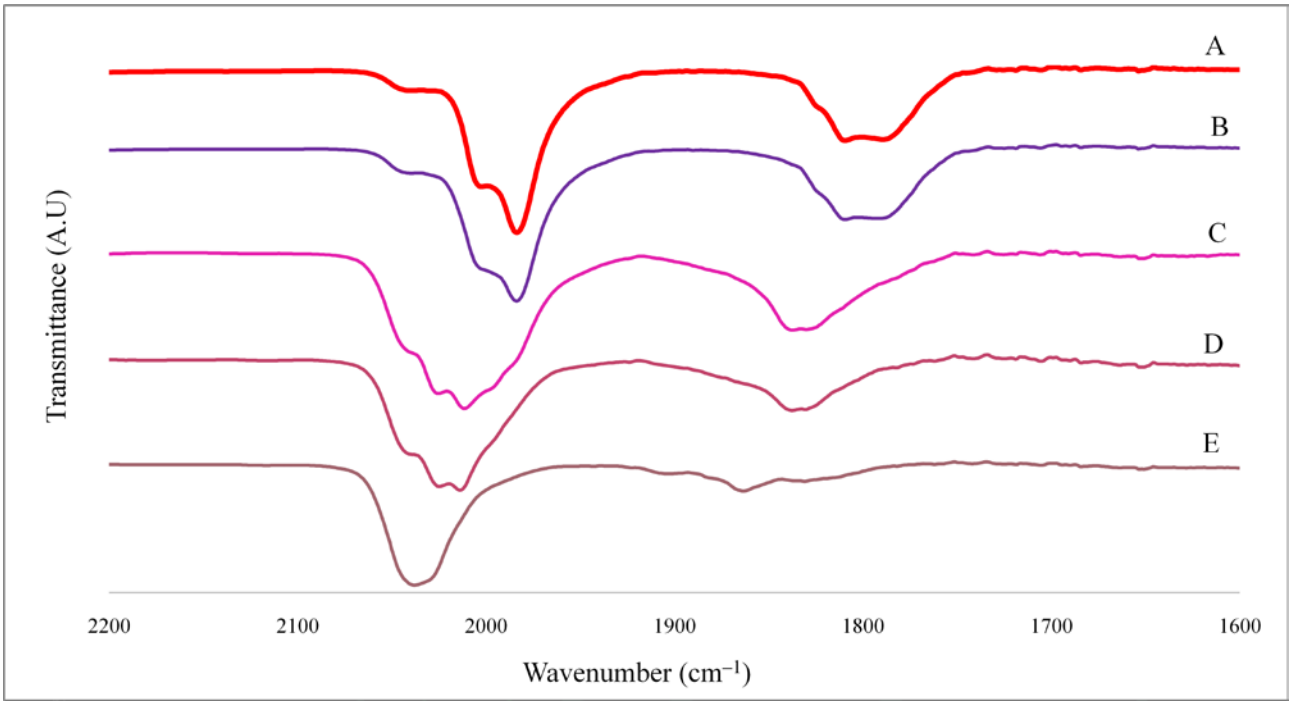


Figure S14

IR spectrum (ν_{CO} region) recorded in CH_3CN of a mixture of $[NBu_4]_2[Pt_6(CO)_{12}]$ + $[NBu_4]_2[Ni_6(CO)_{12}]$ (1:2 molar ratio) after heating at 85 °C for 90 minutes.

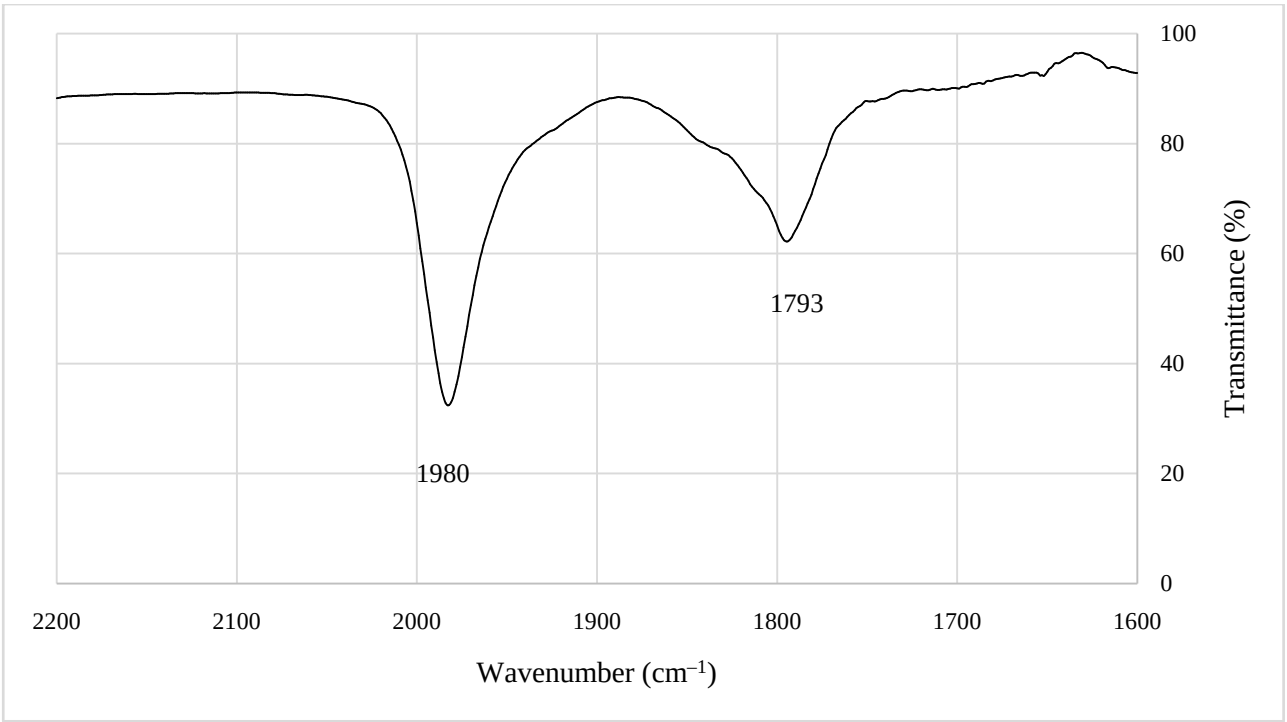


Figure S15

IR spectrum (ν_{CO} region) recorded in CH_3CN of a mixture of $[NBu_4]_2[Pt_9(CO)_{18}]$ + $[NBu_4]_2[Ni_6(CO)_{12}]$ (1:1.16 molar ratio) after heating at 85 °C for 90 minutes.

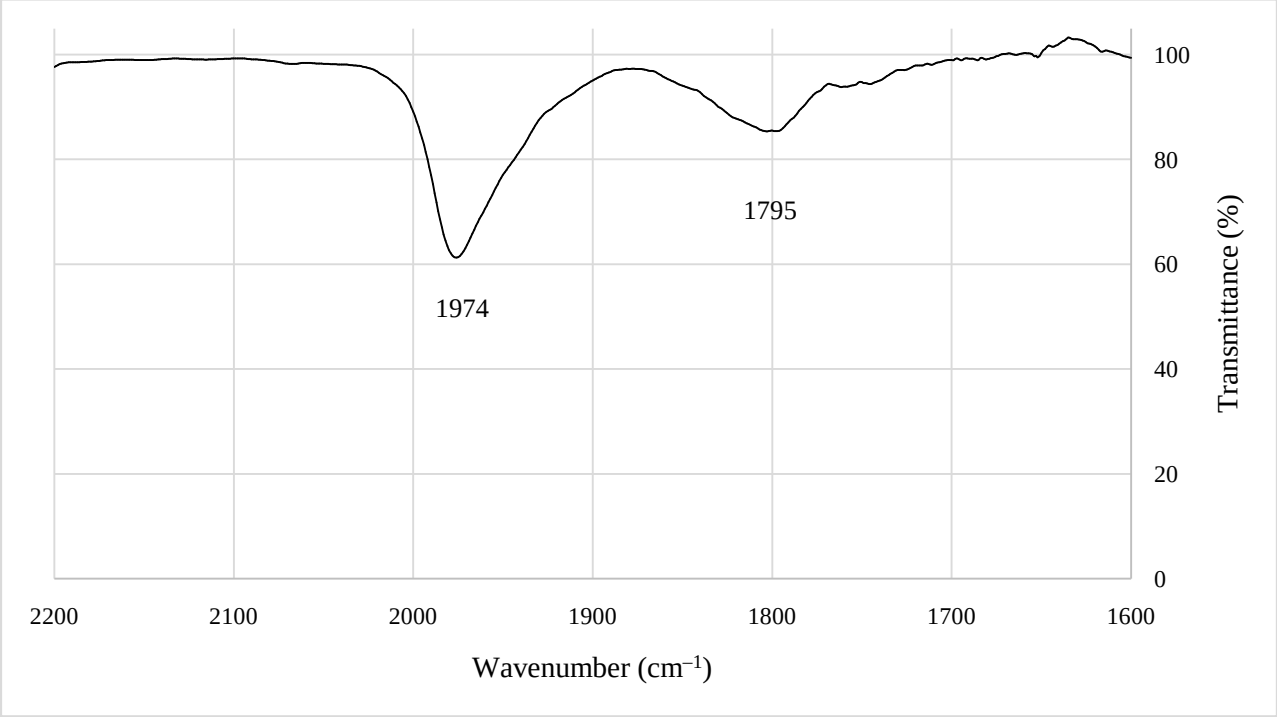


Figure S16

IR spectrum (ν_{CO} region) recorded in thf of $[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]$ (x = 2.90).

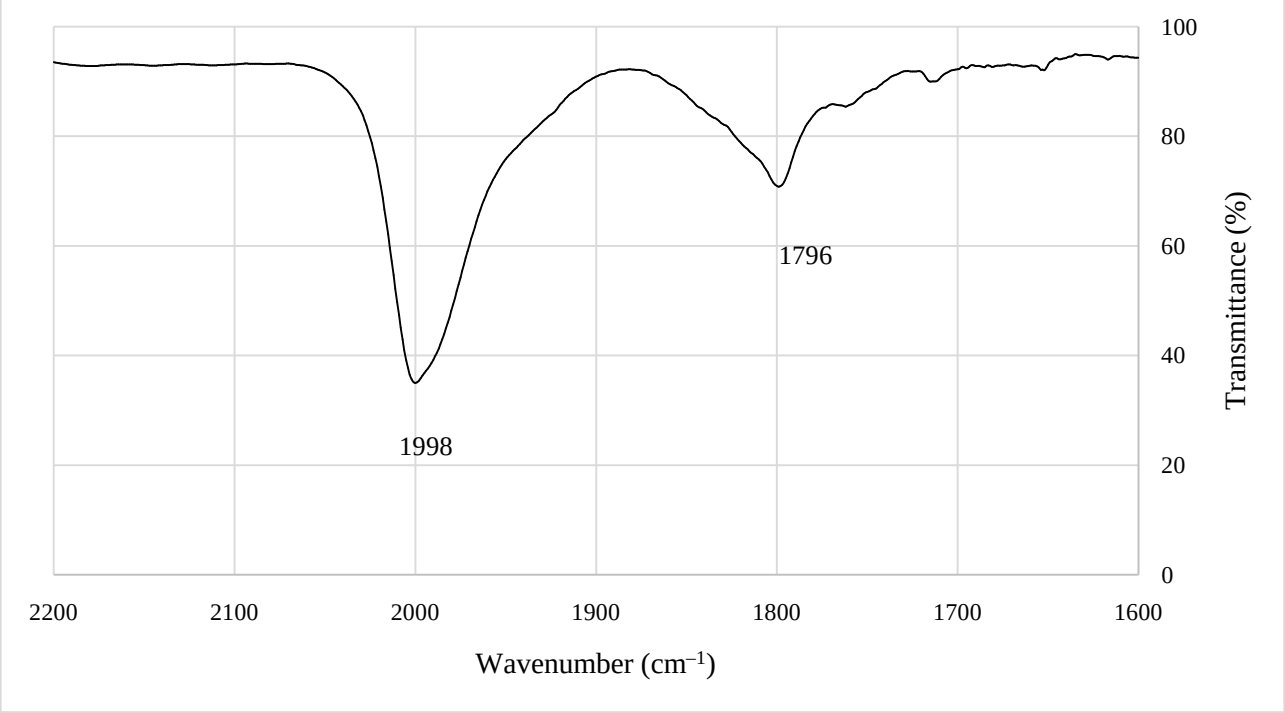


Figure S17

Molecular structure of $[Pt_{12-x}Ni_x(CO)_{21}]^{4-}$ (x = 3.72) (purple, Pt; yellow, Ni ≈ 21-32% and Pt ≈ 68-79%; orange, Ni ≈68-73% and Pt ≈ 27-32%; red, O; grey, C).

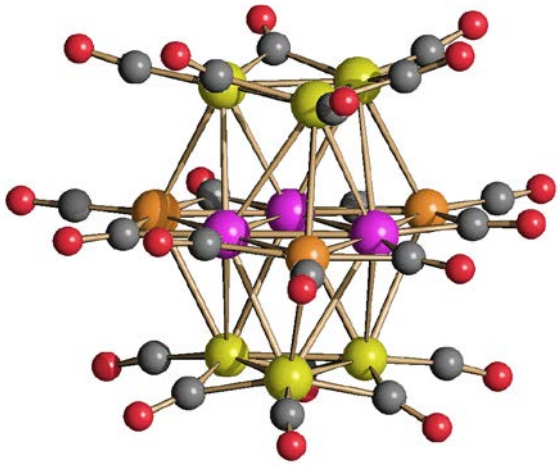


Figure S18

Molecular structure of $[Pt_{12-x}Ni_x(CO)_{21}]^{4-}$ (x = 5.82) (purple, Pt; yellow, Ni ≈ 49-58% and Pt ≈ 42-51%; orange, Ni ≈ 84-90% and Pt ≈ 10-16%; red, O; grey, C).

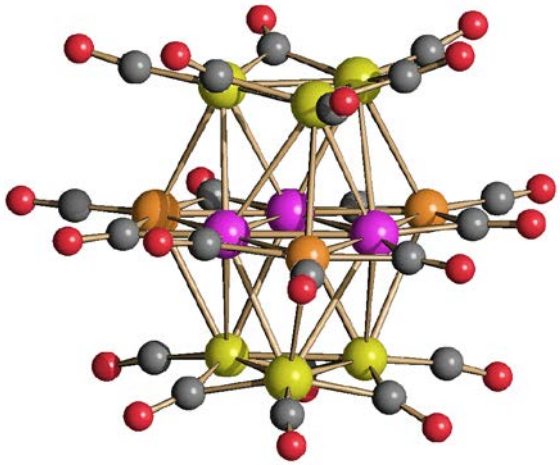


Figure S19

Molecular structure of $[Pt_{12-x}Ni_x(CO)_{21}]^{4-}$ (x = 6.45) (purple, Pt; yellow, Ni ≈ 25-96% and Pt ≈ 4-75%; orange, Ni ≈ 81-92% and Pt ≈ 8-19%; red, O; grey, C).

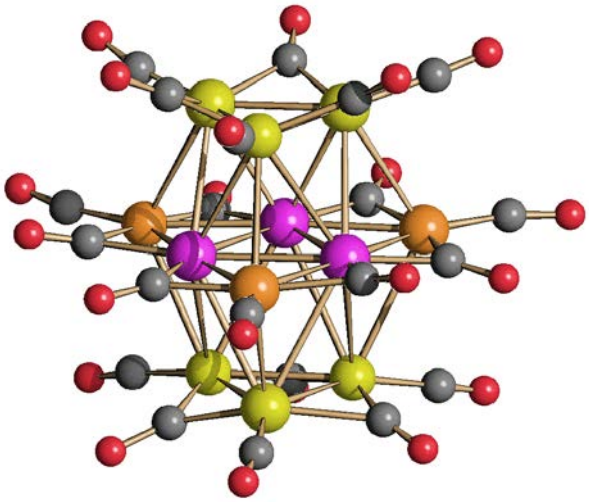


Figure S20

Molecular structure of $[Pt_{19-x}Ni_x(CO)_{22}]^{4-}$ (x = 2.23) (purple, Pt; yellow, Ni ≈ 7-41% and Pt ≈ 59-93%; red, O; grey, C).

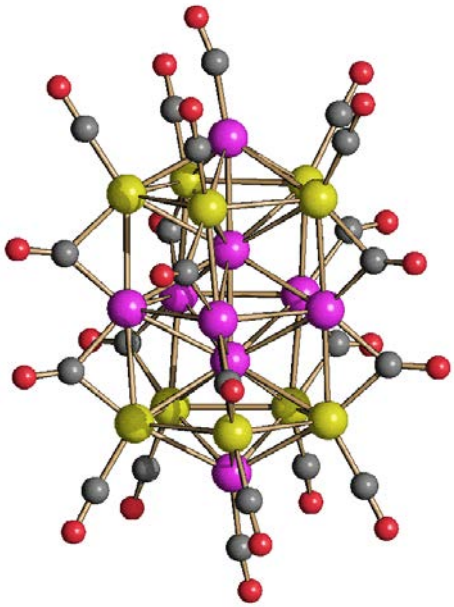
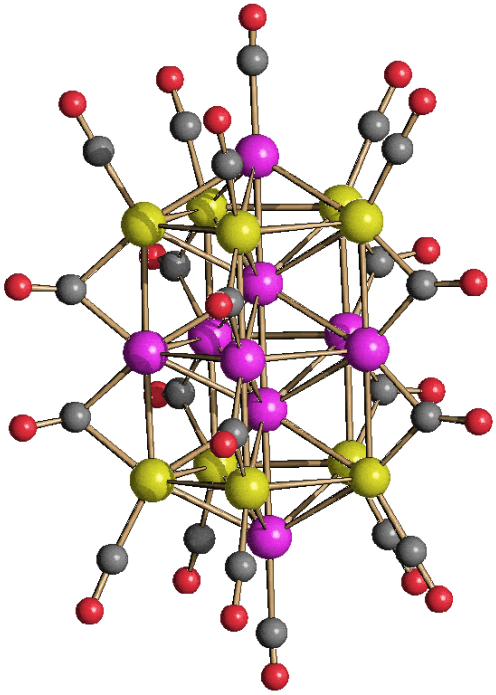


Figure S21

Molecular structure of $[Pt_{19-x}Ni_x(CO)_{22}]^{4-}$ (x = 3.11) (purple, Pt; yellow, Ni ≈ 27-35% and Pt ≈ 65-73%; red, O; grey, C).



X-ray Crystallographic Study

Crystal data and collection details for the structures deposited with CCDC, that is $[NBu_4]_4[Pt_{6-x}Ni_x(CO)_{12}]$ (x = 4.20), $[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]$ (x = 3.72), $[NBu_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 2CH_3COCH_3$ (x = 5.82), $[NEt_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3COCH_3$ (x = 2.23), $[NBu_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3CN$ (x = 3.11), $[NMe_4]_5[HPt_{14+x}Ni_{24-x}(CO)_{44}]\cdot 3CH_3COCH_3$ (x = 0.70) are reported in Table S5.

The structures of $[NMe_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 2CH_3CN$ (x = 6.25), $[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 1.79CH_3CN$ (x = 6.45), $[NBu_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3CN$ (x = 5.26) were of low quality and poorly diffracting. The resulting structures allowed to determine the overall geometry composition and connectivity of the clusters. These compared very well with related homometallic and heterometallic carbonyl clusters. Their cif files were included as Supplementary Material (cifSI.cif), but they were not deposited with CCDC. Their crystal data and collection details are reported in Table S6.

The diffraction experiments were carried out on a Bruker APEX II diffractometer equipped with a PHOTON2 detector using Mo–Kα radiation. Data were corrected for Lorentz polarization and absorption effects (empirical absorption correction SADABS).[1] Structures were solved by direct methods and refined by full-matrix least-squares based on all data using F^2.[2] Hydrogen atoms were fixed at calculated positions and refined by a riding model. All non-hydrogen atoms were refined with anisotropic displacement parameters, unless otherwise stated.

Structures deposited with CCDC

$[NBu_4]_4[Pt_{6-x}Ni_x(CO)_{12}]$ (x = 4.20): The asymmetric unit of the unit cell contains half of a cluster anion (located on an inversion centre) and one $[NBu_4]^+$ cation (located on a general position). The positions occupied by M(1), M(2) and M(3) are disordered Pt/Ni. These have been refined applying dummy atoms constraints (EADP and EXYZ lines in SHLEXL) resulting in the following refined occupancy factors: M(1) = 0.368(2) Pt and 0.632(2) Ni; M(2) = 0.356(2) Pt and 0.644(2) Ni; M(3) = 0.182(2) Pt and 0.818(2) Ni.

$[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]$ (x = 3.72): The asymmetric unit of the unit cell contains half of a cluster anion (located on 2) and two $[NEt_4]^+$ cations (located on general positions). The positions occupied by M(3), M(4), M(5), M(6) and M(7) are disordered Pt/Ni. These have been refined applying dummy atoms constraints (EADP and EXYZ lines in SHLEXL) resulting in the following refined occupancy factors: M(3) = 0.794(4) Pt and 0.206(4) Ni; M(4) = 0.730(4) Pt and 0.270(4) Ni; M(5) = 0.682(4) Pt and 0.318(4) Ni; M(6) = 0.325(5) Pt and 0.675(5) Ni; M(7) = 0.272(4) Pt and 0.728(4) Ni. The two $[NEt_4]^+$ cations are disordered and, therefore, they have been split into two positions and refined anisotropically employing one occupancy factor per disordered group. The $[NEt_4]^+$

cations have been restrained to have similar thermal parameters (SIMU line in SHELXL, s.u. 0.02) and similar geometries (SAME line in SHELXL, s.u. 0.04). Restraints to bond distances were applied as follow (s.u. 0.02): 1.47 Å for C–N and 1.53 Å for C–C in $[NEt_4]^+$.

$[NBu_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 2CH_3COCH_3$ (x = 5.82): The asymmetric unit of the unit cell contains half of a cluster anion (located on 2), two $[NBu_4]^+$ cations and one CH_3COCH_3 molecule (located on general positions). The positions occupied by M(3), M(4), M(5), M(6) and M(7) are disordered Pt/Ni. These have been refined applying dummy atoms constraints (EADP and EXYZ lines in SHLEXL) resulting in the following refined occupancy factors: M(3) = 0.508(7) Pt and 0.492(7) Ni; M(4) = 0.449(7) Pt and 0.551(7) Ni; M(5) = 0.424(7) Pt and 0.576(7) Ni; M(6) = 0.158(6) Pt and 0.842(6) Ni; M(7) = 0.104(9) Pt and 0.896(9) Ni. The $[NBu_4]^+$ cations and CH_3COCH_3 molecule have been restrained to have similar thermal parameters (SIMU line in SHELXL, s.u. 0.01). Restraints to bond distances were applied as follow (s.u. 0.02): 1.47 Å for C–N and 1.53 Å for C–C in $[NBu_4]^+$; 1.21 Å for C–O and 1.51 Å for C–C in CH_3COCH_3.

$[NEt_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3COCH_3$ (x = 2.23): The asymmetric unit of the unit cell contains half of a cluster anion (located on 2),two $[NEt_4]^+$ cations and one CH_3COCH_3 molecule (located on general positions). The positions occupied by M(6), M(7), M(8), M(9) and M(10) are disordered Pt/Ni. These have been refined applying dummy atoms constraints (EADP and EXYZ lines in SHLEXL) resulting in the following refined occupancy factors: M(6) = 0.930(9) Pt and 0.070(9) Ni; M(7) = 0.828(9) Pt and 0.172(9) Ni; M(8) = 0.748(9) Pt and 0.252(9) Ni; M(9) = 0.786(9) Pt and 0.214(9) Ni; M(10) = 0.594(9) Pt and 0.404(9) Ni. One $[NEt_4]^+$ cation is disordered and, therefore, it has been split into two positions and refined anisotropically employing one occupancy factor per disordered group. The $[NEt_4]^+$ cations have been restrained to have similar thermal parameters (SIMU line in SHELXL, s.u. 0.02). Restraints to bond distances were applied as follow (s.u. 0.02): 1.47 Å for C–N and 1.53 Å for C–C in $[NBu_4]^+$; 1.21 Å for C–O and 1.51 Å for C–C in CH_3COCH_3.

$[NBu_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3CN$ (x = 3.11): The asymmetric unit of the unit cell contains one fourth of a cluster anion (located on a site of symmetry *mm*2), two halves of $[NBu_4]^+$ cations (located on *m*), and one half of a CH_3CN molecule (located on *m*). The positions occupied by M(6), M(7) and M(8) are disordered Pt/Ni. These have been refined applying dummy atoms constraints (EADP and EXYZ lines in SHLEXL) resulting in the following refined occupancy factors: M(6) = 0.73(2) Pt and 0.27(2) Ni; M(7) = 0.646(14) Pt and 0.354(14) Ni; M(8) = 0.683(14) Pt and 0.317(15) Ni. The unit cell contains an additional total potential solvent accessible void of 335 $Å^3$ (*ca*. 5.7% of the Cell Volume), which is likely to be occupied by further highly disordered CH_3CN molecules. These voids have been treated using the SQUEEZE routine of PLATON.[3] Similar *U*

restraints have been applied to all C, O and N atoms (SIMU line in SHELXL, s.u. 0.01). Restraints to bond distances were applied as follow (s.u. 0.02): 1.47 Å for C–N and 1.53 Å for C–C in $[NBu_4]^+$; 1.14 Å for C–N and 1.49 Å for C–C in CH_3CN.

$[NMe_4]_5[HPt_{14+x}Ni_{24-x}(CO)_{44}]\cdot 3CH_3COCH_3$ (x = 0.70): The asymmetric unit of the unit cell contains one sixth of a cluster anion (located on $\bar{3}$), one third of a $[NMe_4]^+$ cation (located on $\bar{3}$), and one $[NMe_4]^+$ cation and one CH_3COCH_3 molecule. The latter cation and solvent molecules are disordered on the same general position and display 0.5 occupancy factor each. The position occupied by M(7) is disordered Pt/Ni. This has been refined applying dummy atoms constraints (EADP and EXYZ lines in SHLEXL) resulting in the following refined occupancy factor: M(4) = 0.116(3) Pt and 0.884(3) Ni. Restraints to bond distances were applied as follow (s.u. 0.02): 1.47 Å for C–N in $[NMe_4]^+$.

<u>Structures not deposited with CCDC</u>

$[NMe_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 2CH_3CN$ (x = 6.25): The asymmetric unit of the unit cell contains half of a cluster anion (located on 2), two $[NMe_4]^+$ cations and one CH_3CN molecule (located on general positions). The positions occupied by M(3), M(4), M(5), M(6) and M(7) are disordered Pt/Ni. These have been refined applying dummy atoms constraints (EADP and EXYZ lines in SHLEXL) resulting in the following refined occupancy factors: M(3) = 0.474(5) Pt and 0.526(5) Ni; M(4) = 0.372(4) Pt and 0.628(4) Ni; M(5) = 0.327(4) Pt and 0.673(4) Ni; M(6) = 0.147(5) Pt and 0.853(5) Ni; M(7) = 0.131(4) Pt and 0.869(4) Ni. The CO ligands has been restrained to isotropic behaviour (ISOR line in SHELXL, s.u. 0.005). One $[NMe_4]^+$ cation is disordered and, therefore, it has been split into two positions and refined anisotropically employing one occupancy factor per disordered group. The $[NMe_4]^+$ cations have been restrained to have similar thermal parameters (SIMU line in SHELXL, s.u. 0.02) and similar geometries (SAME line in SHELXL, s.u. 0.04).

$[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 1.78CH_3CN$ (x = 6.45): The asymmetric unit of the unit cell contains one cluster anion, four $[NEt_4]^+$ cations and two CH_3CN molecules (located on general positions). The positions occupied by M(4), M(5), M(6), M(7), M(8), M(9), M(10), M(11) and M(12) are disordered Pt/Ni. These have been refined applying dummy atoms constraints (EADP and EXYZ lines in SHLEXL) resulting in the following refined occupancy factors: M(4) = 0.754(12) Pt and 0.246(12) Ni; M(5) = 0.696(12) Pt and 0.304(12) Ni; M(6) = 0.513(12) Pt and 0.487(12) Ni; M(7) = 0.073(11) Pt and 0.927(11) Ni; M(8) = 0.040(11) Pt and 0.960(11) Ni; M(9) = 0.046(11) Pt and 0.954(12) Ni; M(10) = 0.082(12) Pt and 0.918(12) Ni; M(11) = 0.192(12) Pt and 0.808(12) Ni; M(12) = 0.160(12) Pt and 0.840(12) Ni. All the C, O and N atoms have been restrained to isotropic behaviour (ISOR line in SHELXL, s.u. 0.01). The $[NEt_4]^+$ cations have been restrained to have

similar geometries (SAME line in SHELXL, s.u. 0.04). One $[NEt_4]^+$ cation is disordered and, therefore, it has been split into two positions and refined anisotropically employing one occupancy factor per disordered group. The disorder model involves also one CH_3CN molecule which, therefore, possesses a partial occupation factor, that is 0.790(3). Restraints to bond distances were applied as follow (s.u. 0.02): 1.47 Å for C–N and 1.53 Å for C–C in $[NEt_4]^+$; 1.14 Å for C–N and 1.49 Å for C–C in CH_3CN.

$[NBu_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3CN$ (x = 5.26): The asymmetric unit of the unit cell contains one fourth of a cluster anion (located on a site of symmetry *mm*2), two halves of $[NBu_4]^+$ cations (located on *m*), and one half of a CH_3CN molecule (located on *m*). The positions occupied by M(6), M(7) and M(8) are disordered Pt/Ni. These have been refined applying dummy atoms constraints (EADP and EXYZ lines in SHLEXL) resulting in the following refined occupancy factors: M(6) = 0.533(13) Pt and 0.467(13) Ni; M(7) = 0.421(8) Pt and 0.5793(84) Ni; M(8) = 0.496(9) Pt and 0.504(9) Ni. The crystals appeared to be non-merohedrally twinned. The TwinRotMat routine of PLATON.[3] was used to determine the twinning matrices and to write the reflection data file (.hkl) containing the twin components. Refinement was performed using the instruction HKLF 5 in SHELXL and two BASF parameters, which refined as 0.250(8) and 0.165(7).The CO ligands has been restrained to have similar thermal parameters (SIMU line in SHELXL, s.u. 0.01) and to isotropic behaviour (ISOR line in SHELXL, s.u. 0.01). Similar *U* restraints have been applied to the $[NBu_4]^+$ cations (SIMU line in SHELXL, s.u. 0.001). The $[NBu_4]^+$ cations have been refined as rigid group (AFIX 6 line in SHELXL).

Table S5

Crystal data and experimental details for $[NBu_4]_4[Pt_{6-x}Ni_x(CO)_{12}]$ (x = 4.20), $[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]$ (x = 3.72), $[NBu_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 2CH_3COCH_3$ (x = 5.82), $[NEt_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3COCH_3$ (x = 2.23), $[NBu_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3CN$ (x = 3.11), $[NMe_4]_5[HPt_{14+x}Ni_{24-x}(CO)_{44}]\cdot 3CH_3COCH_3$ (x = 0.70). These structures have been deposited with CCDC.

	$[NBu_4]_4[Pt_{6-x}Ni_x(CO)_{12}]$ (x = 4.20)	**$[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]$ (x = 3.72)**	**$[NBu_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 2CH_3COCH_3$ (x = 5.82)**
Formula	$C_{44}H_{72}N_2Ni_{4.20}O_{12}Pt_{1.80}$	$C_{53}H_{80}N_4Ni_{3.72}O_{21}Pt_{8.28}$	$C_{91}H_{156}N_4Ni_{5.82}O_{23}Pt_{6.18}$
Fw	1418.78	2942.95	3221.88
T, K	100(2)	100(2)	100(2)
λ, Å	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Orthorhombic
Space Group	$P\bar{1}$	$C2/c$	$Pbcn$
a, Å	11.0302(12)	21.4147(14)	17.409(5)
b, Å	11.8415(14)	13.4345(8)	25.656(7)
c, Å	11.9367(14)	24.8815(15)	24.249(6)
α, °	89.874(4)	90	90
β, °	64.953(4)	109.099(2)	90
γ, °	70.960(4)	90	90
Cell Volume, $Å^3$	1318.3(3)	6764.3(7)	10830(5)
Z	1	4	4
D_c, g cm^{-3}	1.787	2.890	1.976
μ, mm^{-1}	6.282	18.128	9.001
F(000)	704	5376	6236
Crystal size, mm	0.18×0.16×0.12	0.18×0.16×0.12	0.18×0.16×0.13
θ limits, °	1.907–27.000	1.732–25.998	1.414–25.050
Index ranges	$-14 \le h \le 14$ $-15 \le k \le 15$ $-15 \le l \le 15$	$-26 \le h \le 26$ $-16 \le k \le 16$ $-30 \le l \le 30$	$-20 \le h \le 20$ $-30 \le k \le 30$ $-28 \le l \le 28$
Reflections collected	24906	43980	79829
Independent reflections	5738 [R_{int} = 0.0834]	6602 [R_{int} = 0.0539]	9569 [R_{int} = 0.1330]
Completeness to θ max	99.9%	99.4%	99.7%
Data / restraints / parameters	5738 / 0 / 296	6602 / 244 / 389	9569/ 302 / 593

Goodness on fit on F^2	1.017	1.237	1.125
R_1 ($I > 2\sigma(I)$)	0.0332	0.0498	0.0967
wR_2 (all data)	0.0762	0.0962	0.2643
Largest diff. peak and hole, e Å^{-3}	1.153 / –0.870	1.727 / –2.928	3.952 / –2.626

	$[NEt_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3COCH_3$ (x = 2.23)	**$[NBu_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3CN$ (x = 3.11)**	**$[NMe_4]_5[HPt_{14+x}Ni_{24-x}(CO)_{22}]\cdot 3CH_3COCH_3$ (x = 0.70)**
Formula	$C_{60}H_{92}N_4Ni_{2.23}O_{24}Pt_{16.77}$	$C_{90}H_{150}N_6Ni_{3.11}O_{22}Pt_{15.89}$	$C_{73}H_{78}N_5Ni_{23.20}O_{47}Pt_{14.70}$
Fw	4656.29	4950.72	6012.97
T, K	100(2)	100(2)	100(2)
λ, Å	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Orthorhombic	Trigonal
Space Group	*C*2/*c*	*Pmmn*	$R\bar{3}$
a, Å	25.210(2)	17.067(4)	16.2307(19)
b, Å	13.3089(11)	20.438(5)	16.2307(19)
c, Å	26.112(2)	16.797(4)	36.437(5)
α, °	90	90	90
β, °	105.662(3)	90	90
γ, °	90	90	120
Cell Volume, Å^3	8435.7(12)	5859(2)	8313(2)
Z	4	2	3
D_c, g cm^{-3}	3.666	2.806	3.603
μ, mm^{-1}	28.236	19.429	22.395
F(000)	8170	4469	8178
Crystal size, mm	0.19×0.15×0.11	0.18×0.16×0.12	0.16×0.15×0.13
θ limits, °	1.745–25.099	1.971–25.000	1.677–25.994
Index ranges	-29 ≤ h ≤ 29 -15 ≤ k ≤ 15 -31 ≤ l ≤ 31	-20 ≤ h ≤ 20 -24 ≤ k ≤ 24 -19 ≤ l ≤ 19	-20 ≤ h ≤ 20 -20 ≤ k ≤ 20 -44 ≤ l ≤ 44
Reflections collected	47303	52911	41806
Independent reflections	7357 [R_{int} = 0.0825]	5476 [R_{int} = 0.0887]	3617 [R_{int} = 0.1759]
Completeness to θ max	99.2%	99.2%	99.9%
Data / restraints / parameters	7357 / 382 / 561	5467/ 85 / 202	3617 / 55 / 238

Goodness on fit on F^2	1.174	1.128	1.050
R_1 ($I > 2\sigma(I)$)	0.0878	0.1507	0.0446
wR_2 (all data)	0.2307	0.4267	0.1287
Largest diff. peak and hole, e $Å^{-3}$	4.233 / –2.786	5.642 / –2.750	3.175 / –2.525

Table S6

Crystal data and experimental details for $[NMe_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 2CH_3CN$ (x = 6.25), $[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 1.79CH_3CN$ (x = 6.45), $[NBu_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3CN$ (x = 5.26). These structures have not been deposited with CCDC.

	$[NMe_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 2CH_3CN$ (x = 6.25)	**$[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 1.79CH_3CN$ (x = 6.45)**	**$[NBu_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3CN$ (x = 5.26)**
Formula	$C_{41}H_{54}N_6Ni_{6.25}O_{21}Pt_{5.75}$	$C_{56.58}H_{85.37}N_{5.79}Ni_{6.45}O_{21}Pt_{5.56}$	$C_{90}H_{150}N_6Ni_{5.26}O_{22}Pt_{13.73}$
Fw	2455.60	2644.80	4656.82
T, K	100(2)	100(2)	100(2)
λ, Å	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Orthorhombic
Space Group	*C*2/*c*	$P\bar{1}$	*Pmmn*
a, Å	19.316(3)	13.2466(19)	17.121(5)
b, Å	13.933(2)	14.556(2)	20.403(6)
c, Å	21.955(3)	18.866(3)	16.642(6)
α, °	90	91.855(4)	90
β, °	103.199(4)	92.379(4)	90
γ, °	90	91.164(4)	90
Cell Volume, $Å^3$	5752.6(16)	3631.7(9)	5814(3)
Z	4	2	2
D_c, g cm^{-3}	2.835	2.419	2.660
μ, mm^{-1}	15.991	12.350	17.339
F(000)	4534	2494	4254
Crystal size, mm	0.15×0.13×0.12	0.16×0.13×0.11	0.16×0.13×0.12
θ limits, °	1.819–24.999	1.539–24.997	1.706–25.011
Index ranges	-22 ≤ h ≤ 22 -16 ≤ k ≤ 16 -26 ≤ l ≤ 26	-15 ≤ h ≤ 15 -17 ≤ k ≤ 17 -22 ≤ l ≤ 22	-20 ≤ h ≤ 20 -24 ≤ k ≤ 24 -19 ≤ l ≤ 19
Reflections collected	28086	40409	30201
Independent reflections	4997 [R_{int} = 0.0893]	12476 [R_{int} = 0.1260]	5418 [R_{int} = 0.1469]
Completeness to θ max	98.7%	97.4%	99.2%
Data / restraints / parameters	4997 / 400 / 386	12476 / 1101 / 919	5418/ 154 / 210
Goodness on fit	1.073	1.081	1.356

on F^2			
R_1 ($I > 2\sigma(I)$)	0.0706	0.1570	0.1433
wR_2 (all data)	0.1796	0.4208	0.4018
Largest diff. peak and hole, e $Å^{-3}$	2.659 / –2.176	4.155 / –1.561	7.162 / –6.474

Figure S22

IR spectral changes of a CH_3CN solution of $[Pt_{19}(CO)_{22}]^{4-}$ recorded in an OTTLE cell during the progressive increase of the potential from –0.4 to +0.2 V *vs* Ag pseudo-reference electrode (scan rate 1 mV sec^{-1}). $[N^nBu_4][PF_6]$ (0.1 mol dm^{-3}) as the supporting electrolyte. The absorptions of the solvent and supporting electrolyte have been subtracted.

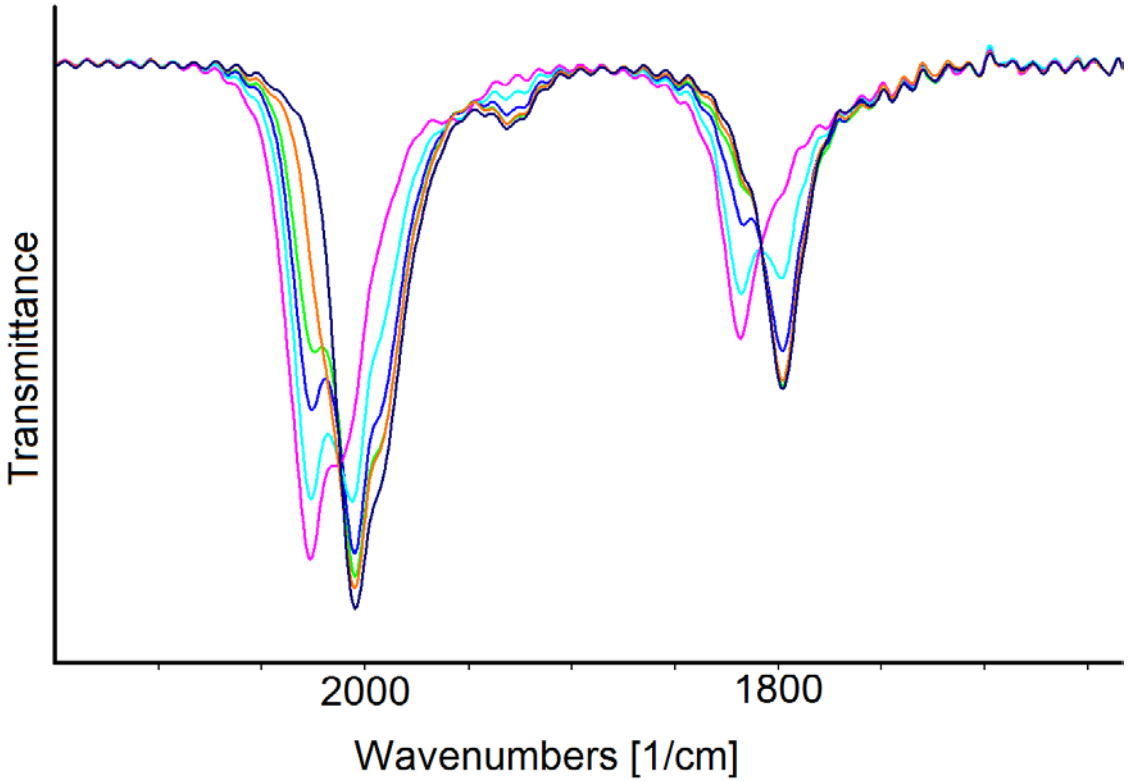
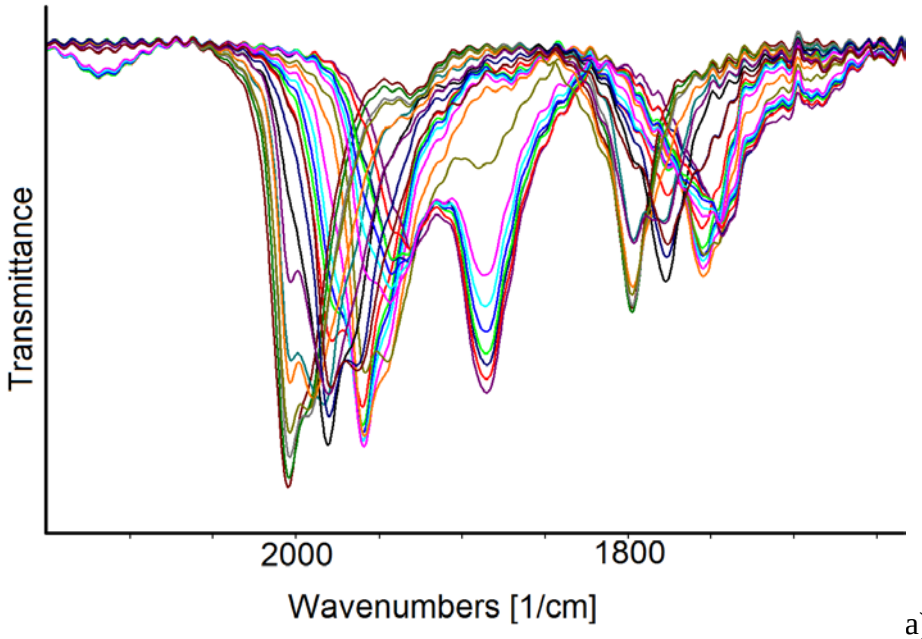
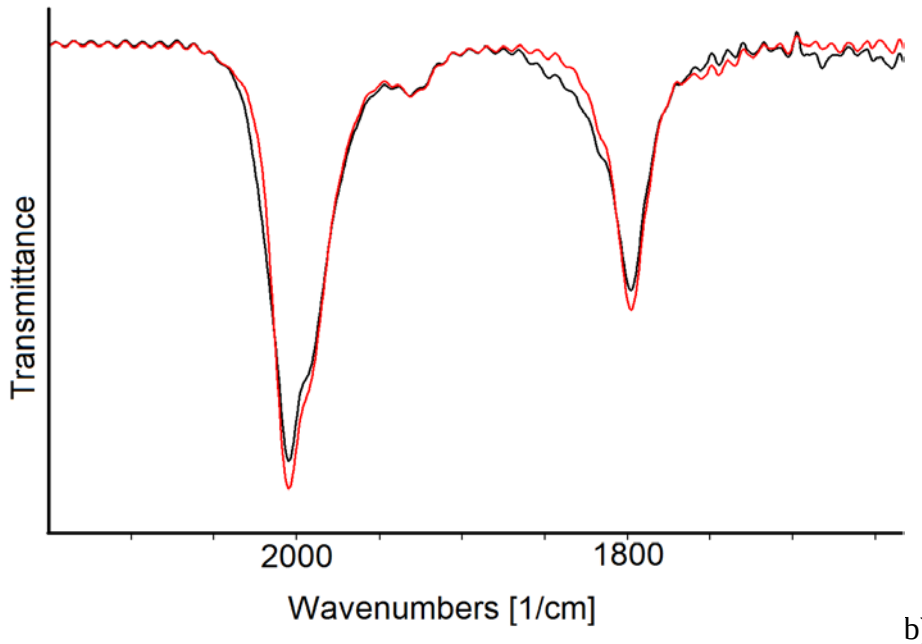


Figure S23

IR spectral changes of a CH_3CN solution of $[Pt_{19}(CO)_{22}]^{4-}$ recorded in an OTTLE cell a) during the progressive decrease of the potential from –0.7 to –2.5V *vs* Ag pseudo-reference electrode (scan rate 2 mV sec^{-1}); b) before (red line) and after (black line) the cyclic voltammetry between –0.7 and –2.5V (*vs* Ag pseudo reference electrode, scan rate 2 mV sec^{-1}).$[N^nBu_4][PF_6]$ (0.1 mol dm^{-3}) as the supporting electrolyte. The absorptions of the solvent and supporting electrolyte have been subtracted.



a)



b)

Figure S24

CV response of $[Pt_{19-x}Ni_x(CO)_{22}]^{4-}$ (x= 3.11) at a GC (blue line) and at a Pt (red line) electrodes in CH_3CN solution of $[N^nBu_4][PF_6]$ (0.1 mol dm^{-3}) supporting electrolyte. Scan rate: 0.1 V s^{-1}.

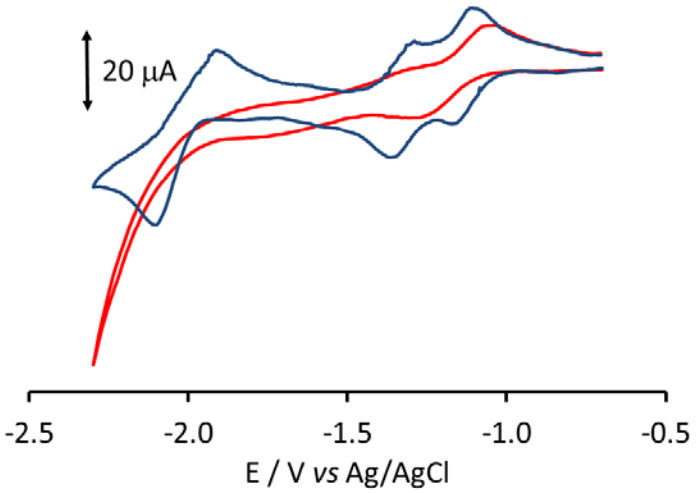


Figure S25

ORTEP drawing of the cluster anion of $[NBu_4]_4[Pt_{6-x}Ni_x(CO)_{12}]$ (x = 4.20). Thermal ellipsoids are at the 50% probability level (orange, disordered Pt/Ni; red, O; black, C). CCDC 2217067

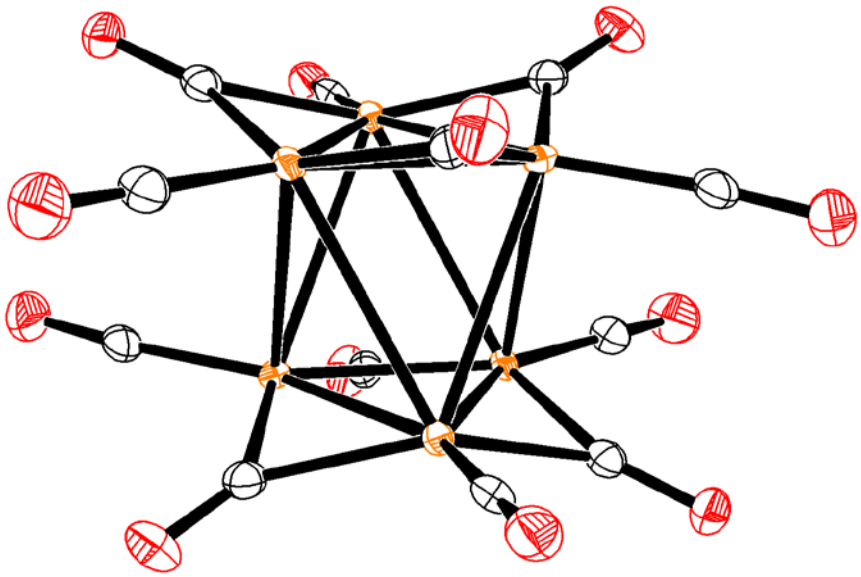


Figure S26

ORTEP drawing of the cluster anion of $[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]$ (x = 3.72). Thermal ellipsoids are at the 50% probability level (purple, Pt; orange, disordered Pt/Ni; red, O; black, C). CCDC 2217068

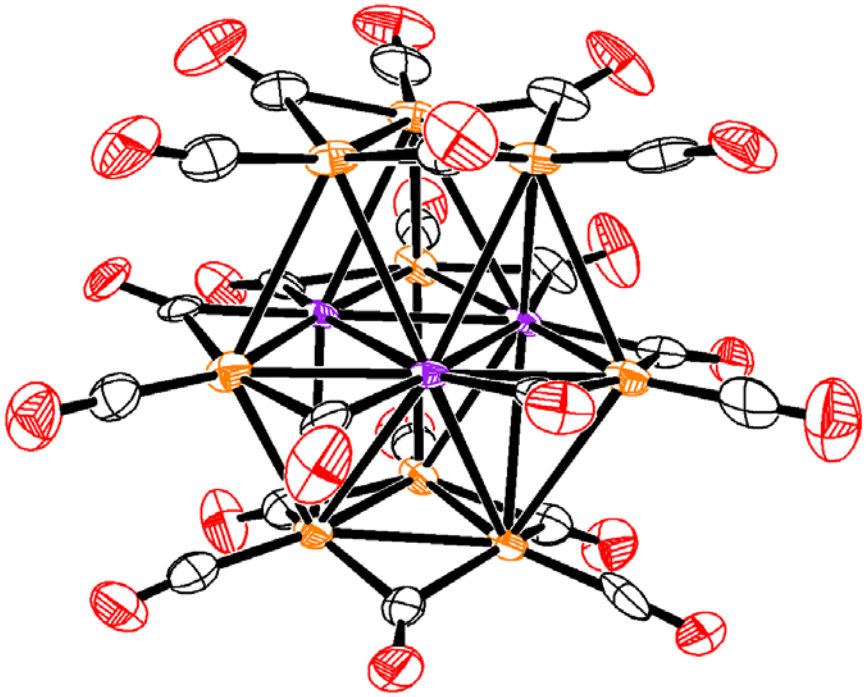


Figure S27

ORTEP drawing of the cluster anion of $[NBu_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 2CH_3COCH_3$ (x = 5.82). Thermal ellipsoids are at the 50% probability level (purple, Pt; orange, disordered Pt/Ni; red, O; black, C). CCDC 2217069

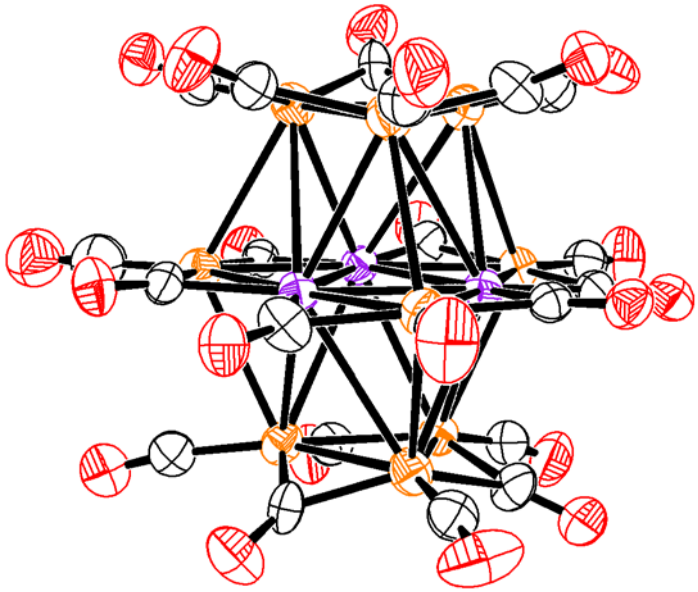


Figure S28

ORTEP drawing of the cluster anion of $[NEt_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3COCH_3$ (x = 2.23). Thermal ellipsoids are at the 50% probability level (purple, Pt; orange, disordered Pt/Ni; red, O; black, C). CCDC 2217072

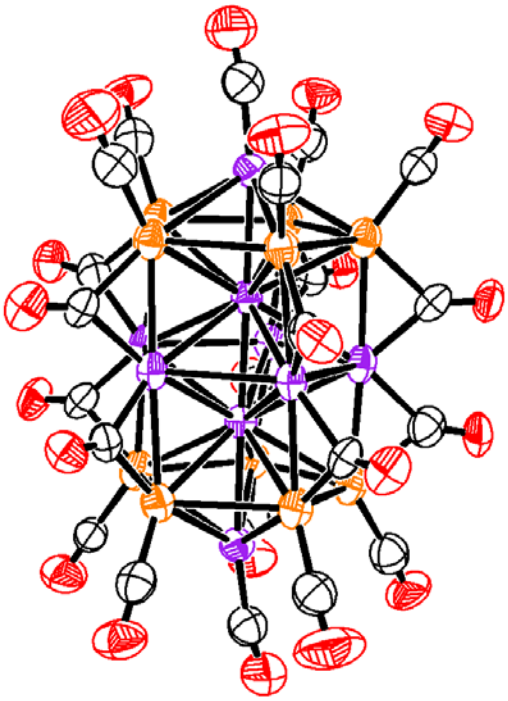


Figure S29

ORTEP drawing of the cluster anion of $[NBu_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3CN$ (x = 3.11). Thermal ellipsoids are at the 50% probability level (purple, Pt; orange, disordered Pt/Ni; red, O; black, C). CCDC 2217073

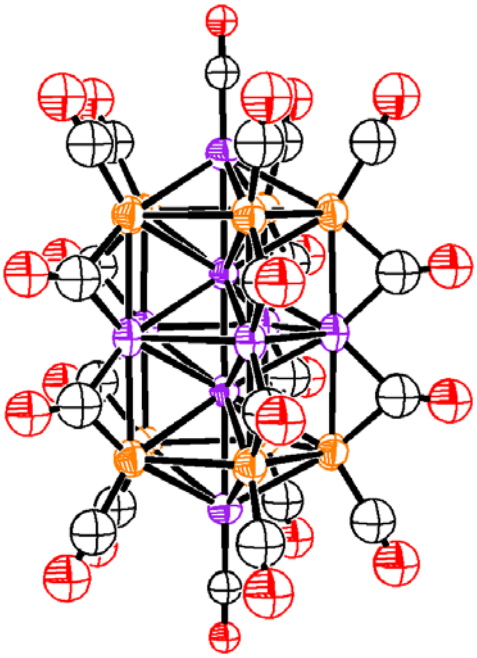


Figure S30

ORTEP drawing of the cluster anion of $[NMe_4]_5[HPt_{14+x}Ni_{24-x}(CO)_{44}]\cdot 3CH_3COCH_3$ (x = 0.70). Thermal ellipsoids are at the 50% probability level (purple, Pt; green, Ni; yellow, disordered Pt/Ni; red, O; black, C). CCDC 2217076

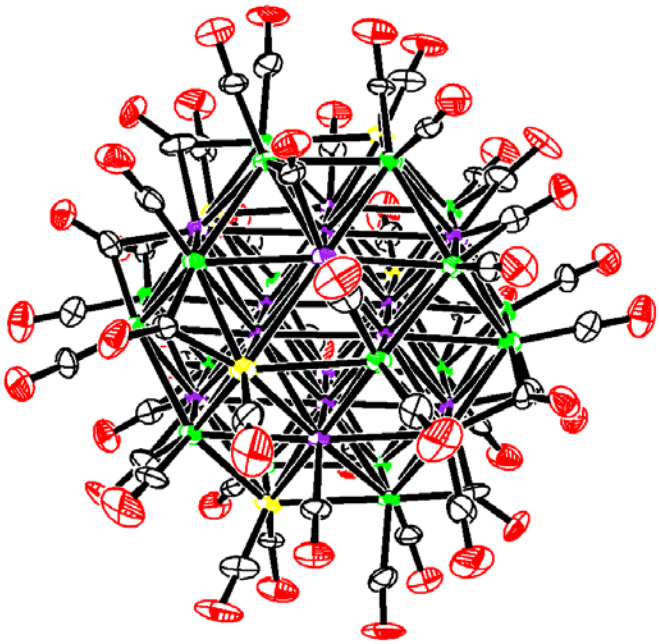


Figure S31

ORTEP drawing of the cluster anion of $[NMe_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 2CH_3CN$ (x = 6.25). Thermal ellipsoids are at the 50% probability level (purple, Pt; orange, disordered Pt/Ni; red, O; black, C).

No CCDC

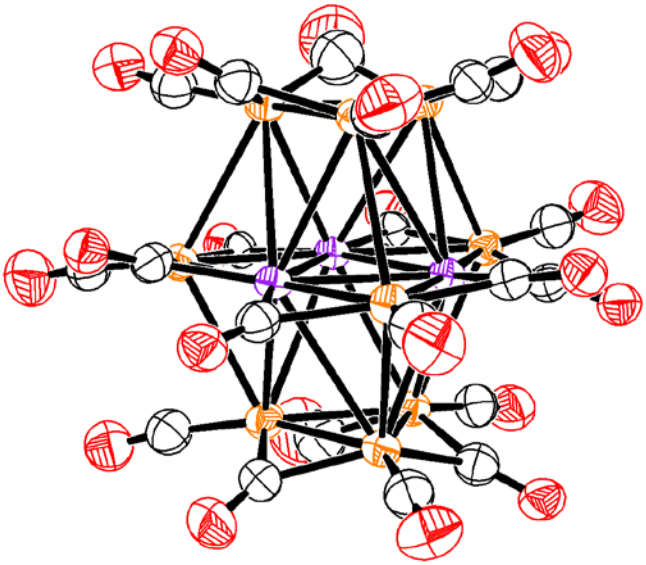


Figure S32

ORTEP drawing of the cluster anion of $[NEt_4]_4[Pt_{12-x}Ni_x(CO)_{21}]\cdot 1.79CH_3CN$ (x = 6.45). Thermal ellipsoids are at the 50% probability level (purple, Pt; orange, disordered Pt/Ni; red, O; black, C).

No CCDC

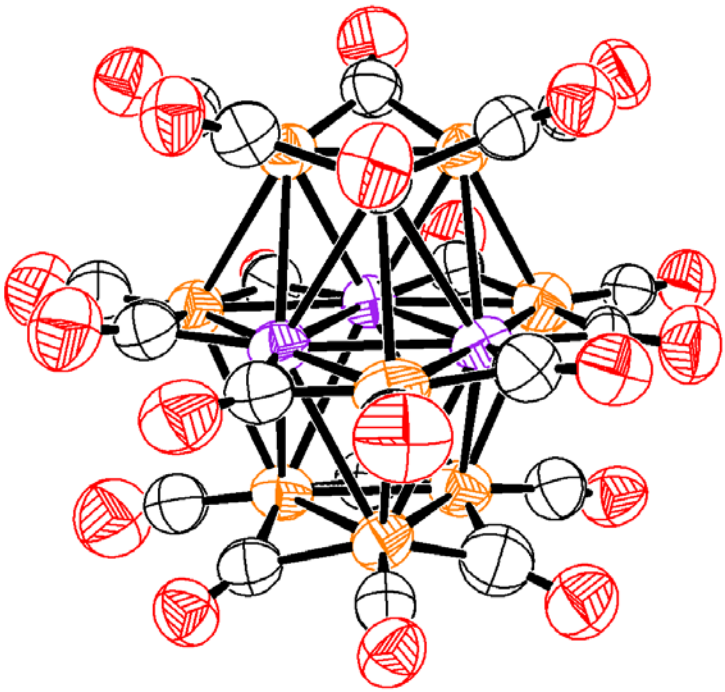
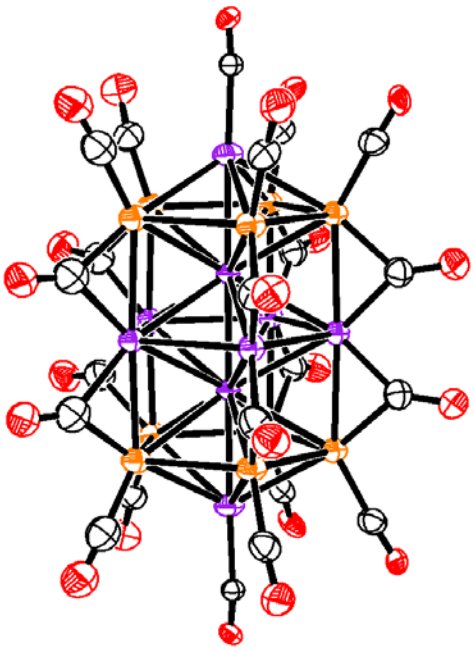


Figure S33

ORTEP drawing of the cluster anion of $[NBu_4]_4[Pt_{19-x}Ni_x(CO)_{22}]\cdot 2CH_3CN$ (x = 5.26). Thermal ellipsoids are at the 50% probability level (purple, Pt; orange, disordered Pt/Ni; red, O; black, C).

No CCDC



Cartesian coordinates, energy values and computed frequencies

$[PtNi_{11}(CO)_{21}]^{4-}$ isA (E = -19076.480479556431 a.u., G^{298K} = -19076.38614915 a.u.)

54
PtNi11C21O21

Ni	0.007703467	0.033995620	-1.524729403
Ni	-1.357425337	0.048644165	0.839745193
Ni	-0.057297097	-2.315129106	1.470857261
Pt	1.245348273	-2.552500306	-0.704060784
Ni	-1.287743928	-2.266130012	-0.670837669
Ni	0.013940708	-0.007361859	2.850398195
Ni	-2.420001924	0.087373602	-1.352879317
C	-2.798212971	-2.641012731	-1.460716187
C	-0.211403122	-2.856108225	-2.117790380
C	2.782955222	-3.140493178	-1.595578188
C	1.709034575	-2.962723871	1.256034432
C	-0.172416246	-2.724411390	3.164368427
C	-1.860538687	-2.691196001	1.070101583
C	-3.905617387	0.182029864	-2.233578686
C	-3.140833298	0.082243739	0.421075536
C	0.025115433	0.033316117	4.580583171
C	-1.227819934	-0.054745567	-2.857134837
C	-1.882144008	0.092228867	2.591706811
O	-3.748189856	-3.050999830	-1.962538513
O	-0.305610638	-3.304889734	-3.193899769
O	3.702724840	-3.586499620	-2.132689070
O	2.571930037	-3.469717378	1.861642730
O	-0.255027004	-3.158790125	4.226047923
O	-2.811686793	-3.105921571	1.609286672
O	-4.892474178	0.264468377	-2.822776531
O	-4.232417740	0.090138024	0.840913566
O	0.033197834	0.072280657	5.732201466
O	-1.412584362	-0.170946264	-4.006478197
O	-2.784465697	0.159405341	3.333212940
Ni	1.377107213	-0.021731930	0.842841710
Ni	0.060853888	2.289979333	1.456398798
Ni	-1.143846560	2.326777031	-0.627750754
Ni	1.276023308	2.260364744	-0.629084878
Ni	2.431867597	-0.072380752	-1.348534736
C	2.740236610	2.705335478	-1.468800058
C	0.077279650	2.828629943	-1.962386036
C	-2.571992020	2.866388151	-1.466248228
C	-1.707981505	2.824738916	1.093246239
C	0.079896283	2.790644962	3.123165280
C	1.846001920	2.755620912	1.090378987
C	3.911525352	-0.214109707	-2.228011485
C	3.162237840	0.049185110	0.416504586
C	1.269057040	0.153200124	-2.851958922
C	1.912482549	-0.163154393	2.575789081
O	3.669419210	3.129384747	-1.999509941
O	0.088373623	3.340162422	-3.014320715
O	-3.465399802	3.365407126	-1.994847761
O	-2.618735907	3.325369800	1.630219046
O	0.099327097	3.253037593	4.177859327
O	2.768902910	3.233009356	1.627614751
O	4.892001674	-0.327487985	-2.823117027
O	4.248895673	0.173713162	0.830389250
O	1.454064753	0.346384803	-3.990456690
O	2.814361424	-0.305016553	3.307532650

Computed frequencies (cm^{-1})

1:	13.46	61:	233.94	121:	535.81
2:	15.44	62:	243.02	122:	537.27
3:	25.07	63:	250.87	123:	539.06
4:	27.56	64:	251.03	124:	546.79
5:	34.73	65:	252.12	125:	548.20
6:	35.91	66:	257.83	126:	548.42
7:	40.62	67:	261.79	127:	563.57
8:	41.81	68:	275.03	128:	576.62
9:	49.86	69:	275.63	129:	582.64
10:	53.69	70:	285.04	130:	598.30
11:	58.69	71:	305.54	131:	601.32
12:	60.79	72:	309.78	132:	613.85
13:	63.37	73:	384.17	133:	615.57
14:	64.04	74:	389.31	134:	617.78
15:	64.74	75:	393.48	135:	648.09
16:	67.28	76:	393.66	136:	1911.69
17:	70.18	77:	399.66	137:	1912.73
18:	71.30	78:	400.76	138:	1922.70
19:	71.57	79:	403.65	139:	1931.27
20:	73.16	80:	405.45	140:	1931.78
21:	74.48	81:	410.13	141:	1942.45
22:	74.89	82:	411.24	142:	1943.46
23:	77.35	83:	420.41	143:	1954.09
24:	78.71	84:	423.66	144:	1963.36
25:	79.77	85:	427.44	145:	1990.89
26:	81.73	86:	428.11	146:	1992.20
27:	82.75	87:	428.80	147:	2003.26
28:	84.67	88:	429.38	148:	2079.17
29:	84.84	89:	431.34	149:	2083.18
30:	86.10	90:	432.63	150:	2089.85
31:	88.14	91:	434.69	151:	2097.72
32:	90.24	92:	440.68	152:	2099.15
33:	96.39	93:	443.54	153:	2119.48
34:	102.41	94:	445.32	154:	2127.64
35:	104.22	95:	446.28	155:	2128.48
36:	106.03	96:	453.68	156:	2169.08
37:	108.51	97:	459.66		
38:	114.67	98:	460.24		
39:	115.99	99:	462.75		
40:	120.78	100:	463.46		
41:	121.52	101:	465.50		
42:	122.20	102:	467.44		
43:	124.77	103:	470.54		
44:	132.24	104:	471.79		
45:	142.00	105:	475.86		
46:	146.68	106:	477.08		
47:	153.70	107:	481.24		
48:	154.19	108:	482.78		
49:	156.78	109:	483.75		
50:	157.62	110:	488.19		
51:	159.17	111:	490.45		
52:	177.02	112:	494.32		
53:	180.26	113:	497.93		
54:	183.99	114:	510.00		
55:	185.72	115:	510.27		
56:	206.56	116:	515.02		
57:	208.45	117:	517.36		
58:	215.56	118:	525.12		
59:	216.85	119:	528.83		
60:	222.73	120:	534.11		

$[PtNi_{11}(CO)_{21}]^{4-}$ is B_e (E = -19076.474610605354 a.u., G^{298K} = -19076.37934703 a.u.)

54
PtNi11C21O21

Ni	-0.000339093	0.000836530	-1.486317744
Ni	-1.410295294	0.050302594	0.891708546
Ni	-0.079645345	-2.354060785	1.416199771
Ni	1.121617415	-2.323776019	-0.665678128
Ni	-1.297126389	-2.238311631	-0.653912400
Pt	-0.000611689	-0.000415566	3.092393303
Ni	-2.424376102	0.082239728	-1.339816935
C	-2.756988580	-2.667362898	-1.504365211
C	-0.114804171	-2.773724684	-2.009745211
C	2.549268096	-2.864184231	-1.506813259
C	1.688262084	-2.863476520	1.042416985
C	-0.104136371	-2.928688497	3.066659174
C	-1.882389595	-2.732794879	1.065883077
C	-3.914816857	0.154826149	-2.221193758
C	-3.174590665	-0.035009237	0.405072975
C	-0.000796825	0.000145979	4.949221366
C	-1.233321615	0.187145832	-2.830711035
C	-2.045444289	0.225114194	2.603309476
O	-3.676366973	-3.095630255	-2.050266328
O	-0.138649171	-3.254660425	-3.076006287
O	3.443746332	-3.362256288	-2.034079137
O	2.599901053	-3.384264735	1.558768866
O	-0.132271461	-3.426985304	4.103443033
O	-2.822748106	-3.185582654	1.594465737
O	-4.906668221	0.208289796	-2.803882351
O	-4.271304716	-0.154088085	0.794367410
O	-0.001175335	0.000127288	6.106557724
O	-1.391507976	0.346415125	-3.977869636
O	-2.971743775	0.426734357	3.287056311
Ni	1.410012445	-0.050554327	0.891680339
Ni	0.079485500	2.353990860	1.416987226
Ni	-1.121243982	2.324857645	-0.665136050
Ni	1.297303075	2.238277438	-0.652906172
Ni	2.423373112	-0.080783243	-1.341042044
C	2.757453172	2.667794017	-1.502501885
C	0.115520311	2.773525103	-2.009335797
C	-2.548848387	2.864758669	-1.506731248
C	-1.687719347	2.865814997	1.042296067
C	0.104512611	2.928513736	3.067399472
C	1.883503764	2.728813248	1.067591426
C	3.913647749	-0.152283654	-2.222890719
C	3.174338647	0.028570937	0.404138013
C	1.231764509	-0.187023528	-2.831413024
C	2.044906711	-0.219907994	2.604012707
O	3.677071793	3.096568475	-2.047646876
O	0.139759523	3.253691409	-3.075945231
O	-3.443816343	3.362776805	-2.033237718
O	-2.598819929	3.387956173	1.558232023
O	0.133631611	3.426690849	4.104213279
O	2.824787704	3.178774108	1.596964252
O	4.905512389	-0.205040835	-2.805622305
O	4.271932346	0.140472350	0.792981306
O	1.389218598	-0.348890706	-3.978286405
O	2.972036053	-0.414267412	3.288733881

Computed frequencies (cm^{-1})

1:	i14.99	61:	243.98	121:	531.26
2:	10.98	62:	250.65	122:	531.56
3:	26.63	63:	250.70	123:	534.51
4:	29.80	64:	251.65	124:	535.12
5:	30.77	65:	252.00	125:	546.89
6:	33.18	66:	260.02	126:	553.00
7:	38.12	67:	261.79	127:	563.79
8:	40.65	68:	262.82	128:	563.79
9:	50.37	69:	274.42	129:	594.60
10:	55.90	70:	290.32	130:	598.82
11:	58.31	71:	291.96	131:	600.42
12:	58.89	72:	313.89	132:	604.59
13:	59.66	73:	394.72	133:	610.82
14:	60.03	74:	394.82	134:	628.79
15:	66.96	75:	395.01	135:	641.55
16:	68.43	76:	395.86	136:	1911.24
17:	69.89	77:	398.88	137:	1913.87
18:	72.67	78:	402.83	138:	1924.02
19:	73.68	79:	405.66	139:	1930.82
20:	73.83	80:	408.96	140:	1932.20
21:	75.34	81:	410.17	141:	1941.88
22:	75.85	82:	416.58	142:	1942.70
23:	76.59	83:	419.31	143:	1954.14
24:	77.24	84:	424.59	144:	1960.16
25:	78.60	85:	426.11	145:	1990.95
26:	80.56	86:	426.76	146:	1995.86
27:	81.49	87:	429.72	147:	2007.47
28:	85.06	88:	432.38	148:	2075.13
29:	85.74	89:	432.90	149:	2083.17
30:	86.72	90:	432.96	150:	2090.44
31:	86.93	91:	434.29	151:	2093.52
32:	89.24	92:	436.61	152:	2097.50
33:	91.66	93:	442.18	153:	2117.36
34:	101.28	94:	446.98	154:	2121.42
35:	101.43	95:	450.00	155:	2128.02
36:	103.97	96:	452.64	156:	2166.71
37:	107.58	97:	455.68		
38:	108.77	98:	458.29		
39:	114.29	99:	462.02		
40:	115.73	100:	462.27		
41:	120.03	101:	463.79		
42:	122.38	102:	465.42		
43:	125.84	103:	466.51		
44:	132.62	104:	475.47		
45:	138.54	105:	477.53		
46:	143.18	106:	479.80		
47:	147.01	107:	483.27		
48:	149.34	108:	483.71		
49:	152.80	109:	484.39		
50:	162.27	110:	485.35		
51:	164.32	111:	488.46		
52:	182.45	112:	497.42		
53:	182.77	113:	497.98		
54:	184.73	114:	506.11		
55:	188.70	115:	506.20		
56:	193.81	116:	512.25		
57:	202.58	117:	513.37		
58:	214.49	118:	520.73		
59:	234.86	119:	527.44		
60:	235.94	120:	528.74		

$[PtNi_{11}(CO)_{21}]^{4-}$ isB$_i$ (E = -19076.502016993978 a.u., G^{298K} = -19076.40802153 a.u.)

54
PtNi11C21O21

Pt	-0.000162958	0.000284301	-1.445342732
Ni	-1.434095324	0.041343558	0.849643430
Ni	-0.071387567	-2.270600927	1.413045140
Ni	1.141024448	-2.434507037	-0.664621560
Ni	-1.301554509	-2.342002579	-0.667311830
Ni	-0.000467224	-0.000270851	2.826727973
Ni	-2.528969770	0.111356286	-1.356909851
C	-2.765092356	-2.762533368	-1.509449951
C	-0.105204553	-2.994752168	-1.975648780
C	2.569345229	-2.983527881	-1.489434529
C	1.698230828	-2.847739667	1.074304199
C	-0.098420317	-2.738701147	3.091100177
C	-1.872194119	-2.736323290	1.072528780
C	-4.043306940	0.183574967	-2.168748455
C	-3.210808611	-0.003785764	0.449071344
C	-0.000602544	-0.000751304	4.558717096
C	-1.375240834	0.177097966	-2.885201680
C	-1.912239936	0.146294716	2.595753090
O	-3.697750979	-3.165810745	-2.051373797
O	-0.125492474	-3.535428072	-3.011925967
O	3.471271116	-3.476995238	-2.008451761
O	2.595438429	-3.342530978	1.638029434
O	-0.126133287	-3.207395907	4.142905748
O	-2.792991326	-3.182665375	1.638503471
O	-5.059894692	0.234332856	-2.708640100
O	-4.295253449	-0.091956309	0.880353300
O	-0.000773844	-0.001208323	5.710600855
O	-1.493900520	0.299854772	-4.043935099
O	-2.787888554	0.270075490	3.361582667
Ni	1.433849465	-0.041686523	0.849648218
Ni	0.071456692	2.270330985	1.413074351
Ni	-1.140749988	2.434804244	-0.664658520
Ni	1.301838521	2.341854043	-0.667217048
Ni	2.528491532	-0.111218137	-1.357309442
C	2.765506307	2.762345849	-1.509062568
C	0.105728179	2.995347968	-1.975337897
C	-2.568891830	2.983932548	-1.489678797
C	-1.697889405	2.848383458	1.074170728
C	0.098645750	2.738335954	3.091166033
C	1.872721062	2.734916900	1.072825789
C	4.042673736	-0.182389032	-2.169581894
C	3.210620958	0.000731791	0.448754849
C	1.374451701	-0.176865113	-2.885582933
C	1.911724057	-0.143831401	2.595971999
O	3.698289534	3.165641548	-2.050775294
O	0.126207301	3.535652272	-3.011811779
O	-3.470490322	3.477588384	-2.009092711
O	-2.594762457	3.343897633	1.637783067
O	0.126630282	3.206901308	4.143016960
O	2.793907493	3.180229568	1.638979442
O	5.059087261	-0.232542425	-2.709857683
O	4.295277126	0.086634921	0.879928125
O	1.492875520	-0.299942963	-4.044289976
O	2.787318162	-0.263781766	3.362467216

Computed frequencies (cm^{-1})

1:	13.09	61:	232.44	121:	536.76
2:	21.75	62:	243.37	122:	548.32
3:	28.38	63:	243.66	123:	549.32
4:	32.86	64:	247.72	124:	551.95
5:	32.92	65:	248.45	125:	552.09
6:	35.79	66:	253.24	126:	561.83
7:	40.20	67:	254.19	127:	562.00
8:	41.02	68:	262.11	128:	567.55
9:	45.57	69:	263.45	129:	590.58
10:	51.55	70:	272.23	130:	594.76
11:	52.20	71:	294.63	131:	597.89
12:	55.65	72:	303.50	132:	601.45
13:	57.88	73:	387.73	133:	620.32
14:	60.12	74:	388.40	134:	639.63
15:	64.35	75:	394.06	135:	665.20
16:	65.00	76:	399.64	136:	1910.39
17:	68.42	77:	400.62	137:	1915.98
18:	70.04	78:	401.33	138:	1927.10
19:	71.01	79:	401.84	139:	1932.89
20:	72.27	80:	405.37	140:	1933.81
21:	73.59	81:	410.97	141:	1944.69
22:	75.08	82:	413.04	142:	1944.89
23:	75.60	83:	417.59	143:	1954.01
24:	77.08	84:	419.27	144:	1962.18
25:	78.69	85:	422.94	145:	1979.96
26:	79.78	86:	425.06	146:	1990.36
27:	80.07	87:	427.05	147:	1999.26
28:	81.23	88:	428.50	148:	2082.93
29:	85.88	89:	429.79	149:	2087.51
30:	87.27	90:	430.00	150:	2093.97
31:	88.89	91:	433.43	151:	2097.05
32:	90.23	92:	433.94	152:	2097.85
33:	91.57	93:	448.04	153:	2121.66
34:	96.35	94:	448.63	154:	2126.87
35:	100.84	95:	452.81	155:	2128.07
36:	101.23	96:	453.51	156:	2169.85
37:	104.05	97:	455.26		
38:	106.64	98:	457.57		
39:	109.96	99:	460.34		
40:	110.20	100:	462.51		
41:	121.36	101:	464.00		
42:	123.28	102:	464.30		
43:	128.68	103:	467.16		
44:	132.24	104:	476.45		
45:	134.71	105:	478.88		
46:	137.72	106:	478.94		
47:	141.63	107:	481.42		
48:	145.34	108:	484.11		
49:	156.53	109:	484.91		
50:	160.07	110:	487.15		
51:	178.53	111:	487.91		
52:	178.87	112:	494.17		
53:	179.41	113:	512.92		
54:	180.44	114:	514.07		
55:	182.79	115:	514.32		
56:	201.36	116:	517.80		
57:	206.85	117:	517.90		
58:	210.05	118:	525.00		
59:	229.12	119:	532.37		
60:	230.32	120:	535.76		

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isAA (E = -17688.412020313470 a.u., G^{298K} = -17688.31980550 a.u.)

54
Pt2Ni10C21O21

Ni	0.004688000	0.032016000	-1.530233000
Ni	-1.359836000	0.085671000	0.850849000
Pt	-0.092889000	-2.535100000	1.614865000
Pt	1.265383000	-2.580893000	-0.686215000
Ni	-1.322209000	-2.314526000	-0.664988000
Ni	0.007290000	0.028529000	2.862583000
Ni	-2.421253000	0.077872000	-1.335673000
C	-2.799843000	-2.610516000	-1.545050000
C	-0.200193000	-2.834763000	-2.104341000
C	2.786165000	-3.043881000	-1.679251000
C	1.859115000	-3.123287000	1.217515000
C	-0.232951000	-2.926965000	3.441716000
C	-2.035660000	-2.828727000	1.014552000
C	-3.919417000	0.187258000	-2.194293000
C	-3.134410000	0.013188000	0.450212000
C	0.016900000	0.037205000	4.591203000
C	-1.242906000	0.016218000	-2.854226000
C	-1.875429000	0.237385000	2.607105000
O	-3.732532000	-2.989008000	-2.098312000
O	-0.276042000	-3.238541000	-3.198906000
O	3.700529000	-3.423072000	-2.269658000
O	2.757547000	-3.640096000	1.758934000
O	-0.321148000	-3.259888000	4.541568000
O	-3.022836000	-3.245516000	1.481994000
O	-4.916056000	0.282816000	-2.763972000
O	-4.224503000	-0.058089000	0.868452000
O	0.026593000	0.059196000	5.743286000
O	-1.438053000	-0.009655000	-4.007537000
O	-2.775018000	0.429984000	3.329222000
Ni	1.382608000	0.011176000	0.855118000
Ni	0.070258000	2.314852000	1.440632000
Ni	-1.135083000	2.331895000	-0.647731000
Ni	1.279494000	2.259672000	-0.651391000
Ni	2.431765000	-0.081834000	-1.341245000
C	2.739304000	2.706058000	-1.495367000
C	0.084474000	2.800848000	-1.998121000
C	-2.563870000	2.871328000	-1.483905000
C	-1.686445000	2.871343000	1.066051000
C	0.101039000	2.828948000	3.105570000
C	1.856804000	2.761832000	1.065565000
C	3.931031000	-0.157312000	-2.199414000
C	3.160521000	0.027518000	0.433203000
C	1.271411000	0.063806000	-2.856546000
C	1.909757000	-0.078894000	2.600787000
O	3.664879000	3.130826000	-2.031884000
O	0.094539000	3.285598000	-3.062575000
O	-3.458660000	3.368258000	-2.011757000
O	-2.591160000	3.395061000	1.590530000
O	0.132225000	3.294169000	4.158195000
O	2.786472000	3.235592000	1.593951000
O	4.931898000	-0.196375000	-2.769088000
O	4.252189000	0.117679000	0.842894000
O	1.460723000	0.172744000	-4.005292000
O	2.812801000	-0.159604000	3.339822000

Computed frequencies (cm^{-1})

1:	9.74	61:	224.46	121:	535.71
2:	15.51	62:	233.68	122:	536.32
3:	22.55	63:	246.16	123:	537.83
4:	23.76	64:	250.16	124:	546.55
5:	35.00	65:	251.61	125:	547.11
6:	35.77	66:	251.78	126:	549.06
7:	37.38	67:	261.28	127:	563.27
8:	39.13	68:	273.76	128:	575.81
9:	42.66	69:	274.33	129:	598.71
10:	44.42	70:	284.60	130:	601.56
11:	52.64	71:	305.94	131:	608.96
12:	59.21	72:	307.70	132:	611.48
13:	60.34	73:	363.83	133:	615.19
14:	63.77	74:	380.06	134:	615.88
15:	64.25	75:	392.99	135:	648.21
16:	64.37	76:	394.36	136:	1911.92
17:	66.80	77:	398.08	137:	1912.96
18:	68.24	78:	400.80	138:	1923.13
19:	69.87	79:	401.22	139:	1932.87
20:	71.20	80:	404.69	140:	1933.91
21:	71.53	81:	409.02	141:	1943.67
22:	73.70	82:	409.87	142:	1945.38
23:	76.34	83:	411.85	143:	1955.70
24:	77.14	84:	423.80	144:	1968.52
25:	77.31	85:	426.15	145:	1990.99
26:	79.17	86:	426.82	146:	1992.62
27:	82.66	87:	427.39	147:	2004.54
28:	83.04	88:	428.37	148:	2083.78
29:	83.31	89:	431.67	149:	2085.00
30:	84.35	90:	432.03	150:	2093.46
31:	85.53	91:	433.99	151:	2097.28
32:	86.68	92:	435.11	152:	2102.60
33:	89.96	93:	440.38	153:	2122.37
34:	91.29	94:	442.98	154:	2127.41
35:	101.92	95:	446.32	155:	2132.75
36:	102.77	96:	453.79	156:	2170.02
37:	105.01	97:	457.18		
38:	109.62	98:	458.81		
39:	114.68	99:	460.63		
40:	117.76	100:	461.79		
41:	118.52	101:	463.86		
42:	119.08	102:	466.99		
43:	122.62	103:	468.69		
44:	126.94	104:	470.06		
45:	134.39	105:	470.13		
46:	136.16	106:	474.75		
47:	146.91	107:	477.09		
48:	148.23	108:	481.73		
49:	149.19	109:	483.01		
50:	157.28	110:	486.88		
51:	157.91	111:	487.28		
52:	158.50	112:	490.22		
53:	175.87	113:	494.32		
54:	184.63	114:	498.16		
55:	184.75	115:	511.07		
56:	189.47	116:	513.97		
57:	198.95	117:	514.05		
58:	206.92	118:	521.50		
59:	207.19	119:	526.59		
60:	220.91	120:	533.98		

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isAA'-1 (E = -17688.412068707108 a.u., G^{298K} = -17688.32102956 a.u.)

54
Pt2Ni10C21O21

Ni	-0.000617000	-0.000023000	-1.515150000
Ni	-1.382395000	0.053926000	0.862227000
Pt	-0.104476000	-2.514499000	1.567105000
Ni	1.157395000	-2.357125000	-0.641114000
Ni	-1.314125000	-2.268842000	-0.659154000
Ni	0.000217000	-0.001412000	2.865946000
Ni	-2.431438000	0.088191000	-1.335726000
C	-2.744019000	-2.648564000	-1.584328000
C	-0.079819000	-2.763829000	-1.995580000
C	2.577531000	-2.812301000	-1.548271000
C	1.814861000	-2.985666000	1.020759000
C	-0.143660000	-3.058766000	3.358908000
C	-2.065064000	-2.778201000	1.003007000
C	-3.941377000	0.135171000	-2.183093000
C	-3.146916000	0.160833000	0.456908000
C	0.000770000	0.000598000	4.593426000
C	-1.258718000	-0.019369000	-2.843324000
C	-1.900158000	0.043789000	2.629252000
O	-3.650010000	-3.059784000	-2.160924000
O	-0.086069000	-3.212052000	-3.075520000
O	3.462337000	-3.282574000	-2.112843000
O	2.754236000	-3.504706000	1.486181000
O	-0.170579000	-3.466773000	4.438079000
O	-3.064727000	-3.174152000	1.463235000
O	-4.949340000	0.167813000	-2.739686000
O	-4.239118000	0.248674000	0.866487000
O	0.001426000	0.002420000	5.745805000
O	-1.444488000	-0.087817000	-3.996286000
O	-2.802275000	0.046221000	3.372401000
Ni	1.382136000	-0.053228000	0.861789000
Pt	0.103100000	2.512994000	1.568582000
Ni	-1.157178000	2.356135000	-0.640824000
Ni	1.315068000	2.266989000	-0.657441000
Ni	2.429919000	-0.091676000	-1.337144000
C	2.745394000	2.647031000	-1.581935000
C	0.081570000	2.759797000	-1.995310000
C	-2.576018000	2.811947000	-1.549734000
C	-1.812655000	2.993063000	1.018439000
C	0.141776000	3.055184000	3.360931000
C	2.062429000	2.782166000	1.004835000
C	3.939263000	-0.140427000	-2.185750000
C	3.147309000	-0.141171000	0.454781000
C	1.256755000	0.016470000	-2.844145000
C	1.900172000	-0.058770000	2.628829000
O	3.651983000	3.057230000	-2.158274000
O	0.088531000	3.207050000	-3.075658000
O	-3.460671000	3.281402000	-2.115124000
O	-2.749328000	3.519204000	1.481432000
O	0.168832000	3.461268000	4.440850000
O	3.060360000	3.181505000	1.465942000
O	4.946667000	-0.174381000	-2.743229000
O	4.241201000	-0.205117000	0.864159000
O	1.441905000	0.083958000	-3.997256000
O	2.802091000	-0.079803000	3.371927000

Computed frequencies (cm^{-1})

1:	1.49	61:	217.11	121:	533.11
2:	12.40	62:	219.70	122:	533.62
3:	21.37	63:	242.95	123:	536.62
4:	26.07	64:	243.19	124:	545.36
5:	29.88	65:	250.07	125:	546.83
6:	33.39	66:	258.35	126:	548.63
7:	41.51	67:	259.92	127:	576.50
8:	41.85	68:	272.36	128:	577.01
9:	49.33	69:	273.39	129:	582.89
10:	50.69	70:	285.25	130:	586.29
11:	53.64	71:	304.30	131:	612.36
12:	54.26	72:	310.35	132:	615.80
13:	56.66	73:	383.63	133:	617.69
14:	56.85	74:	386.52	134:	617.99
15:	62.12	75:	388.12	135:	647.52
16:	62.56	76:	392.07	136:	1912.13
17:	63.86	77:	395.83	137:	1915.32
18:	65.10	78:	399.48	138:	1924.54
19:	68.78	79:	400.16	139:	1931.92
20:	68.93	80:	401.74	140:	1932.37
21:	70.75	81:	408.29	141:	1941.10
22:	72.18	82:	410.56	142:	1943.12
23:	72.27	83:	411.06	143:	1957.77
24:	75.59	84:	417.78	144:	1965.37
25:	77.00	85:	422.96	145:	1991.68
26:	78.81	86:	423.21	146:	1992.84
27:	79.60	87:	426.18	147:	2005.48
28:	80.50	88:	429.40	148:	2081.56
29:	82.68	89:	430.65	149:	2087.13
30:	84.16	90:	431.36	150:	2091.49
31:	85.17	91:	433.27	151:	2095.18
32:	88.04	92:	441.09	152:	2102.76
33:	92.50	93:	441.31	153:	2123.83
34:	96.49	94:	444.40	154:	2125.40
35:	96.55	95:	445.52	155:	2131.80
36:	105.48	96:	447.54	156:	2169.54
37:	109.10	97:	447.74		
38:	111.64	98:	460.99		
39:	115.67	99:	463.76		
40:	116.62	100:	464.10		
41:	118.79	101:	464.57		
42:	119.50	102:	466.40		
43:	120.82	103:	469.82		
44:	130.10	104:	471.77		
45:	131.66	105:	472.60		
46:	143.18	106:	475.17		
47:	145.01	107:	476.34		
48:	149.23	108:	477.63		
49:	150.68	109:	479.44		
50:	153.53	110:	484.81		
51:	155.35	111:	486.64		
52:	155.59	112:	492.35		
53:	175.21	113:	492.47		
54:	180.51	114:	495.08		
55:	180.85	115:	509.84		
56:	204.65	116:	510.82		
57:	206.29	117:	515.23		
58:	215.43	118:	523.53		
59:	215.67	119:	525.55		
60:	216.52	120:	528.93		

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isAA'-2 (E = -17688.412784592023 a.u., G^{298K} = -17688.32030848 a.u.)

54
Pt2Ni10C21O21

Ni	-0.005987000	-0.035476000	-1.519614000
Ni	-1.363474000	0.052673000	0.846133000
Pt	-0.113172000	-2.493963000	1.591132000
Ni	1.170082000	-2.350746000	-0.610782000
Ni	-1.307294000	-2.304380000	-0.651285000
Ni	-0.018452000	0.046399000	2.858989000
Ni	-2.433767000	0.056814000	-1.331786000
C	-2.735112000	-2.658694000	-1.595909000
C	-0.057620000	-2.793500000	-1.972463000
C	2.592965000	-2.822344000	-1.502562000
C	1.831238000	-2.913340000	1.069756000
C	-0.166352000	-3.012234000	3.388603000
C	-2.014159000	-2.955955000	0.975177000
C	-3.922695000	0.210289000	-2.194966000
C	-3.132537000	-0.140251000	0.451861000
C	-0.049586000	-0.042248000	4.586024000
C	-1.274599000	-0.045936000	-2.848337000
C	-1.896558000	0.326536000	2.568890000
O	-3.641872000	-3.045437000	-2.186772000
O	-0.050177000	-3.257217000	-3.045535000
O	3.481425000	-3.298234000	-2.056439000
O	2.775655000	-3.397044000	1.562230000
O	-0.210341000	-3.414047000	4.469999000
O	-2.959477000	-3.491535000	1.409355000
O	-4.900929000	0.336266000	-2.790755000
O	-4.202366000	-0.352742000	0.874523000
O	-0.072801000	-0.121210000	5.735328000
O	-1.462403000	-0.114708000	-4.000667000
O	-2.786995000	0.604577000	3.274910000
Ni	1.366383000	-0.020315000	0.858314000
Ni	0.085296000	2.357997000	1.470696000
Pt	-1.263974000	2.555817000	-0.679154000
Ni	1.273631000	2.261260000	-0.696326000
Ni	2.427056000	-0.089100000	-1.335183000
C	2.760561000	2.635679000	-1.527427000
C	0.162842000	2.796447000	-2.138620000
C	-2.816983000	3.135300000	-1.548684000
C	-1.640536000	3.095295000	1.267581000
C	0.235073000	2.753847000	3.167157000
C	1.875891000	2.738901000	1.020351000
C	3.929384000	-0.143974000	-2.194501000
C	3.141106000	-0.086061000	0.450800000
C	1.240158000	-0.071225000	-2.848178000
C	1.880176000	0.005758000	2.619770000
O	3.693029000	3.046744000	-2.060508000
O	0.230985000	3.203303000	-3.233033000
O	-3.748163000	3.575876000	-2.069918000
O	-2.450783000	3.690533000	1.865740000
O	0.338226000	3.173543000	4.232200000
O	2.833330000	3.174312000	1.530706000
O	4.931460000	-0.184581000	-2.761211000
O	4.233180000	-0.113689000	0.868667000
O	1.430466000	-0.087068000	-4.002168000
O	2.779569000	0.023091000	3.367294000

Computed frequencies (cm^{-1})

1:	12.42	61:	217.25	121:	534.11
7:	18.24	62:	221.72	122:	535.88
3:	23.66	63:	242.99	123:	537.92
4:	27.07	64:	243.34	124:	545.43
5:	31.07	65:	250.99	125:	547.49
6:	35.87	66:	256.98	126:	548.19
7:	37.61	67:	258.87	127:	575.60
8:	42.48	68:	273.29	128:	575.96
9:	48.77	69:	274.98	129:	585.98
10:	51.27	70:	282.42	130:	589.06
11:	54.20	71:	303.14	131:	612.83
12:	56.76	72:	308.82	132:	615.13
13:	61.09	73:	382.45	133:	618.54
14:	61.88	74:	384.02	134:	619.61
15:	62.65	75:	388.77	135:	647.49
16:	64.06	76:	390.01	136:	1910.80
17:	66.58	77:	393.06	137:	1912.63
18:	67.44	78:	397.62	138:	1922.94
19:	69.46	79:	400.04	139:	1932.35
20:	70.51	80:	402.00	140:	1932.95
21:	71.21	81:	408.41	141:	1943.34
22:	74.09	82:	408.93	142:	1944.74
23:	74.39	83:	410.50	143:	1956.93
24:	76.21	84:	419.75	144:	1965.26
25:	78.62	85:	421.58	145:	1989.59
26:	79.43	86:	424.60	146:	1992.57
27:	80.60	87:	427.14	147:	2003.74
28:	81.33	88:	428.47	148:	2080.06
29:	83.25	89:	429.09	149:	2081.72
30:	85.59	90:	431.47	150:	2091.31
31:	88.30	91:	435.03	151:	2101.41
32:	90.23	92:	439.76	152:	2102.36
33:	90.88	93:	441.35	153:	2119.18
34:	96.55	94:	442.54	154:	2130.44
35:	97.72	95:	446.40	155:	2132.41
36:	105.97	96:	447.93	156:	2169.53
37:	108.39	97:	448.62		
38:	110.94	98:	459.02		
39:	112.62	99:	461.43		
40:	115.45	100:	463.67		
41:	119.79	101:	466.78		
42:	120.26	102:	467.75		
43:	123.48	103:	468.02		
44:	127.40	104:	470.81		
45:	137.77	105:	474.00		
46:	138.64	106:	474.62		
47:	144.81	107:	475.18		
48:	150.69	108:	477.79		
49:	151.95	109:	482.76		
50:	153.22	110:	487.01		
51:	155.06	111:	493.97		
52:	155.24	112:	494.46		
53:	175.90	113:	494.73		
54:	178.40	114:	499.02		
55:	179.10	115:	508.34		
56:	204.87	116:	508.84		
57:	207.65	117:	515.78		
58:	214.91	118:	522.48		
59:	215.65	119:	526.18		
60:	216.18	120:	529.41		

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isAB$_e$-1 (E = -17688.406584257413 a.u., G^{298K} = -17688.31265799 a.u.)

54
Pt2Ni10C21O21

Ni	0.009274000	-0.011676000	-1.485139000
Ni	-1.410663000	0.106836000	0.898498000
Pt	-0.125584000	-2.581611000	1.553095000
Ni	1.137507000	-2.376081000	-0.641519000
Ni	-1.336175000	-2.277400000	-0.658464000
Pt	0.021765000	0.030990000	3.099558000
Ni	-2.407849000	0.105038000	-1.340463000
C	-2.775040000	-2.631531000	-1.581199000
C	-0.100810000	-2.789736000	-1.991042000
C	2.554600000	-2.834599000	-1.550382000
C	1.827222000	-2.958859000	1.019018000
C	-0.163065000	-3.173340000	3.334036000
C	-2.089563000	-2.801309000	1.003089000
C	-3.889927000	0.216760000	-2.234359000
C	-3.166839000	0.090888000	0.411256000
C	0.033960000	0.043333000	4.954816000
C	-1.232243000	-0.107755000	-2.829775000
C	-2.031654000	0.216253000	2.624456000
O	-3.693929000	-3.016250000	-2.155307000
O	-0.111122000	-3.246382000	-3.067216000
O	3.432235000	-3.319937000	-2.114397000
O	2.786480000	-3.436563000	1.487080000
O	-0.194973000	-3.619830000	4.396818000
O	-3.092557000	-3.200505000	1.452857000
O	-4.869442000	0.312162000	-2.831494000
O	-4.272219000	0.063499000	0.791670000
O	0.051814000	0.077498000	6.111537000
O	-1.402586000	-0.268683000	-3.975164000
O	-2.958906000	0.361179000	3.320146000
Ni	1.425967000	-0.019071000	0.897161000
Ni	0.088174000	2.374994000	1.405705000
Ni	-1.122439000	2.329104000	-0.669808000
Ni	1.296950000	2.233509000	-0.675429000
Ni	2.432997000	-0.140748000	-1.326343000
C	2.753943000	2.663617000	-1.532677000
C	0.092545000	2.759181000	-2.027536000
C	-2.547597000	2.874222000	-1.508991000
C	-1.679690000	2.880798000	1.043256000
C	0.120945000	2.948135000	3.058912000
C	1.870376000	2.793595000	1.032112000
C	3.923819000	-0.225383000	-2.208298000
C	3.177119000	0.100705000	0.413227000
C	1.258807000	0.062226000	-2.821235000
C	2.063512000	-0.229737000	2.608330000
O	3.675748000	3.081404000	-2.080931000
O	0.108371000	3.231871000	-3.097486000
O	-3.435342000	3.380600000	-2.040187000
O	-2.592288000	3.397621000	1.561805000
O	0.154759000	3.442258000	4.097236000
O	2.801437000	3.286737000	1.540204000
O	4.910722000	-0.283980000	-2.798149000
O	4.263244000	0.317404000	0.790176000
O	1.437521000	0.228067000	-3.964616000
O	2.990688000	-0.459516000	3.280950000

Computed frequencies (cm^{-1})

1:	i22.03	61:	234.34	121:	530.33
2:	22.76	62:	242.22	122:	530.76
3:	24.16	63:	243.48	123:	531.01
4:	29.05	64:	250.97	124:	535.09
5:	33.08	65:	252.35	125:	547.33
6:	36.41	66:	257.67	126:	552.65
7:	39.89	67:	260.85	127:	563.20
8:	41.19	68:	261.50	128:	574.01
9:	44.39	69:	273.74	129:	582.42
10:	52.77	70:	286.96	130:	598.22
11:	53.69	71:	291.40	131:	603.69
12:	56.58	72:	312.60	132:	611.00
13:	59.13	73:	383.70	133:	614.05
14:	59.99	74:	390.61	134:	628.39
15:	62.02	75:	393.46	135:	643.66
16:	62.25	76:	394.21	136:	1913.96
17:	64.78	77:	396.81	137:	1914.95
18:	67.94	78:	398.72	138:	1924.86
19:	69.57	79:	400.59	139:	1932.19
20:	71.44	80:	405.83	140:	1933.67
21:	73.57	81:	409.69	141:	1942.81
22:	75.27	82:	412.19	142:	1945.33
23:	76.30	83:	416.26	143:	1956.81
24:	76.68	84:	416.94	144:	1965.77
25:	78.11	85:	423.77	145:	1992.44
26:	79.72	86:	424.79	146:	1996.26
27:	80.18	87:	428.22	147:	2009.25
28:	80.68	88:	429.73	148:	2074.41
29:	84.58	89:	431.41	149:	2086.08
30:	85.11	90:	432.40	150:	2092.46
31:	87.28	91:	434.26	151:	2097.26
32:	89.22	92:	435.47	152:	2100.21
33:	90.01	93:	439.87	153:	2114.75
34:	93.24	94:	441.61	154:	2123.82
35:	96.85	95:	445.08	155:	2131.93
36:	102.39	96:	448.31	156:	2168.07
37:	104.25	97:	452.14		
38:	107.44	98:	455.69		
39:	109.88	99:	460.56		
40:	114.78	100:	462.44		
41:	116.25	101:	463.24		
42:	119.61	102:	464.36		
43:	124.86	103:	464.72		
44:	127.21	104:	471.24		
45:	131.91	105:	475.59		
46:	137.79	106:	477.72		
47:	142.89	107:	478.24		
48:	145.61	108:	480.05		
49:	146.94	109:	482.17		
50:	150.40	110:	484.64		
51:	157.22	111:	490.23		
52:	163.74	112:	492.76		
53:	181.71	113:	496.10		
54:	182.60	114:	498.49		
55:	185.11	115:	503.69		
56:	191.44	116:	510.47		
57:	201.81	117:	512.81		
58:	212.57	118:	518.85		
59:	216.70	119:	524.91		
60:	217.50	120:	527.46		

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isAB$_e$-2 (E = -17688.407460733724 a.u., G^{298K} = -17688.31484838 a.u.)

54
Pt2Ni10C21O21

Ni	-0.009774000	0.019464000	-1.563706000
Ni	-1.416990000	0.091935000	0.880227000
Pt	-0.071246000	-2.495194000	1.596380000
Ni	1.164106000	-2.366482000	-0.633097000
Ni	-1.305296000	-2.335831000	-0.628010000
Ni	0.006970000	0.042421000	2.866278000
Pt	-2.624699000	0.141607000	-1.429613000
C	-2.740272000	-2.755855000	-1.541894000
C	-0.079438000	-2.765013000	-1.989845000
C	2.570466000	-2.812777000	-1.567014000
C	1.815896000	-3.044964000	1.009616000
C	-0.091611000	-2.987803000	3.402395000
C	-1.998084000	-2.911602000	1.031725000
C	-4.223768000	0.279996000	-2.365288000
C	-3.206967000	-0.089563000	0.604811000
C	0.031761000	-0.035658000	4.596450000
C	-1.186746000	-0.077861000	-2.964332000
C	-1.854199000	0.324792000	2.649774000
O	-3.643878000	-3.182664000	-2.107707000
O	-0.081695000	-3.206875000	-3.072447000
O	3.445143000	-3.274296000	-2.153537000
O	2.730525000	-3.620703000	1.457047000
O	-0.112245000	-3.373222000	4.490524000
O	-2.944095000	-3.415601000	1.500749000
O	-5.209042000	0.404105000	-2.959109000
O	-4.256870000	-0.315150000	1.066509000
O	0.050038000	-0.104509000	5.745768000
O	-1.333389000	-0.245863000	-4.111535000
O	-2.720676000	0.596400000	3.387261000
Ni	1.339313000	-0.029153000	0.846534000
Ni	0.091704000	2.322866000	1.435358000
Ni	-1.105497000	2.417931000	-0.646957000
Ni	1.294897000	2.250229000	-0.659518000
Ni	2.432003000	-0.095321000	-1.311799000
C	2.757444000	2.675945000	-1.506708000
C	0.103205000	2.781942000	-2.026455000
C	-2.511457000	3.048403000	-1.472762000
C	-1.668185000	2.901394000	1.070430000
C	0.122170000	2.838116000	3.101795000
C	1.874887000	2.777616000	1.037978000
C	3.972147000	-0.109910000	-2.107265000
C	3.093453000	-0.339763000	0.478655000
C	1.307414000	0.092655000	-2.836870000
C	1.890615000	0.174257000	2.585876000
O	3.684309000	3.105623000	-2.037876000
O	0.131886000	3.234851000	-3.104593000
O	-3.386240000	3.587461000	-1.990454000
O	-2.563307000	3.425580000	1.610610000
O	0.148510000	3.305194000	4.153287000
O	2.803279000	3.267056000	1.554430000
O	5.007722000	-0.107079000	-2.610740000
O	4.143208000	-0.617145000	0.913503000
O	1.525925000	0.228301000	-3.977895000
O	2.806670000	0.379718000	3.282456000

Computed frequencies (cm^{-1})

1:	12.98	61:	235.66	121:	530.56
2:	21.99	62:	242.18	122:	531.71
3:	26.29	63:	243.53	123:	533.42
4:	29.00	64:	251.16	124:	535.04
5:	32.95	65:	251.64	125:	548.11
6:	34.07	66:	257.88	126:	550.74
7:	41.31	67:	261.34	127:	563.97
8:	42.23	68:	261.60	128:	578.36
9:	46.19	69:	273.20	129:	589.11
10:	48.47	70:	284.77	130:	599.23
11:	53.68	71:	286.98	131:	602.79
12:	56.15	72:	308.39	132:	610.30
13:	58.87	73:	383.21	133:	621.84
14:	62.36	74:	388.28	134:	626.88
15:	63.97	75:	393.29	135:	643.61
16:	66.24	76:	394.46	136:	1911.60
17:	67.79	77:	397.31	137:	1913.68
18:	70.57	78:	400.87	138:	1922.92
19:	71.87	79:	403.27	139:	1931.58
20:	73.66	80:	405.41	140:	1934.52
21:	74.19	81:	406.41	141:	1944.21
22:	76.76	82:	410.54	142:	1946.74
23:	77.19	83:	415.57	143:	1956.51
24:	78.23	84:	418.59	144:	1964.13
25:	79.51	85:	420.13	145:	1991.38
26:	80.05	86:	422.80	146:	1993.91
27:	80.65	87:	426.34	147:	2006.69
28:	81.14	88:	429.13	148:	2076.14
29:	82.81	89:	431.02	149:	2081.47
30:	87.03	90:	432.69	150:	2089.29
31:	87.47	91:	433.48	151:	2098.73
32:	90.75	92:	435.38	152:	2103.13
33:	91.14	93:	439.68	153:	2120.01
34:	94.47	94:	444.93	154:	2127.15
35:	96.67	95:	449.05	155:	2130.77
36:	102.81	96:	450.56	156:	2167.44
37:	103.30	97:	451.88		
38:	108.65	98:	455.93		
39:	110.68	99:	457.91		
40:	112.17	100:	461.59		
41:	117.02	101:	462.43		
42:	119.72	102:	463.52		
43:	122.72	103:	466.08		
44:	127.59	104:	471.63		
45:	131.84	105:	473.55		
46:	133.88	106:	474.62		
47:	143.86	107:	479.53		
48:	147.14	108:	482.22		
49:	147.85	109:	483.59		
50:	150.66	110:	488.29		
51:	155.32	111:	494.26		
52:	162.32	112:	495.59		
53:	176.26	113:	498.56		
54:	182.85	114:	500.83		
55:	184.81	115:	503.81		
56:	192.54	116:	505.84		
57:	200.69	117:	511.53		
58:	214.48	118:	517.09		
59:	215.22	119:	523.75		
60:	217.10	120:	527.25		

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isAB$_i$-1 (E = -17688.435276497021 a.u., G^{298K} =-17688.34203306 a.u.)

54
Pt2Ni10C21O21

Ni	-0.030530000	-0.000811000	-1.584509000
Pt	-1.296383000	0.052712000	0.813986000
Pt	-0.152668000	-2.594241000	1.616706000
Ni	1.108243000	-2.324725000	-0.592935000
Ni	-1.365496000	-2.363871000	-0.647033000
Ni	0.049222000	0.046911000	2.959193000
Ni	-2.490062000	0.078940000	-1.420370000
C	-2.782849000	-2.723043000	-1.596396000
C	-0.098391000	-2.778991000	-1.972835000
C	2.541763000	-2.764322000	-1.489576000
C	1.799272000	-2.915382000	1.075715000
C	-0.177443000	-3.151774000	3.396395000
C	-2.077588000	-3.015022000	0.987175000
C	-3.956224000	0.185735000	-2.314294000
C	-3.236991000	0.083914000	0.348127000
C	0.092406000	0.013725000	4.678872000
C	-1.270507000	0.004983000	-2.915751000
C	-1.845345000	0.185132000	2.740047000
O	-3.687518000	-3.104346000	-2.195138000
O	-0.064943000	-3.225670000	-3.052571000
O	3.422775000	-3.259510000	-2.039507000
O	2.768157000	-3.380753000	1.536506000
O	-0.181622000	-3.570206000	4.473148000
O	-3.041204000	-3.516077000	1.419674000
O	-4.937206000	0.270623000	-2.911697000
O	-4.307314000	0.100491000	0.822593000
O	0.118303000	-0.017887000	5.830066000
O	-1.444037000	-0.028286000	-4.072868000
O	-2.784733000	0.324350000	3.424368000
Ni	1.420141000	-0.020286000	0.913505000
Ni	0.097370000	2.402875000	1.454791000
Ni	-1.147840000	2.416639000	-0.641643000
Ni	1.265352000	2.222156000	-0.654632000
Ni	2.406684000	-0.117452000	-1.326228000
C	2.719045000	2.636221000	-1.521689000
C	0.070775000	2.767845000	-2.016353000
C	-2.575095000	2.962253000	-1.471354000
C	-1.642416000	3.043052000	1.074869000
C	0.157040000	2.916725000	3.115083000
C	1.894349000	2.746756000	1.045908000
C	3.918736000	-0.148180000	-2.173965000
C	3.166668000	-0.093206000	0.459000000
C	1.248977000	-0.024436000	-2.870251000
C	1.956775000	0.002792000	2.656372000
O	3.635225000	3.068449000	-2.069238000
O	0.105903000	3.223939000	-3.092676000
O	-3.471235000	3.453289000	-2.002313000
O	-2.523389000	3.600625000	1.602496000
O	0.210115000	3.375861000	4.169653000
O	2.857273000	3.192820000	1.536922000
O	4.930017000	-0.163978000	-2.724336000
O	4.275735000	-0.108017000	0.829324000
O	1.480875000	0.012704000	-4.016073000
O	2.871835000	0.017958000	3.385141000

Computed frequencies (cm^{-1})

1:	i8.02	61:	228.99	121:	536.39
2:	9.41	62:	230.75	122:	546.73
3:	24.06	63:	239.91	123:	548.05
4:	26.91	64:	243.12	124:	551.11
5:	33.81	65:	248.59	125:	551.51
6:	36.44	66:	254.64	126:	561.95
7:	37.31	67:	255.95	127:	566.70
8:	39.81	68:	262.12	128:	574.94
9:	43.56	69:	262.92	129:	582.17
10:	48.46	70:	270.05	130:	592.89
11:	50.87	71:	294.92	131:	600.60
12:	52.29	72:	303.48	132:	615.22
13:	55.02	73:	380.64	133:	620.78
14:	58.06	74:	383.58	134:	639.41
15:	58.87	75:	388.42	135:	665.00
16:	62.72	76:	394.44	136:	1911.99
17:	64.59	77:	398.06	137:	1918.67
18:	65.37	78:	399.76	138:	1928.31
19:	65.95	79:	400.75	139:	1933.07
20:	69.45	80:	404.65	140:	1935.04
21:	71.50	81:	407.44	141:	1943.85
22:	74.11	82:	409.78	142:	1945.13
23:	75.04	83:	412.25	143:	1956.13
24:	76.05	84:	418.90	144:	1965.30
25:	76.48	85:	419.29	145:	1982.35
26:	77.71	86:	421.72	146:	1991.68
27:	79.30	87:	423.35	147:	2001.41
28:	80.53	88:	428.26	148:	2082.88
29:	81.44	89:	429.82	149:	2086.63
30:	85.36	90:	430.70	150:	2093.76
31:	87.13	91:	432.17	151:	2097.94
32:	89.11	92:	433.59	152:	2102.08
33:	90.30	93:	441.65	153:	2121.12
34:	92.39	94:	446.53	154:	2128.98
35:	95.47	95:	450.07	155:	2131.36
36:	98.86	96:	451.15	156:	2170.12
37:	101.50	97:	454.09		
38:	102.01	98:	456.51		
39:	104.82	99:	457.96		
40:	111.54	100:	459.90		
41:	116.35	101:	462.67		
42:	120.24	102:	464.22		
43:	123.65	103:	466.74		
44:	130.46	104:	475.05		
45:	132.90	105:	477.19		
46:	135.66	106:	478.82		
47:	140.55	107:	479.76		
48:	143.40	108:	482.02		
49:	145.09	109:	483.59		
50:	156.05	110:	484.41		
51:	158.05	111:	485.72		
52:	174.67	112:	494.57		
53:	178.61	113:	499.03		
54:	180.36	114:	510.40		
55:	181.65	115:	512.47		
56:	200.29	116:	513.92		
57:	205.38	117:	518.30		
58:	208.78	118:	523.34		
59:	210.28	119:	526.43		
60:	215.11	120:	530.67		

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isAB$_i$-2 (E = -17688.434994151510 a.u., G^{298K} =-17688.34250172 a.u.)

54
Pt2Ni10C21O21

Pt	0.005081000	0.000428000	-1.434939000
Ni	-1.430108000	0.063175000	0.866159000
Pt	-0.087885000	-2.494467000	1.575412000
Ni	1.167616000	-2.464334000	-0.647883000
Ni	-1.337127000	-2.371040000	-0.650741000
Ni	0.002831000	0.052435000	2.845378000
Ni	-2.524965000	0.091526000	-1.339021000
C	-2.774093000	-2.720960000	-1.571660000
C	-0.103545000	-2.919082000	-1.980444000
C	2.577082000	-2.915348000	-1.568456000
C	1.814247000	-3.052081000	1.022806000
C	-0.109640000	-2.955953000	3.389579000
C	-2.033899000	-2.883483000	1.026810000
C	-4.036926000	0.201745000	-2.151572000
C	-3.197647000	-0.042992000	0.478768000
C	0.002514000	-0.012599000	4.574295000
C	-1.378875000	0.118383000	-2.873752000
C	-1.900376000	0.255032000	2.612264000
O	-3.693201000	-3.091763000	-2.154509000
O	-0.120016000	-3.388419000	-3.050362000
O	3.465525000	-3.360823000	-2.146165000
O	2.725896000	-3.599617000	1.509543000
O	-0.126204000	-3.337188000	4.478743000
O	-2.985716000	-3.354509000	1.516407000
O	-5.045947000	0.287953000	-2.700377000
O	-4.279161000	-0.168699000	0.908793000
O	0.006413000	-0.067153000	5.724948000
O	-1.503386000	0.198052000	-4.035571000
O	-2.770623000	0.468023000	3.364220000
Ni	1.433483000	-0.039287000	0.871371000
Ni	0.078012000	2.291711000	1.378969000
Ni	-1.144591000	2.440358000	-0.697155000
Ni	1.294099000	2.358834000	-0.709788000
Ni	2.534148000	-0.098859000	-1.329159000
C	2.753462000	2.780499000	-1.555483000
C	0.089194000	2.996834000	-2.019735000
C	-2.579307000	2.975447000	-1.518820000
C	-1.683168000	2.889708000	1.038961000
C	0.110249000	2.778870000	3.054547000
C	1.876772000	2.767259000	1.018432000
C	4.069559000	-0.091654000	-2.104468000
C	3.182996000	-0.295304000	0.497405000
C	1.398818000	-0.074761000	-2.870017000
C	1.914450000	0.132403000	2.616863000
O	3.683636000	3.188140000	-2.098232000
O	0.100895000	3.525342000	-3.062116000
O	-3.485587000	3.460373000	-2.037781000
O	-2.570271000	3.407552000	1.597071000
O	0.139029000	3.257327000	4.101280000
O	2.799179000	3.226168000	1.570897000
O	5.103535000	-0.072959000	-2.611974000
O	4.246069000	-0.531796000	0.926960000
O	1.529259000	-0.101131000	-4.033609000
O	2.798217000	0.292685000	3.366311000

Computed frequencies (cm^{-1})

1:	14.02	61:	229.85	121:	537.17		
2:	25.32	62:	231.74	122:	547.23		
3:	26.40	63:	241.73	123:	549.58		
4:	30.88	64:	242.66	124:	550.90		
5:	34.67	65:	248.52	125:	552.14		
6:	36.84	66:	248.79	126:	562.22		
7:	38.78	67:	253.62	127:	567.91		
8:	41.33	68:	260.79	128:	572.12		
9:	44.59	69:	261.73	129:	589.61		
10:	48.16	70:	272.05	130:	593.22		
11:	50.53	71:	291.29	131:	601.92		
12:	51.74	72:	298.73	132:	614.85		
13:	59.19	73:	382.12	133:	619.93		
14:	60.75	74:	387.12	134:	640.09		
15:	63.19	75:	392.11	135:	664.90		
16:	64.55	76:	393.28	136:	1910.36		
17:	65.65	77:	395.83	137:	1914.98		
18:	66.64	78:	399.37	138:	1926.29		
19:	68.94	79:	400.55	139:	1934.56		
20:	70.43	80:	403.21	140:	1934.82		
21:	71.41	81:	405.30	141:	1946.24		
22:	73.27	82:	408.83	142:	1947.91		
23:	75.21	83:	410.60	143:	1956.61		
24:	75.71	84:	415.77	144:	1966.36		
25:	76.78	85:	416.98	145:	1980.95		
26:	77.14	86:	424.12	146:	1988.87		
27:	78.24	87:	424.26	147:	1999.61		
28:	80.20	88:	428.18	148:	2082.17		
29:	84.63	89:	428.56	149:	2089.98		
30:	85.36	90:	428.93	150:	2093.83		
31:	85.58	91:	432.82	151:	2101.31		
32:	86.27	92:	436.06	152:	2104.25		
33:	89.92	93:	438.82	153:	2123.46		
34:	92.22	94:	445.74	154:	2129.64		
35:	98.53	95:	446.42	155:	2132.07		
36:	99.17	96:	452.45	156:	2170.91		
37:	100.93	97:	453.95				
38:	101.04	98:	456.36				
39:	108.15	99:	458.15				
40:	109.45	100:	461.04				
41:	119.20	101:	463.38				
42:	120.87	102:	464.56				
43:	121.60	103:	467.36				
44:	127.01	104:	472.36				
45:	129.84	105:	475.04				
46:	134.08	106:	476.29				
47:	138.18	107:	479.96				
48:	139.69	108:	482.16				
49:	144.58	109:	485.68				
50:	153.48	110:	490.18				
51:	156.91	111:	492.70				
52:	171.01	112:	495.10				
53:	177.96	113:	496.91				
54:	180.90	114:	511.46				
55:	182.16	115:	512.78				
56:	199.67	116:	513.42				
57:	206.16	117:	519.40				
58:	207.47	118:	523.11				
59:	208.98	119:	528.50				
60:	214.43	120:	534.51				

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isB_eB_e(E = -17688.399509772160 a.u., G^{298K} =-17688.30519335 a.u.)

54
Pt2Ni10C21O21

Ni	-0.017088000	0.007732000	-1.554610000
Ni	-1.487955000	0.049765000	0.911034000
Ni	-0.053798000	-2.360190000	1.432649000
Ni	1.137073000	-2.322607000	-0.659890000
Ni	-1.276116000	-2.306815000	-0.629600000
Pt	-0.008683000	0.002098000	3.079316000
Pt	-2.626550000	0.085284000	-1.460953000
C	-2.730709000	-2.815669000	-1.460587000
C	-0.101164000	-2.802366000	-1.997943000
C	2.567153000	-2.851739000	-1.504936000
C	1.711540000	-2.862634000	1.044653000
C	-0.064008000	-2.931064000	3.084928000
C	-1.854773000	-2.765420000	1.098193000
C	-4.236012000	0.157881000	-2.388879000
C	-3.273256000	-0.100976000	0.528687000
C	0.003218000	-0.022375000	4.939443000
C	-1.156576000	0.261256000	-2.972101000
C	-2.040613000	0.280628000	2.644606000
O	-3.635727000	-3.291390000	-1.987815000
O	-0.116220000	-3.290111000	-3.061288000
O	3.464138000	-3.344970000	-2.032182000
O	2.626472000	-3.383597000	1.555053000
O	-0.081264000	-3.424994000	4.123854000
O	-2.782366000	-3.228123000	1.640761000
O	-5.244175000	0.204852000	-2.953470000
O	-4.344061000	-0.287307000	0.959998000
O	0.010017000	-0.043758000	6.095423000
O	-1.256926000	0.494687000	-4.112081000
O	-2.938796000	0.536132000	3.348053000
Ni	1.391181000	-0.048719000	0.879596000
Ni	0.090311000	2.351700000	1.420409000
Ni	-1.088738000	2.395629000	-0.669403000
Ni	1.319384000	2.245028000	-0.644482000
Ni	2.413584000	-0.077844000	-1.344639000
C	2.784548000	2.667459000	-1.489165000
C	0.156186000	2.812699000	-2.007079000
C	-2.493535000	3.019124000	-1.505205000
C	-1.673059000	2.884992000	1.044939000
C	0.113172000	2.917634000	3.075098000
C	1.895505000	2.725334000	1.080988000
C	3.919831000	-0.135607000	-2.208075000
C	3.158849000	0.041293000	0.400543000
C	1.267199000	-0.239843000	-2.846131000
C	2.031955000	-0.233681000	2.591765000
O	3.706657000	3.093416000	-2.032022000
O	0.204111000	3.306007000	-3.067102000
O	-3.371443000	3.555324000	-2.019833000
O	-2.579730000	3.407037000	1.568398000
O	0.142985000	3.414417000	4.112500000
O	2.835337000	3.170418000	1.617220000
O	4.920510000	-0.176869000	-2.774352000
O	4.251889000	0.160094000	0.797369000
O	1.448584000	-0.459294000	-3.979674000
O	2.961954000	-0.439958000	3.267420000

Computed frequencies (cm^{-1})

1:	i18.55	61:	239.30	121:	525.58
2:	i4.12	62:	249.10	122:	525.85
3:	22.99	63:	250.51	123:	532.30
4:	27.36	64:	251.69	124:	533.34
5:	30.95	65:	252.02	125:	537.44
6:	31.45	66:	257.02	126:	552.97
7:	33.77	67:	260.45	127:	563.37
8:	38.06	68:	261.91	128:	563.72
9:	46.92	69:	262.18	129:	596.95
10:	51.62	70:	276.56	130:	600.99
11:	52.48	71:	290.30	131:	602.73
12:	56.79	72:	304.45	132:	605.82
13:	57.58	73:	386.87	133:	614.74
14:	58.59	74:	392.78	134:	631.88
15:	59.35	75:	393.86	135:	633.18
16:	60.32	76:	395.68	136:	1911.35
17:	68.05	77:	396.26	137:	1914.87
18:	70.07	78:	401.73	138:	1925.17
19:	71.08	79:	402.18	139:	1930.77
20:	71.98	80:	407.04	140:	1932.61
21:	72.58	81:	410.48	141:	1942.48
22:	74.10	82:	412.56	142:	1943.26
23:	75.27	83:	414.09	143:	1955.61
24:	75.87	84:	417.49	144:	1960.88
25:	76.79	85:	421.69	145:	1991.66
26:	77.81	86:	422.27	146:	1997.81
27:	78.64	87:	425.40	147:	2011.86
28:	79.32	88:	428.76	148:	2077.75
29:	80.69	89:	432.48	149:	2080.67
30:	83.73	90:	433.24	150:	2089.61
31:	84.37	91:	433.93	151:	2096.23
32:	85.57	92:	434.30	152:	2100.92
33:	90.45	93:	437.31	153:	2113.76
34:	91.48	94:	440.23	154:	2123.88
35:	93.24	95:	448.19	155:	2125.61
36:	100.85	96:	448.61	156:	2164.37
37:	101.48	97:	451.10		
38:	103.57	98:	451.54		
39:	104.57	99:	460.73		
40:	110.84	100:	462.36		
41:	118.99	101:	463.34		
42:	119.94	102:	464.15		
43:	121.83	103:	465.55		
44:	127.44	104:	467.78		
45:	128.34	105:	475.16		
46:	136.72	106:	478.53		
47:	139.65	107:	479.16		
48:	143.41	108:	482.25		
49:	145.35	109:	484.06		
50:	148.21	110:	484.87		
51:	149.20	111:	485.93		
52:	172.33	112:	491.21		
53:	182.41	113:	494.10		
54:	183.46	114:	498.95		
55:	186.49	115:	502.10		
56:	188.71	116:	502.44		
57:	197.73	117:	507.59		
58:	198.77	118:	508.32		
59:	235.36	119:	520.92		
60:	236.86	120:	523.71		

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isB$_e$B$_i$-1(E = -17688.432325128389 a.u., G^{298K} =-17688.34022078 a.u.)

54
Pt2Ni10C21O21

Ni	-0.029207000	-0.002274000	-1.540980000
Pt	-1.316421000	0.048220000	0.865879000
Ni	-0.129667000	-2.463177000	1.422631000
Ni	1.090403000	-2.321682000	-0.649802000
Ni	-1.331686000	-2.334218000	-0.683715000
Pt	0.069721000	0.017001000	3.187356000
Ni	-2.481236000	0.073916000	-1.399340000
C	-2.776755000	-2.743854000	-1.562667000
C	-0.111202000	-2.791847000	-2.028079000
C	2.537116000	-2.829215000	-1.478848000
C	1.651566000	-2.905709000	1.056604000
C	-0.171944000	-3.013820000	3.076927000
C	-1.905482000	-2.947158000	1.009496000
C	-3.947205000	0.140198000	-2.305403000
C	-3.247402000	0.020490000	0.334110000
C	0.176240000	0.046261000	5.028914000
C	-1.249065000	0.169987000	-2.883689000
C	-1.986499000	0.194701000	2.758228000
O	-3.691352000	-3.151349000	-2.132029000
O	-0.092166000	-3.260121000	-3.099500000
O	3.434571000	-3.330024000	-1.998271000
O	2.570837000	-3.429207000	1.555065000
O	-0.212857000	-3.492007000	4.122324000
O	-2.831759000	-3.457656000	1.507709000
O	-4.928857000	0.188690000	-2.904373000
O	-4.324181000	-0.030421000	0.791113000
O	0.247752000	0.068018000	6.183705000
O	-1.403163000	0.318196000	-4.033370000
O	-2.955285000	0.340911000	3.397174000
Ni	1.456908000	-0.072660000	0.945435000
Ni	0.061789000	2.486527000	1.443065000
Ni	-1.148324000	2.413876000	-0.662199000
Ni	1.267268000	2.227100000	-0.623377000
Ni	2.403155000	-0.084068000	-1.321436000
C	2.732186000	2.626356000	-1.480553000
C	0.103119000	2.763070000	-2.010526000
C	-2.567146000	2.940616000	-1.520831000
C	-1.689079000	3.054348000	1.035234000
C	0.081660000	3.052108000	3.091513000
C	1.872077000	2.782274000	1.081480000
C	3.896634000	-0.163065000	-2.200741000
C	3.189627000	0.056117000	0.422742000
C	1.229328000	-0.174710000	-2.844336000
C	2.107589000	-0.266935000	2.640286000
O	3.647949000	3.063532000	-2.025152000
O	0.162317000	3.218643000	-3.085874000
O	-3.459870000	3.423797000	-2.064476000
O	-2.593613000	3.601180000	1.534650000
O	0.103785000	3.535970000	4.135039000
O	2.829747000	3.229536000	1.581216000
O	4.890490000	-0.223084000	-2.778053000
O	4.295652000	0.209984000	0.771852000
O	1.429879000	-0.321660000	-3.986552000
O	3.042058000	-0.501702000	3.303825000

Computed frequencies (cm^{-1})

1:	13.34	61:	231.49	121:	533.66
2:	16.19	62:	245.22	122:	534.48
3:	23.47	63:	245.55	123:	540.77
4:	27.85	64:	247.34	124:	543.62
5:	29.37	65:	248.90	125:	548.66
6:	30.27	66:	253.45	126:	562.20
7:	35.14	67:	254.71	127:	562.65
8:	40.30	68:	255.93	128:	568.84
9:	45.23	69:	265.91	129:	593.02
10:	49.16	70:	270.23	130:	597.58
11:	51.23	71:	285.78	131:	597.76
12:	54.62	72:	305.84	132:	601.99
13:	57.46	73:	380.62	133:	618.94
14:	57.68	74:	389.57	134:	649.05
15:	59.61	75:	390.38	135:	661.66
16:	61.13	76:	394.74	136:	1912.28
17:	66.11	77:	401.76	137:	1918.52
18:	67.51	78:	402.52	138:	1929.15
19:	68.97	79:	403.15	139:	1934.57
20:	70.54	80:	406.24	140:	1935.57
21:	73.04	81:	407.92	141:	1945.31
22:	73.76	82:	410.28	142:	1946.34
23:	75.33	83:	418.48	143:	1957.05
24:	75.83	84:	420.41	144:	1963.74
25:	76.62	85:	424.84	145:	1983.06
26:	77.92	86:	426.45	146:	1993.01
27:	79.89	87:	427.32	147:	2004.14
28:	81.09	88:	428.71	148:	2083.00
29:	81.98	89:	430.28	149:	2086.00
30:	83.88	90:	431.10	150:	2094.34
31:	85.50	91:	432.75	151:	2095.47
32:	89.42	92:	435.86	152:	2100.95
33:	90.57	93:	440.82	153:	2121.25
34:	92.92	94:	445.09	154:	2124.58
35:	97.47	95:	451.55	155:	2131.19
36:	100.65	96:	453.76	156:	2168.56
37:	101.85	97:	454.84		
38:	104.51	98:	455.35		
39:	106.05	99:	458.64		
40:	109.09	100:	460.48		
41:	110.76	101:	462.15		
42:	118.48	102:	464.80		
43:	121.77	103:	466.17		
44:	124.60	104:	472.93		
45:	127.14	105:	478.88		
46:	132.85	106:	479.78		
47:	137.21	107:	481.30		
48:	146.15	108:	483.31		
49:	146.40	109:	484.81		
50:	152.96	110:	485.94		
51:	158.20	111:	488.77		
52:	176.99	112:	496.48		
53:	177.38	113:	509.32		
54:	182.39	114:	511.52		
55:	183.55	115:	512.45		
56:	190.68	116:	514.60		
57:	197.27	117:	515.25		
58:	207.79	118:	516.71		
59:	215.00	119:	526.12		
60:	230.28	120:	528.38		

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isB_eB_i-2(E = -17688.429924836251 a.u., G^{298K} =-17688.33735572 a.u.)

54
Pt2Ni10C21O21

Pt	-0.001523000	0.000638000	-1.317604000
Ni	-1.524584000	0.033538000	0.925633000
Ni	-0.077558000	-2.333882000	1.359619000
Ni	1.138289000	-2.459432000	-0.709572000
Ni	-1.306210000	-2.356687000	-0.716431000
Pt	-0.002766000	-0.001606000	3.060460000
Ni	-2.537777000	0.110312000	-1.317078000
C	-2.771702000	-2.751530000	-1.568053000
C	-0.108847000	-3.012184000	-2.020442000
C	2.567382000	-3.014113000	-1.526319000
C	1.702032000	-2.866222000	1.035726000
C	-0.109469000	-2.847631000	3.032468000
C	-1.873484000	-2.798988000	1.015356000
C	-4.023969000	0.220958000	-2.180550000
C	-3.275648000	-0.073150000	0.444604000
C	-0.002304000	-0.004979000	4.921252000
C	-1.352038000	0.217819000	-2.795810000
C	-2.093531000	0.180212000	2.638018000
O	-3.707210000	-3.135272000	-2.119183000
O	-0.130287000	-3.548157000	-3.058965000
O	3.472260000	-3.505975000	-2.041606000
O	2.605205000	-3.356093000	1.594379000
O	-0.140067000	-3.345689000	4.069505000
O	-2.788998000	-3.274871000	1.565459000
O	-5.013743000	0.299807000	-2.762978000
O	-4.365406000	-0.230884000	0.842999000
O	-0.002655000	-0.008432000	6.077205000
O	-1.419414000	0.372914000	-3.953547000
O	-2.982195000	0.345533000	3.378500000
Ni	1.522868000	-0.035186000	0.925111000
Ni	0.077572000	2.332160000	1.358527000
Ni	-1.136886000	2.461816000	-0.711468000
Ni	1.307269000	2.355944000	-0.717025000
Ni	2.534609000	-0.110426000	-1.319876000
C	2.773584000	2.750964000	-1.566838000
C	0.111724000	3.013185000	-2.021763000
C	-2.565435000	3.017195000	-1.528583000
C	-1.699723000	2.871766000	1.032921000
C	0.110689000	2.845922000	3.031462000
C	1.875945000	2.790802000	1.016037000
C	4.020876000	-0.216616000	-2.184359000
C	3.274554000	0.055185000	0.442455000
C	1.347639000	-0.215220000	-2.797666000
C	2.090883000	-0.163781000	2.638937000
O	3.709888000	3.135062000	-2.116433000
O	0.134175000	3.549525000	-3.060071000
O	-3.470298000	3.509290000	-2.043663000
O	-2.601289000	3.365607000	1.590618000
O	0.143229000	3.344237000	4.068284000
O	2.793320000	3.261131000	1.567835000
O	5.010988000	-0.291819000	-2.766649000
O	4.366855000	0.195071000	0.840560000
O	1.413428000	-0.369784000	-3.955526000
O	2.979750000	-0.307985000	3.383527000

Computed frequencies (cm^{-1})

1:	i11.84	61:	231.26	121:	535.74
2:	18.39	62:	242.40	122:	536.07
3:	26.35	63:	243.19	123:	546.61
4:	26.75	64:	248.39	124:	547.11
5:	29.03	65:	248.73	125:	557.12
6:	29.77	66:	250.81	126:	561.38
7:	35.61	67:	251.73	127:	561.89
8:	36.62	68:	253.66	128:	570.64
9:	38.78	69:	258.57	129:	590.33
10:	40.89	70:	270.74	130:	595.05
11:	48.83	71:	284.87	131:	601.76
12:	51.58	72:	297.76	132:	603.98
13:	53.89	73:	386.27	133:	635.72
14:	56.39	74:	387.70	134:	636.48
15:	58.50	75:	387.75	135:	662.81
16:	60.18	76:	392.37	136:	1912.29
17:	64.17	77:	396.47	137:	1920.19
18:	64.44	78:	401.26	138:	1926.49
19:	68.66	79:	401.31	139:	1935.12
20:	70.30	80:	406.40	140:	1936.92
21:	70.80	81:	406.47	141:	1944.32
22:	71.92	82:	411.14	142:	1946.98
23:	73.94	83:	411.99	143:	1958.18
24:	74.01	84:	417.08	144:	1963.49
25:	74.88	85:	419.80	145:	1986.00
26:	75.87	86:	423.02	146:	1990.53
27:	77.14	87:	426.17	147:	2005.09
28:	77.49	88:	426.59	148:	2078.76
29:	79.80	89:	428.44	149:	2089.62
30:	80.62	90:	429.77	150:	2097.32
31:	84.55	91:	430.38	151:	2097.51
32:	85.57	92:	431.42	152:	2097.75
33:	87.25	93:	443.33	153:	2118.40
34:	89.58	94:	445.25	154:	2122.77
35:	90.74	95:	448.30	155:	2132.13
36:	95.30	96:	452.73	156:	2168.29
37:	100.26	97:	452.88		
38:	100.43	98:	455.59		
39:	102.79	99:	456.45		
40:	105.01	100:	458.29		
41:	109.47	101:	464.78		
42:	112.49	102:	465.90		
43:	120.01	103:	466.86		
44:	125.32	104:	471.70		
45:	126.96	105:	476.34		
46:	129.22	106:	478.73		
47:	134.32	107:	481.01		
48:	140.52	108:	482.06		
49:	145.55	109:	482.12		
50:	145.59	110:	482.26		
51:	172.01	111:	486.71		
52:	176.60	112:	494.54		
53:	178.40	113:	496.32		
54:	180.11	114:	504.11		
55:	180.61	115:	504.69		
56:	181.54	116:	514.25		
57:	199.20	117:	518.41		
58:	200.51	118:	519.10		
59:	220.01	119:	522.10		
60:	229.74	120:	530.75		

$[Pt_2Ni_{10}(CO)_{21}]^{4-}$ isBiBi (E = -17688.454147015927 a.u., G^{298K} =-17688.36210154 a.u.)

54
Pt2Ni10C21O21

Pt	-0.037900000	-0.002192000	-1.559551000
Pt	-1.420919000	0.042598000	0.837446000
Ni	-0.074673000	-2.368912000	1.451003000
Ni	1.141177000	-2.413049000	-0.642506000
Ni	-1.300848000	-2.435142000	-0.657480000
Ni	0.009962000	0.012265000	2.912435000
Ni	-2.605163000	0.118811000	-1.442648000
C	-2.761716000	-2.843112000	-1.507264000
C	-0.079653000	-3.021428000	-1.964145000
C	2.585038000	-2.920508000	-1.468654000
C	1.703439000	-2.872478000	1.089205000
C	-0.093541000	-2.828926000	3.128042000
C	-1.847236000	-2.944126000	1.067325000
C	-4.087203000	0.197678000	-2.296848000
C	-3.341585000	0.082016000	0.353334000
C	0.078893000	0.040490000	4.634314000
C	-1.415707000	0.133204000	-2.976199000
C	-1.912512000	0.094479000	2.754160000
O	-3.699121000	-3.229151000	-2.052786000
O	-0.065732000	-3.569448000	-2.996269000
O	3.493386000	-3.404061000	-1.985511000
O	2.614117000	-3.369953000	1.627948000
O	-0.109558000	-3.268478000	4.192155000
O	-2.746260000	-3.455532000	1.611218000
O	-5.085009000	0.257533000	-2.869123000
O	-4.417836000	0.080450000	0.818385000
O	0.119750000	0.066483000	5.784469000
O	-1.546466000	0.212530000	-4.138491000
O	-2.814122000	0.151051000	3.500737000
Ni	1.398839000	-0.048096000	0.861179000
Ni	0.082411000	2.377276000	1.458102000
Ni	-1.136601000	2.520056000	-0.640891000
Ni	1.297068000	2.320003000	-0.635163000
Ni	2.478005000	-0.101402000	-1.375135000
C	2.761035000	2.728618000	-1.482659000
C	0.115850000	2.959333000	-1.976868000
C	-2.559438000	3.066924000	-1.474644000
C	-1.662691000	3.034820000	1.090449000
C	0.117513000	2.847395000	3.131471000
C	1.892831000	2.738648000	1.099992000
C	4.006677000	-0.164295000	-2.167845000
C	3.164211000	0.008117000	0.437751000
C	1.363108000	-0.150420000	-2.951116000
C	1.912892000	-0.180606000	2.597606000
O	3.689645000	3.144538000	-2.021870000
O	0.164544000	3.462910000	-3.030360000
O	-3.458151000	3.556837000	-2.001812000
O	-2.540271000	3.574222000	1.642389000
O	0.154559000	3.299268000	4.190207000
O	2.838224000	3.164726000	1.640088000
O	5.031445000	-0.207343000	-2.690701000
O	4.255672000	0.103095000	0.847496000
O	1.541392000	-0.251208000	-4.104816000
O	2.808230000	-0.346508000	3.331846000

Computed frequencies (cm^{-1})

1:	15.73	61:	228.28	121:	544.86
2:	23.76	62:	233.86	122:	546.28
3:	26.23	63:	241.13	123:	553.14
4:	30.18	64:	242.59	124:	556.20
5:	32.56	65:	245.45	125:	560.31
6:	35.03	66:	246.52	126:	561.66
7:	38.94	67:	251.50	127:	567.98
8:	39.72	68:	252.21	128:	571.56
9:	41.80	69:	252.38	129:	589.31
10:	47.10	70:	262.15	130:	593.52
11:	49.30	71:	273.55	131:	596.54
12:	50.42	72:	300.16	132:	601.52
13:	52.55	73:	383.67	133:	629.73
14:	53.76	74:	386.98	134:	658.01
15:	57.01	75:	393.41	135:	680.15
16:	58.95	76:	394.84	136:	1911.78
17:	62.42	77:	395.82	137:	1916.71
18:	65.25	78:	400.37	138:	1928.54
19:	68.82	79:	401.33	139:	1933.97
20:	70.13	80:	403.22	140:	1934.79
21:	71.61	81:	408.21	141:	1946.59
22:	73.16	82:	408.84	142:	1947.18
23:	73.73	83:	415.54	143:	1954.33
24:	74.19	84:	417.64	144:	1964.73
25:	74.68	85:	421.36	145:	1973.42
26:	75.77	86:	423.01	146:	1982.02
27:	77.65	87:	424.15	147:	1997.33
28:	79.10	88:	425.68	148:	2088.22
29:	79.25	89:	427.58	149:	2091.24
30:	81.60	90:	428.76	150:	2097.07
31:	84.20	91:	431.97	151:	2099.33
32:	85.46	92:	435.70	152:	2103.46
33:	87.72	93:	440.30	153:	2124.33
34:	87.95	94:	447.71	154:	2130.99
35:	95.64	95:	450.65	155:	2131.13
36:	98.40	96:	452.84	156:	2171.71
37:	99.21	97:	455.28		
38:	100.26	98:	455.94		
39:	100.83	99:	456.54		
40:	105.26	100:	457.27		
41:	114.88	101:	458.23		
42:	116.07	102:	461.69		
43:	123.34	103:	463.34		
44:	124.71	104:	468.12		
45:	129.42	105:	477.13		
46:	129.79	106:	479.23		
47:	133.02	107:	480.26		
48:	133.82	108:	481.06		
49:	142.72	109:	483.33		
50:	156.99	110:	484.35		
51:	173.64	111:	488.47		
52:	173.97	112:	493.51		
53:	174.69	113:	510.20		
54:	175.64	114:	516.59		
55:	183.81	115:	517.02		
56:	190.00	116:	517.60		
57:	204.63	117:	519.34		
58:	205.00	118:	524.16		
59:	223.75	119:	535.48		
60:	225.34	120:	536.38		

$[Pt_{18}Ni(CO)_{22}]^{4-}$ isA(E = -6144.906719533445 a.u.)

63
Pt18NiC22O22

Pt	-0.212174151	0.114595587	1.297379925
Ni	-2.010619139	1.457981921	0.004327744
Pt	2.395415034	-0.040839423	0.541812606
Pt	-0.012464848	0.042238750	3.979485942
Pt	0.733537691	2.403762399	-0.199140495
Pt	2.309793300	0.138827156	-2.240283791
Pt	-1.844110197	1.736886256	2.679495302
Pt	1.140433578	2.159865861	2.523103857
C	3.286765344	0.263926480	-3.804407893
C	3.735431339	0.466570708	-0.834096218
C	1.489761120	3.623101925	1.168268632
C	1.783447423	2.939325895	4.067413591
C	0.069513154	0.066080764	5.803558742
C	-2.576256774	2.809620100	3.991769180
C	-3.274019753	1.922493036	1.260539788
O	3.899929296	0.339858472	-4.772462942
O	4.836048803	0.862995845	-0.891081644
O	1.972462538	4.686415665	1.270710066
O	2.171652219	3.420144901	5.035391084
O	0.130929148	0.090497145	6.956580608
O	-3.018943781	3.466787840	4.824752243
O	-4.411784175	2.154175166	1.394156548
Pt	-0.210581123	0.117262904	-1.313752280
Pt	-2.114767822	-1.443180241	0.139384628
Pt	-0.050758960	-0.013005132	-3.987958805
Pt	0.764657409	-2.269626981	-0.476950849
Pt	2.652374965	-0.294813541	3.263568566
Pt	-1.768542252	-1.742200600	-2.582754701
Pt	1.075056206	-2.421247305	-3.194554231
C	3.610464876	-0.569136605	4.813100049
C	3.899210633	-0.636145586	1.724060648
C	1.796493796	-3.508786076	-1.669120306
C	1.617961136	-3.229670401	-4.759212093
C	-0.029849705	-0.070002136	-5.812441588
C	-2.304339707	-2.586141741	-4.133623778
C	-3.076605397	-2.495792509	-1.235823178
O	4.252816269	-0.755275128	5.751860081
O	4.991745073	-1.048793716	1.639337637
O	2.527679198	-4.419907110	-1.590631268
O	1.979464103	-3.766907898	-5.712376516
O	-0.024690150	-0.115269060	-6.966646896
O	-2.634630830	-3.100088784	-5.106320551
O	-3.965346713	-3.252375172	-1.345065941
Pt	-2.180455635	-1.250984383	2.875372030
Pt	0.615370089	-2.252772801	2.296982552
C	0.704787370	-3.708642919	0.891174445
C	0.819256118	-3.207493390	3.867407517
C	-2.974567331	-1.694964756	4.472016344
C	-3.478441315	-1.962679851	1.492978938
O	0.655612156	-4.877555029	0.943536952
O	0.948352998	-3.808166074	4.837814758
O	-3.493366572	-1.970018024	5.461707850
O	-4.555848545	-2.411244673	1.585746247
Pt	-2.222569322	1.244833490	-2.673772805
Pt	0.509331889	2.458152096	-2.927016620
C	0.746590718	3.892382767	-1.523353033
C	0.672351323	3.363160916	-4.518594655
C	-3.421545792	1.661308087	-4.013469539
C	-2.839767921	2.535543066	-1.246956166
O	0.796285882	5.060609607	-1.585739658
O	0.765565756	3.953363493	-5.502359639
O	-4.148126528	1.919092844	-4.866460510
O	-3.405373512	3.550865904	-1.368366511

$[Pt_{18}Ni(CO)_{22}]^{4-}$ isA'(E = -6144.911455623183 a.u.)

63
Pt18NiC22O22

Pt	0.296116195	0.006781470	1.321345873
Pt	-1.905215647	1.354297371	0.538681729
Pt	2.722948141	-0.024167155	-0.024802500
Pt	0.056709498	0.025805143	4.006860876
Pt	0.840802470	2.405555135	-0.118474308
Pt	2.584358952	-0.000398460	-2.776057664
Ni	-1.953187100	1.432084247	3.119029351
Pt	0.604002692	2.395670960	2.626416377
C	3.495267589	0.026588344	-4.370012795
C	4.097776348	-0.253200763	-1.428975234
C	0.948016852	3.835704750	1.255267794
C	0.718497421	3.323994766	4.213091849
C	-0.030248730	0.120574326	5.833350230
C	-2.694244310	1.898105863	4.606591075
C	-2.860073066	2.463315139	1.906407532
O	4.064985850	0.042952077	-5.369267827
O	5.242093664	-0.456066728	-1.569284112
O	1.084755397	4.996328381	1.343203665
O	0.787698412	3.894122154	5.208524781
O	-0.086532723	0.160333796	6.986487657
O	-3.180096646	2.217239965	5.595150269
O	-3.597022528	3.373700763	1.953813660
Pt	0.274635807	0.027033474	-1.300306857
Pt	-1.954213975	-1.391095181	-0.565934640
Pt	0.043672415	0.025091311	-3.971957199
Pt	0.799280013	-2.392269365	0.163455776
Pt	2.590846534	-0.010326573	2.734306633
Pt	-2.133769335	-1.562145453	-3.302720341
Pt	0.644300462	-2.362881070	-2.588888801
C	3.520360035	-0.009258854	4.320293977
C	4.092192281	0.218687099	1.371442068
C	1.270949514	-3.718737497	-1.244745078
C	0.830077319	-3.275608776	-4.181619632
C	-0.085184953	-0.035970384	-5.793554733
C	-2.932195840	-2.162125145	-4.848482059
C	-2.971985501	-2.593681118	-1.797291565
O	4.097745912	-0.006119726	5.315065868
O	5.238386121	0.417775539	1.507124452
O	1.739996061	-4.787157730	-1.354121098
O	0.945135442	-3.837289740	-5.176960674
O	-0.172094395	-0.050159355	-6.944853835
O	-3.459685826	-2.575669461	-5.786212211
O	-3.693849171	-3.515935425	-1.753580972
Pt	-1.909800832	-1.185865137	2.243668051
Pt	0.755739407	-2.381964253	2.917129539
C	0.997005496	-3.823251197	1.514860250
C	0.964903071	-3.324901085	4.485093894
C	-2.715971197	-1.812417620	3.775978851
C	-3.302557379	-1.748657578	0.842194333
O	1.166572520	-4.978013864	1.617055908
O	1.100483059	-3.905951001	5.468473011
O	-3.203293712	-2.210876869	4.737285570
O	-4.427043003	-2.057408909	0.940244886
Pt	-1.930669426	1.220503299	-2.265995932
Pt	0.774493732	2.413260082	-2.865622513
C	1.452383279	3.708867577	-1.474102486
C	0.968120608	3.374927669	-4.425332261
C	-2.769513448	1.893708046	-3.762227130
C	-3.249939058	1.867353233	-0.821796883
O	2.011708242	4.734081682	-1.568522187
O	1.098048604	3.964609034	-5.404272537
O	-3.270145128	2.314558285	-4.706268866
O	-4.336532484	2.294960490	-0.905650853

$[Pt_{18}Ni(CO)_{22}]^{4-}$ isB (E = -6144.876970262768 a.u.)

63
Pt18NiC22O22

Ni	-0.187345347	-0.405281944	1.355077961
Pt	-1.813564821	1.413492213	0.323519744
Pt	2.228572890	-0.052684771	0.293919816
Pt	0.126805388	0.128824918	3.998098321
Pt	0.773868355	2.383965007	-0.853005310
Pt	2.298481594	0.230128019	-2.525827287
Pt	-2.101790102	1.405470805	3.029706188
Pt	0.651540220	1.952434930	1.909943963
C	3.518905496	0.233054519	-3.931861740
C	3.556881322	0.598029568	-1.028949465
C	0.873201133	3.629816135	0.687019179
C	1.049396214	2.812645930	3.503731031
C	-0.278413337	-0.120817104	5.769507664
C	-2.976285360	1.944250664	4.564618500
C	-3.337517402	1.837729488	1.527715028
O	4.280438948	0.227258315	-4.789022799
O	4.638353098	1.054977890	-0.989530471
O	0.956044139	4.773049988	0.908002952
O	1.303290343	3.468291248	4.411237051
O	-0.501946529	-0.225714642	6.896605352
O	-3.573065255	2.287074569	5.487162119
O	-4.467978059	2.145308311	1.466505034
Pt	-0.072180121	-0.241056584	-1.184553511
Pt	-2.123204707	-1.553140822	0.084336104
Pt	-0.080999722	-0.073076704	-3.902869874
Pt	0.702689374	-2.554884345	0.052367139
Pt	2.702609847	0.126264478	2.931515676
Pt	-2.112836630	-1.415923914	-2.640932340
Pt	0.677194238	-2.475301422	-2.686743263
C	3.624710917	0.168047357	4.517992572
C	3.799298987	-0.641164647	1.420047425
C	1.364736442	-3.817108185	-1.335842488
C	0.953315641	-3.347756220	-4.290595680
C	0.532690562	0.136656282	-5.596537350
C	-2.892845404	-1.940125569	-4.227951828
C	-3.560582211	-1.875535844	-1.263420834
O	4.227194228	0.170525658	5.500956521
O	4.799801628	-1.232105038	1.324018317
O	1.907208084	-4.850492141	-1.436187252
O	1.125949867	-3.889594557	-5.290591908
O	0.850730831	0.205662419	-6.705051173
O	-3.370747455	-2.273355393	-5.220656443
O	-4.695746966	-2.139687214	-1.325910941
Pt	-1.981932865	-1.569350202	2.820355208
Pt	0.957583526	-2.306739234	2.738030931
C	0.947236554	-3.898517735	1.491315034
C	1.462488959	-2.967928112	4.390834635
C	-2.626147507	-2.161989542	4.457037886
C	-3.070526717	-2.571087633	1.484338783
O	1.038060109	-5.051797932	1.666790477
O	1.767356247	-3.400708121	5.410383392
O	-3.046660025	-2.563208568	5.447833296
O	-3.884298011	-3.410552948	1.586025899
Pt	-1.807538280	1.562384819	-2.429103513
Pt	0.766619750	2.621828848	-3.559686274
C	1.461429220	3.804209083	-2.083248669
C	1.002066325	3.534213262	-5.143795517
C	-2.639413914	2.119681136	-3.978261196
C	-2.552258504	2.770253879	-0.994023698
O	2.018538928	4.834202866	-2.063126937
O	1.182677590	4.187651847	-6.077177766
O	-3.172644059	2.460273773	-4.938176518
O	-3.103497686	3.798028861	-0.963907152

$[Pt_{18}Ni(CO)_{22}]^{4-}$ isC (E = -6144.902429961958 a.u.)

63
Pt18NiC22O22

Pt	-0.393946184	0.001141817	1.496598685
Pt	-2.164698962	1.564797868	0.079311359
Pt	2.602841368	-0.006754967	-0.941909872
Ni	-0.481174872	0.003690675	3.997393338
Pt	0.843154565	2.158971861	0.334772957
Pt	2.699541912	-0.012661624	-3.683341073
Pt	-2.204681377	1.595110087	2.796668328
Pt	0.670978393	2.134965296	3.115206440
C	3.564834864	-0.016855974	-5.312310687
C	4.116676036	-0.026965310	-2.244520861
C	1.095060329	3.539195909	1.719552048
C	0.948105748	3.087364973	4.673904882
C	0.004759507	-0.009918190	5.612743744
C	-2.890729811	2.119389151	4.418496133
C	-3.593887921	2.044637628	1.390172610
O	4.191037638	-0.019865456	-6.281406389
O	5.287132392	-0.043273303	-2.279919539
O	1.311421281	4.685156689	1.839902865
O	1.098722797	3.703618069	5.632925671
O	0.317057254	-0.018005508	6.721164377
O	-3.328645704	2.460352866	5.427677105
O	-4.716712233	2.363108519	1.413137639
Pt	-0.244940190	0.001342803	-1.155337215
Pt	-2.172764056	-1.553766145	0.079978556
Pt	-0.112788524	-0.000007098	-3.827403724
Pt	0.833644316	-2.162130924	0.337585220
Pt	2.351428026	-0.005238657	1.835599291
Pt	-2.059970617	-1.540711791	-2.647847158
Pt	0.991237657	-2.139035639	-2.442072313
C	3.150953394	-0.009011149	3.498792386
C	3.938224636	0.010658904	0.567979481
C	1.654934039	-3.392087097	-1.002295204
C	1.319267010	-3.131015857	-3.962044222
C	0.039228618	0.009536525	-5.633786593
C	-2.734913848	-2.121399370	-4.265223445
C	-3.036859855	-2.682748437	-1.304686096
O	3.705962726	-0.010881552	4.505125402
O	5.096998963	0.026703563	0.727067056
O	2.272493588	-4.384462408	-1.061471557
O	1.507414303	-3.748164982	-4.911887764
O	0.080163688	0.015382291	-6.787087392
O	-3.158248876	-2.487728563	-5.269742226
O	-3.750158789	-3.608534527	-1.389661483
Pt	-2.212982057	-1.582548338	2.798426163
Pt	0.660099949	-2.135332829	3.120139566
C	1.084384871	-3.538571101	1.724926891
C	0.934976443	-3.093862040	4.676149860
C	-2.903615080	-2.104588893	4.419206996
C	-3.600781664	-2.032231284	1.392011169
O	1.301522062	-4.684605535	1.845699663
O	1.083976603	-3.713454972	5.633229401
O	-3.343752908	-2.444188295	5.427799399
O	-4.723547768	-2.351270178	1.415782729
Pt	-2.051819897	1.553861890	-2.648886710
Pt	1.006584734	2.131493623	-2.445568756
C	1.666874584	3.385211907	-1.006011218
C	1.346616257	3.121217723	-3.964417404
C	-2.724107969	2.141018452	-4.265116912
C	-3.023248892	2.698502420	-1.304745288
O	2.284310703	4.377906118	-1.065391740
O	1.541857706	3.737743486	-4.913225136
O	-3.146298168	2.511763398	-5.268516769
O	-3.733202739	3.627033483	-1.389292662

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