Supplementary Material for:
Structure, magnetism and colour in simple bis(phosphine) nickel(II)dihalide complexes: an experimental and theoretical investigation

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Theoretical Investigation of Temperature Independent Paramagnetism

Small magnetic moments are difficult to measure experimentally and are sensitive to impurities from compounds with higher magnetic moments (Walter *et al.*, 2006). In particular, temperature independent paramagnetism (TIP) is difficult to measure accurately, particularly for compounds that can decompose to products with temperature dependent paramagnetism, such as the nickel complexes in this study. It was therefore of interest to investigate whether TIP can be predicted and understood theoretically. Investigation of TIP is not routine in theoretical chemistry and research has mostly been limited to a few well-known small molecules that have not been investigated experimentally (Fowler & Steiner, 1992, 1993; Pelloni *et al.*, 2009; Ruud *et al.*, 1995; Sauer *et al.*, 1993; Stevens & Lipscomb, 1965). An extensive review of the magnetic properties of transition metal complexes and their modelling has appeared (Boça, 2006). Molecules such as the dppe nickel complexes described above have been claimed experimentally to exhibit TIP (Jarrett & Sadler, 1991), but to the best of our knowledge this has not been studied theoretically. In this section we first give the theory behind the theoretical investigation of temperature independent paramagnetism before describing our results.

The energy of a molecule can be expanded in a Taylor series in terms of powers of the magnetic induction **B** around **B**=0 as follows:

$$E(\mathbf{B}) - E(\mathbf{B}=0) = \sum_{i=1}^{3} B_i \left(\frac{\partial E}{\partial B_i}\right)_{\mathbf{B}=0} + \frac{1}{2}\sum_{ij=1}^{3} B_i B_j \left(\frac{\partial^2 E}{\partial B_i \partial B_j}\right)_{\mathbf{B}=0} + \ldots \qquad (1)$$

Truncating the series at second order in **B** and introducing static magnetic moment and magnetisability tensor $\boldsymbol{\xi}$ as the negative first and second partial derivatives of the energy with respect to **B** gives:

$$E(\mathbf{B}) - E(\mathbf{B}=0) \approx -\mathbf{m}^{(0)} \cdot \mathbf{B} - \frac{1}{2}\mathbf{B}^{\mathrm{T}} \xi \mathbf{B} \qquad (2)$$

Temperature dependent paramagnetism results from permanent magnetic moments $\mathbf{m}^{(0)}$ due to spin or angular moments that align with the external magnetic field as a function of temperature. Diamagnetism ($\boldsymbol{\xi}^{\mathrm{D}}$) is present in all media and has an induced magnetic moment oriented antiparallel to the magnetic field. TIP ($\boldsymbol{\xi}^{\mathrm{TIP}}$), also called van Vleck paramagnetism (Cohen-Tannoudji *et al.*, 1977), is characterized by no permanent magnetic moment and an induced magnetic moment parallel to **B**. TIP and diamagnetism are of the same order of magnitude, while temperature dependent paramagnetism is much stronger and dominates, when present. Since molecules are statistically distributed in solution, only an isotropic value of the magnetisability ($\boldsymbol{\xi}$) is measured.

For a homogeneous magnetic field along the z-axis, the Hamiltonian can be written as (Cohen-Tannoudji, et al., 1977):

$$H = H^{(0)} + B\,H^{(1)} + B^2\,H^{(2)} \qquad (3)$$

Here $H^{(0)}$ is the Hamiltionian in absence of a magnetic field and $H^{(1)} = \frac{e}{2m_{\mathrm{e}}}\hat{l}_z = -\hat{m}_z$ and $H^{(2)} = \frac{e^2}{8m_{\mathrm{e}}}(x^2 + y^2)$ are the operators arising from the magnetic field.

The influence of the magnetic field is usually treated within perturbation theory up to second order in B (van Vleck, 1932). Since in the case of the closed shell molecules under consideration there is no permanent magnetic moment, the first-order contribution of $H^{(1)}$ vanishes. If the first-order perturbed ground-state $|0^{(1)}\rangle$ is expanded in the unperturbed excited states $|i^{(0)}\rangle$ one obtains the usual sum-over-states expression for the perturbed ground-state energy:

$$E = E^{(0)} + B^2\langle 0^{(0)}|H^{(2)}|0^{(0)}\rangle - B^2\sum_{i>0}\frac{|\langle 0^{(0)}|H^{(1)}|i^{(0)}\rangle|^2}{\langle i^{(0)}|H^{(0)}|i^{(0)}\rangle - \langle 0^{(0)}|H^{(0)}|0^{(0)}\rangle} \qquad (4)$$

The negative second derivative of the energy with respect to B then gives the zz-component of the magnetizability. The isotropic magnetizability is obtained as the average of xx, yy and zz-components of the magnetizability tensor :

$$\langle\xi\rangle = \frac{1}{3}\langle\xi_{xx} + \xi_{yy} + \xi_{zz}\rangle = \left[-\frac{\langle r^2\rangle}{a_0^2} + \sum_{i>0}\frac{|\mathbf{m}_{0i}|^2}{\Delta E_{0i}}\frac{E_\mathrm{h}}{\mu_0^2}\right]\frac{1}{6}\frac{e^2a_0^2}{m_\mathrm{e}} \qquad (5)$$

The first term in Eq. 5 is negative and is usually called diamagnetic contribution and the second one is positive and called the paramagnetic contribution to the magnetisability. Both terms are gauge-origin dependent and only their sum is gauge-invariant and physically meaningful. Still, it is often useful to study them separately and we will therefore refer to both components as para- and diamagnetic. With a specific gauge-origin, the orbitals of a system can often be related to eigenfunctions of the angular momentum operator present in the magnetic dipole operator in Eq. 5. In the case of single atoms, the gauge-origin can be chosen to lie in the nucleus. Since the Hamiltonian commutes with the angular momentum operator, the paramagnetic term vanishes precisely for closed-shell atoms.

TIP, also called orbital induced paramagnetism (Pelloni, et al., 2009), can usually be explained in terms of simple magnetic-dipole-allowed transitions from an occupied to a virtual orbital. Acting with the angular momentum operator on the virtual orbital rotates it such that it gives a non-vanishing overlap integral with the occupied orbital. Before studying the problem numerically, we will therefore check qualitatively whether TIP is predicted for planar nickel(II) complexes. Magnetisabilities will be discussed in atomic units (a.u.), $e^2a_0^2/m_e$.

For BH and CH^+, TIP is caused by degenerate excitation from a σ_x-orbital (lying in the molecular axis, here the x-axis) to the virtual p_y or p_z-orbital. The corresponding matrix-elements can therefore be computed by $\langle\sigma_x|\hat{l}_z|p_y\rangle = -i\hbar\langle\sigma_x|p_x\rangle$. This can be shown by expanding p_x/p_y in the eigenstates of l_z, $|1,\pm1\rangle$ (Tellgren *et al.*, 2009). One would therefore expect the magnetic dipole transition moment to be ≤ 2 ▪ $_0$, depending on the actual value of the overlap integral, $\langle\sigma_x|p_x\rangle$, which is less than one. Transition moments around 1.4 μ_0 are found (Sauer, et al., 1993). It is perhaps somewhat curious that the mentioned rotation of orbitals is generated by l_z, which is only the second term in the exponential series that constitutes the rotation operator. This becomes clear, however, if one acts with the rotation operator on an eigenstate of the corresponding angular momentum operator (here: z-axis, l_z-operator) one obtains a complex prefactor:

$$\hat{R}(\phi)|l;m_l\rangle = \exp(-i\frac{\phi}{\hbar}\hat{l}_z)|l;m_l\rangle = \exp(-i\phi\, m_l)|l;m_l\rangle \qquad (6)$$

If ▪ times m_l equals $\pm\tilde{\pi}$ ▪, the exponential function gives $\mp i$, i.e. a pure imaginary constant times the eigenstate. Since the real orbitals that are rotated can be written as

linear combinations of $|l,\pm m_l\rangle$ with either real or imaginary coefficients, one obtains rotations of $\tilde{\pi}$ ▪ m_l ▪ ı and $\tilde{\pi}$ ▪ m_l ▪ ▪. by applying the corresponding angular momentum operator (with an imaginary prefactor).

$$\hat{R}(\phi = \frac{\pi}{2m_l})\,[|l;m_l\rangle \pm |l;-m_l\rangle] = -i\,[|l;m_l\rangle \mp |l;-m_l\rangle] = \frac{-i\hat{l}_z}{m_l\hbar}\,[|l;m_l\rangle \pm |l;-m_l\rangle] \qquad (7)$$

Based on crystal-field theory, one would expect the magnetic properties of planar d^8 nickel complexes to arise from the occupation of the *d*-orbitals, i.e. from excitations to the unoccupied $d_{x^2-y^2}$ orbital, $|d_{x^2-y^2}\rangle = \frac{1}{\sqrt{2}}[|2,2\rangle + |2,-2\rangle]$. Working as above in the basis of the eigenstates of l_z, $|2,m\rangle$, and expressing l_y and l_x in terms of the ladder operators it can be shown that:

$$\hat{l}_z|d_{x^2-y^2}\rangle = \frac{2\hbar}{\sqrt{2}}\,[|2,2\rangle - |2,-2\rangle] = 2\hbar|d_{xy}\rangle \qquad (8a)$$

$$\hat{l}_x|d_{x^2-y^2}\rangle = \frac{\hat{l}_+ + \hat{l}_-}{2\sqrt{2}}\,[|2,2\rangle + |2,-2\rangle] = \frac{\hbar}{\sqrt{2}}\,[|2,1\rangle + |2,-1\rangle] = -i\hbar|d_{yz}\rangle \qquad (8b)$$

$$\hat{l}_y|d_{x^2-y^2}\rangle = \frac{\hat{l}_+ - \hat{l}_-}{2i\sqrt{2}}\,[|2,2\rangle + |2,-2\rangle] = \frac{\hbar}{i\sqrt{2}}\,[-|2,1\rangle + |2,-1\rangle] = -i\hbar|d_{xz}\rangle \qquad (8c)$$

The l_z-operator causes a 45°-rotation around the z-axis which explains the prefactor $2\hbar$, which is the values of the transition element for the d_{yz} to $d_{x2\text{-}y2}$ excitation. The rotations caused by l_x and l_y are different because they give a different prefactor and are obviously *not* rotations around x and y-axes. This can be better understood if one works in the eigenstates of the (normalized) linear combinations of l_x and l_y as $\hat{l}_{x\pm y} = \frac{1}{\sqrt{2}}\left(\hat{l}_x \pm \hat{l}_y\right)$. This corresponds to a rotation of the coordinate system by 45° around the z-axis. Abbreviating $|l_{x\pm y}=2;m_{x\pm y}\rangle$ as $|m\rangle_{x\pm y}$ we find:

$$\hat{l}_{x\pm y}|d_{x^2-y^2}\rangle = \frac{-\hat{l}_{x\pm y}}{\sqrt{2}}\,[|-1\rangle_{x\pm y} + |1\rangle_{x\pm y}] = \frac{-\hbar}{\sqrt{2}}\,[-|-1\rangle_{x\pm y} + |1\rangle_{x\pm y}] = -i\hbar\left[\frac{\pm|d_{xz}\rangle - |d_{yz}\rangle}{\sqrt{2}}\right] \qquad (9)$$

In the eigenstates of the $l_{x\pm y}$-operator, the $d_{x2\text{-}y2}$ orbital is a linear combinations of states with m=±1 quantum number, which leads to a rotation by 90° around (x±y)-axis and explains the prefactor $\hbar$. The orbitals obtained are linear combination of d_{xz} and d_{yz}, which is possible in D_{4h} symmetry where these orbitals are degenerate. The nickel bis(phosphine) dihalide complexes being studied here have at most C_{2v} symmetry. In C_{2v} symmetry we find (for KS orbitals) that d_{xz} and d_{yz} mix to give the linear combinations described above, which are in that case only near-degenerate. If the degeneracy of the *d*-orbitals is perturbed by an external crystal field, excitations from d_{xz}, d_{yz} (or linear combinations thereof) and d_{xy} to $d_{x2\text{-}y2}$ can give rise to a paramagnetic contribution to the magnetizibility. These transitions are also found to be magnetic-dipole allowed by applying group theory to the point-groups D_{4h}, C_{2v} or C_2. We therefore expect three metal-to-metal excitations that contribute to the paramagnetic part of ξ with at most 2 to 4 μ_0. As described above, the d_{xy} to $d_{x^2\text{-}y^2}$ transition has already been identified as being responsible for the colour. If one uses the corresponding experimental excitation energy, 75 mEh (606 nm) for the diiodide, for all three excitations together with the maximum possible magnetic transition dipole moment, this gives us $\langle\xi^p\rangle$= 53 a.u. as an upper barrier in terms of crystal field theory.

In computational chemistry, the interaction of molecules with magnetic fields is almost exclusively studied by perturbation theory, which is usually a good

approximation because the magnetic field is sufficiently weak in most experiments. Interestingly, non-perturbative treatment of the magnetic field has recently shown that molecules with TIP become diamagnetic in the presence of strong fields (~ 10^5 T) (Tellgren, et al., 2009).

Accurate magnetisabilities can in general only be computed by gauge-origin invariant methods. We will use DFT and HF with gauge-including atomic orbitals (GIAO) (Ditchfield, 1972; London, 1937; Ruud, et al., 1995; Wolinski *et al.*, 1990), as implemented in the Gaussian Program (Cheeseman *et al.*, 1996; Frisch *et al.*, 2009). The decomposition into paramagnetic and diamagnetic parts is – as noted above – in general not meaningful. For example, one helium atom has no paramagnetic contribution to the magnetisability: ξ^{dia}= -0.4 if the helium atom is chosen as the gauge-origin. If one adds a second helium atom at a non-interacting distance of ~1058 pm the correct ξ is obtained (twice that of one helium atom), however with a paramagnetic contribution of ξ^{para}=100. It is well known that magnetisabilities of diamagnetic compounds are well approximated as being additive in terms of atomic contributions (Ruud, et al., 1995; Ruud *et al.*, 1994). We therefore compare the overall magnetisability of the P_2NiX_2 complexes with the magnetisability of bis(phosphine) ligand and the diamagnetic magnetisabilities from nickel and halide atoms. The difference between the actual [illegible] and the sum of these contributions, which we will call $\Delta\xi$, is then a measure of the deviation from the expected diamagnetic behaviour. (For the non-interacting helium atoms, $\Delta\xi$ is exactly zero.

In order to see how the computed magnetisabilities relate to the transitions predicted by crystal field theory, we carried out linear response TDDFT and TDHF (RPA) calculations. The computed excitation energies E_{0i} and magnetic transition dipole moments m_{0i} were used to obtain the paramagnetic part of the magnetisability (see the SI for details). The nickel atom was chosen as the gauge-origin. Only excitations below -HOMO (the absolute value of the highest occupied KS/HF eigenvalue) were included in the calculation of the paramagnetic contribution.

The computed isotropic magnetisability (in a.u.) of (dtbpe-[illegible]^2P)$NiCl_2$ (structure as above for the **P** isomer and BP86/def2-TZVP) for B3LYP/def2-SV(P) is [illegible] 61.1 and $\Delta\xi$ [illegible] and for HF/def2-SV(P) [illegible] 30.3 and $\Delta\xi$ [illegible] Similar results are obtained for (dtbpe-[illegible]^2P)NiI_2 and B3LYP/def2-SV(P): [illegible] and $\Delta\xi$ [illegible] We therefore see that for HF there is a significant deviation from the expected diamagnetic behaviour and for B3LYP it is still in the same range as for typical temperature-independent paramagnetic molecules such as BH. Obviously, a large part of the diamagnetic contribution comes from the bulky bis(phosphine) ligand.

It was of interest to investigate a smaller molecule, because it allows comparison with more accurate methods. We therefore studied $Ni(PH_3)_2Cl_2$, optimized in C_{2v} symmetry with BP86/def2-SV(P). We find for B3LYP/def2-SV(P) [illegible] and $\Delta\xi$ [illegible] and for HF/def2-SV(P) [illegible] and $\Delta\xi$ [illegible] So, for DFT the difference to (dtbpe-[illegible]^2P)$NiCl_2$ seems to be completely systematic, while for HF the results are still comparable. Computing the excitation energies E_{0i} and magnetic transition dipole moments m_{0i} with RPA/def2-TZVPP (the nickel atom always as the gauge-origin), we find ξ^{para}= 34.2 in good agreement with $\Delta\xi$. The dominant absorptions are those predicted by crystal field theory and the values obtained for several different methods are presented in Table 1.

Table 1 Properties of the main excitations from the 1A1 ground state of C_{2v}-symmetric $(PH_3)_2NiCl_2$ obtained with different methods and the def2-TZVPP-basis. For each method and transition, the excitation energy (E_{0i}/E_h), magnetic transition dipole moment (m_{0i}/μ_0) and the resulting paramagnetic contribution to the magnetisability ($\xi^{para}/e^2a_0^2/m_e$) are tabulated (all in a.u.).

	E_{0i}	m_{0i}	ξ^{para}
RPA			
1B1	0.046	1.2	5.5
1A2	0.047	1.2	5.3
2B2	0.055	2.3	15.8
CC2			
1B1	0.097	0.2	0.4
1A2	0.117	0.2	0.2
2B2	0.108	0.3	0.4
CCSD			
1B1	0.101	0.5	0.5
1A2	0.108	0.5	0.4
2B2	0.102	1.3	2.6
B3LYP			
1B1	0.083	0.4	0.4
1A2	0.090	0.5	0.4
2B2	0.090	1.1	2.2

With the corresponding density difference between ground and excited state, the transitions can be attributed to excitations from the near-degenerate linear combinations $d_{xz}\pm d_{yz}$ and the d_{xy} to the d_{x2-y2} orbital. If E_{0i} and m_{0i} are computed with TDDFT (B3LYP/def2-TZVPP) we find ξ^{para}= 8.26, in good agreement with $\Delta\xi$ from the gauge-invariant DFT-calculations. Improving upon RPA, calculations at the equation of motion (EOM) Coupled Cluster (CC) level of theory agree better with DFT than with HF. Both CC2 (Christiansen *et al.*, 1995; Hellweg *et al.*, 2007) and CCSD (Kállay & Gauss, 2004; Koch & Jørgensen, 1990; Koch *et al.*, 1994; Stanton & Bartlett, 1993) give for all three excitations energies around 100 mE_h, which reduces the paramagnetic magnetisability roughly by one half as compared to RPA. Most importantly, the magnetic transition dipole moment, that enters the magnetisability quadratically, is lower than for RPA.

As for the bis(phosphine) complexes, the triplet-HF wavefunction is lower in energy than the singlet wave function even for (DFT)-singlet optimized structures of (dtbpe-κ^2P)$NiCl_2$ (HF/def2-TZVPP: ΔE=-35 mE_h). With CCSD(T)/def2-TZVPP, we find that the singlet ground-state is more stable by 55 mE_h, which supports our DFT calculations (B3LYP/def2-TZVPP: ΔE=54 mE_h). Overall this leads us to the

conclusion that (time-dependent) HF describes ground state and excitations worse than DFT and probably overestimates paramagnetic contribution to magnetisabilities.

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Calculated Minimum Structures and properties of Nickel(bisphosphine)dihalides

NidtbpeCl2 P structure

Cl	2.5471927	-1.5766442	-0.1504689
Cl	2.5471256	1.5766919	0.1511000
Ni	0.9971296	0.0000092	0.0001288
P	-0.5131563	1.5872791	0.0200176
P	-0.5131356	-1.5872769	-0.0201218
C	-2.1510741	-0.7156613	-0.2725648
H	-2.3099846	-0.7011318	-1.3583231
H	-2.9802207	-1.2986855	0.1565902
C	-2.1511457	0.7156476	0.2720749
H	-2.3103098	0.7011167	1.3577959
H	-2.9801976	1.2986634	-0.1572743
C	-0.7220480	2.5174797	-1.6541618
C	-1.1099919	1.4719283	-2.7142449
H	-2.0991856	1.0291310	-2.5325992
H	-0.3619217	0.6722853	-2.7763492
H	-1.1517662	1.9679109	-3.6969125
C	0.5995491	3.1625071	-2.1086840
H	0.4355488	3.6114765	-3.1021938
H	1.4065766	2.4246480	-2.1841209
H	0.9430608	3.9531183	-1.4339010
C	-1.8292146	3.5859130	-1.6057790
H	-1.5682012	4.4357287	-0.9642039
H	-2.7981065	3.1836237	-1.2767507
H	-1.9728432	3.9803843	-2.6248030
C	-0.4945598	2.8681423	1.4695084
C	0.4114947	4.0768969	1.1701799
H	0.0064501	4.7204915	0.3789581
H	1.4244447	3.7599418	0.8962115
H	0.4737704	4.6889762	2.0845643
C	0.0669127	2.1423379	2.7061939
H	0.1301152	2.8631860	3.5374022
H	1.0714785	1.7434484	2.5154559
H	-0.5890152	1.3259293	3.0364628
C	-1.9083767	3.3846738	1.8094452
H	-1.8131914	4.1064284	2.6365030
H	-2.5830487	2.5912325	2.1567564
H	-2.3901489	3.9075475	0.9751739
C	-0.4941935	-2.8681310	-1.4696159
C	0.4117959	-4.0768843	-1.1700855
H	0.4742828	-4.6889592	-2.0844586
H	0.0065722	-4.7204840	-0.3789597
H	1.4246819	-3.7599275	-0.8958841
C	0.0675606	-2.1423151	-2.7061669
H	0.1309584	-2.8631571	-3.5373657
H	1.0720805	-1.7434222	-2.5151945
H	-0.5882952	-1.3259073	-3.0365813
C	-1.9079291	-3.3846666	-1.8098823
H	-2.5825251	-2.5912257	-2.1573417
H	-2.3898902	-3.9075498	-0.9757260
H	-1.8125498	-4.1064137	-2.6369243
C	-0.7224187	-2.5174913	1.6540004
C	-1.1106339	-1.4719544	2.7139988
H	-2.0997908	-1.0291709	2.5321189
H	-0.3625914	-0.6723001	2.7762898
H	-1.1526368	-1.9679457	3.6966523
C	-1.8295595	-3.5859390	1.6053401
H	-1.9734302	-3.9804208	2.6243258
H	-1.5683795	-4.4357456	0.9638209
H	-2.7983767	-3.1836592	1.2760802
C	0.5990775	-3.1625046	2.1088358
H	1.4060759	-2.4246345	2.1844762
H	0.9427647	-3.9531032	1.4341274
H	0.4348433	-3.6114872	3.1023011

E(BP86/def2-TZVP) = -3822.38175078542
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -3821.13387408111
First ten Excitations energies and properties at B3LYP/def2-TZVPP//BP86/def2-TZVP level

Excitation Energy / Hartree	Oscillator strength /mixed representation
0.1655075008600274	0.7115100186290995E-03
0.1628503474042989	0.1463131583499674E-01
0.1621824320725233	0.5117471118930810E-04
0.1576917536824912	0.1733538028731478E-02
0.1517474313601620	0.1334909282995511E-02
0.1170921536782723	0.4584852770950868E-02
0.9021603739794168E-01	0.8180551363024008E-02
0.8877522950161000E-01	0.2438777753440321E-04
0.8250219940892729E-01	0.2363591335956731E-03
0.8086472666778932E-01	0.3656062411290854E-03

NidtbpeCl2 O structure

Ni	-0.9350261	0.0401186	0.0000240
Cl	-2.4682124	-0.3769874	-1.5470154
Cl	-2.4309447	0.5745107	1.5473760
C	2.1739515	-0.4310501	0.6798733
C	2.2006936	0.2702450	-0.6807292
P	0.5705206	-0.0564703	1.5769516
P	0.5729285	0.0201852	-1.5773027
C	0.4088052	-1.5709532	2.7644006
C	0.2609872	-2.8278115	1.8854530
C	-0.8405530	-1.5186567	3.6631294
C	1.6689989	-1.7138827	3.6388359
C	0.9310047	1.5574377	2.5876902
C	0.1147636	1.6158443	3.8913552
C	0.4996474	2.7495445	1.7160288
C	2.4257619	1.7099429	2.9251196
C	0.8074265	-1.6168399	-2.5879642
C	2.2859205	-1.8842909	-2.9254824

C	0.2853733	-2.7720481	-1.7162206
C	-0.0111198	-1.6121815	-3.8914849
C	0.5281621	1.5425472	-2.7648794
C	1.7948513	1.5872473	-3.6405181
C	0.4790666	2.8072259	-1.8860147
C	-0.7224164	1.5872318	-3.6623200
H	3.0527539	-0.1633327	1.2814755
H	2.2047221	-1.5203865	0.5408019
H	2.3148376	1.3540136	-0.5416753
H	3.0562459	-0.0640071	-1.2825971
H	-0.5920552	-2.7423752	1.1994156
H	0.0793666	-3.6909293	2.5448951
H	1.1634731	-3.0563949	1.3036094
H	-1.7572402	-1.3920982	3.0757344
H	-0.8044165	-0.7168935	4.4059289
H	-0.8988203	-2.4743363	4.2091613
H	2.5929423	-1.7838209	3.0476228
H	1.5851467	-2.6437703	4.2242915
H	1.7751852	-0.8892399	4.3553248
H	-0.9543133	1.4583595	3.7032229
H	0.2422777	2.6206273	4.3260367
H	0.4650043	0.8932644	4.6392554
H	1.0886659	2.8211901	0.7941207
H	0.6633259	3.6796028	2.2846055
H	-0.5636980	2.6840826	1.4521112
H	3.0478529	1.8431385	2.0290475
H	2.8262946	0.8679232	3.5047197
H	2.5488351	2.6175385	3.5376507
H	2.3385908	-2.7988068	-3.5378313
H	2.8959250	-2.0648752	-2.0293957
H	2.7501557	-1.0757549	-3.5052396
H	0.3769887	-3.7120126	-2.2846902
H	-0.7698558	-2.6248892	-1.4525169
H	0.8668617	-2.8886904	-0.7941646
H	0.0386929	-2.6237674	-4.3262649
H	0.3934052	-0.9185833	-4.6394048
H	-1.0648685	-1.3730578	-3.7030144
H	1.8360265	0.7569731	-4.3572189
H	2.7219589	1.5850139	-3.0501395
H	1.7829677	2.5209400	-4.2258056
H	0.3635764	3.6816492	-2.5454524
H	1.3973971	2.9656339	-1.3055736
H	-0.3769382	2.7879024	-1.1986335
H	-0.7503843	0.7839677	-4.4038232
H	-0.7058904	2.5437337	-4.2097787
H	-1.6455010	1.5341233	-3.0737333

E(BP86/def2-TZVP) = -3822.37897704039
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -3821.13122755817
First ten Excitations energies and properties at B3LYP/def2-TZVPP//BP86/def2-TZVP level

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Excitation Energy / Hartree Oscillator strength /mixed representation

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0.1701922579211665 0.3059237287496930E-02
0.1654002630348639 0.3709185413893506E-01
0.1600970809021495 0.7772243330127724E-03
0.1570844469084035 0.6667840241761252E-02
0.1511813502282183 0.1011581127417535E-01
0.1202732110988786 0.3852987438361618E-02
0.8998618022447502E-01 0.6792435129176482E-02
0.8466013179789492E-01 0.2882376555383501E-03
0.8100193566064268E-01 0.1700051596290158E-02
0.7454043411219634E-01 0.1988062507740229E-02

NidtbpeBr2 P structure

Br	2.2600915	-1.6715121	-0.0241928
Br	2.2600956	1.6714978	0.0242979
Ni	0.5828356	-0.0000049	0.0000183
P	-0.9403180	1.5801535	-0.2262493
P	-0.9403322	-1.5801589	0.2262229
C	-2.5743929	-0.7490254	-0.1518458
H	-2.7378502	-0.9111746	-1.2245969
H	-3.4021017	-1.2537547	0.3690187
C	-2.5743978	0.7490257	0.1517479
H	-2.7379024	0.9111756	1.2244916
H	-3.4020820	1.2537573	-0.3691538
C	-1.1273660	2.1993651	-2.0429250
C	-1.4429364	0.9700541	-2.9127410
H	-2.4265350	0.5341457	-2.6894550
H	-0.6721004	0.1968815	-2.8034295
H	-1.4579351	1.2816533	-3.9692285
C	0.1847378	2.8068802	-2.5703254
H	0.0314644	3.0831700	-3.6265678
H	1.0149940	2.0933160	-2.5129750
H	0.4890675	3.7074818	-2.0273928
C	-2.2693173	3.2175015	-2.2118759
H	-2.0556952	4.1760606	-1.7244306
H	-3.2348323	2.8440586	-1.8418567
H	-2.3933805	3.4209750	-3.2878870
C	-0.9983181	3.0994260	0.9778447
C	-0.1257539	4.2725152	0.4943065
H	-0.5299374	4.7524358	-0.4061123
H	0.9067754	3.9573589	0.3038303
H	-0.1129855	5.0355844	1.2893795
C	-0.4596114	2.6213753	2.3387632
H	-0.4531185	3.4768662	3.0333581
H	0.5650283	2.2371964	2.2534962
H	-1.0981703	1.8473670	2.7851011
C	-2.4366450	3.6213813	1.1849027
H	-2.3827983	4.4891725	1.8615749
H	-3.0965456	2.8867510	1.6638958
H	-2.9120684	3.9615957	0.2577064
C	-0.9982833	-3.0994291	-0.9778788
C	-0.1257425	-4.2725242	-0.4943126
H	-0.1129385	-5.0355850	-1.2893932
H	-0.5299671	-4.7524542	0.4060822
H	0.9067786	-3.9573710	-0.3037865
C	-0.4595147	-2.6213734	-2.3387707
H	-0.4529940	-3.4768608	-3.0333698
H	0.5651224	-2.2371983	-2.2534560
H	-1.0980511	-1.8473604	-2.7851328

C -2.4366018 -3.6213791 -1.1850095
H -3.0964768 -2.8867442 -1.6640309
H -2.9120719 -3.9615976 -0.2578391
H -2.3827246 -4.4891665 -1.8616842
C -1.1274591 -2.1993603 2.0428952
C -1.4430626 -0.9700414 2.9126876
H -2.4266494 -0.5341306 2.6893546
H -0.6722185 -0.1968731 2.8034044
H -1.4581095 -1.2816325 3.9691768
C -2.2694214 -3.2174903 2.2118115
H -2.3935292 -3.4209497 3.2878202
H -2.0557840 -4.1760564 1.7243876
H -3.2349199 -2.8440478 1.8417489
C 0.1846214 -2.8068712 2.5703588
H 1.0148812 -2.0933091 2.5130350
H 0.4889726 -3.7074799 2.0274508
H 0.0313026 -3.0831476 3.6265981

E(BP86/def2-TZVP) = -8050.74712032473
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -8048.89870842663
First ten Excitations energies and properties at B3LYP/def2-TZVPP//BP86/def2-TZVP level
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Excitation Energy Oscillator strength
/ Hartree /mixed representation

0.1580022271828264 0.4847780787265710E-01
0.1501832332970819 0.4499221553106105E-03
0.1469356967635924 0.3500344922622727E-01
0.1423242395343819 0.8123571284486054E-04
0.1312616520787026 0.2148055295403870E-02
0.9653844341967593E-01 0.3486846707798013E-02
0.8595290942960558E-01 0.7534564655341978E-02
0.8254794278811080E-01 0.2415919027872073E-03
0.7786325269322250E-01 0.2854513306061185E-03
0.7459904240551836E-01 0.6697751179483663E-03

NidtbpeBr2 O structure

Ni 9.6385431 1.1301020 6.1555908
Br 8.3559049 2.1055730 4.4224015
Br 8.1274383 1.8477868 7.8300240
C 11.9771597 -1.0251898 6.6389618
C 12.6473876 0.0546680 5.7872899
P 10.5212206 -0.2979614 7.5685301
P 11.3561017 0.9853214 4.7977891
C 9.4295157 -1.8587188 7.8900108
C 8.9821842 -2.3908870 6.5147244
C 8.1445088 -1.5584143 8.6823316
C 10.2381995 -2.9517366 8.6142514
C 11.2915127 0.3432802 9.2319994
C 10.2922636 0.2658581 10.4004758
C 11.6634961 1.8225650 9.0305596
C 12.5652706 -0.4322629 9.6178320
C 11.1991505 -0.0283705 3.1486356
C 12.4891701 -0.8034332 2.8199766
C 10.0555790 -1.0408695 3.3336626
C 10.8417078 0.8682860 1.9494985
C 12.2396879 2.6714783 4.4703195
C 13.6072755 2.4498096 3.7967244
C 12.4552408 3.3437940 5.8401265
C 11.4039358 3.6519809 3.6280597
H 12.6978308 -1.5028677 7.3155607
H 11.5738441 -1.8171799 5.9933155
H 13.1392280 0.7931626 6.4348953
H 13.4270259 -0.3730557 5.1434879
H 8.4693257 -1.6167257 5.9280653
H 8.2728278 -3.2174053 6.6775403
H 9.8113437 -2.7952840 5.9197375
H 7.5383998 -0.7850241 8.1962236
H 8.3345858 -1.2380207 9.7104965
H 7.5549349 -2.4886058 8.7271195
H 11.1599552 -3.2240486 8.0811976
H 9.6182733 -3.8605809 8.6787708
H 10.5004961 -2.6657762 9.6409595
H 9.3463736 0.7652564 10.1569266
H 10.7401504 0.7845617 11.2636937
H 10.0907530 -0.7667328 10.7126182
H 12.4338499 1.9533856 8.2610318
H 12.0732257 2.2143559 9.9758160
H 10.7855249 2.4216065 8.7569534
H 13.3864255 -0.2753522 8.9047350
H 12.3988219 -1.5119801 9.7261947
H 12.9127192 -0.0549535 10.5929650
H 12.3477452 -1.3065941 1.8500265
H 12.7085029 -1.5884121 3.5569295
H 13.3711659 -0.1564428 2.7263888
H 9.9295312 -1.6047320 2.3949932
H 9.1090841 -0.5363482 3.5663509
H 10.2719778 -1.7678874 4.1255514
H 10.6180393 0.2130654 1.0919195
H 11.6723911 1.5200571 1.6504573
H 9.9529565 1.4786087 2.1521135
H 13.5110970 2.0619842 2.7744365
H 14.2590173 1.7732466 4.3671194
H 14.1247250 3.4203730 3.7283263
H 12.8630206 4.3525896 5.6701693
H 13.1771949 2.8104815 6.4720577
H 11.5115475 3.4498805 6.3921769
H 11.2451162 3.3136457 2.6003282
H 11.9539883 4.6060466 3.5830479
H 10.4208832 3.8376084 4.0763177

E(BP86/def2-TZVP) = -8050.74591318884
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -8048.89767482787
First ten Excitations energies and properties at B3LYP/def2-TZVPP//BP86/def2-TZVP level
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Excitation Energy Oscillator strength
/ Hartree /mixed representation

0.1582772613198958 0.2049266053039261E-02

0.1577968859790888 0.2780931033091473E-01
0.1457912604317375 0.3054251701670318E-01
0.1398215843592782 0.8586270714304362E-03
0.1304057033984365 0.9384264725095992E-02
0.1005627533156851 0.2726969143253551E-02
0.8521437441546739E-01 0.6135997130965528E-02
0.7731903017713000E-01 0.7340886566272311E-03
0.7627787895194763E-01 0.2307359242079707E-02
0.6781884371412106E-01 0.2067173650963562E-02

NidtbpeI2 P structure

I	1.9954625	-1.7308072	-0.4713829
I	1.9954290	1.7306939	0.4685300
Ni	0.1624346	-0.0003227	-0.0005139
P	-1.3855578	1.5761882	-0.2663823
P	-1.3848260	-1.5772880	0.2669140
C	-3.0262452	-0.7572949	-0.0994285
H	-3.2256015	-0.9920493	-1.1529072
H	-3.8333846	-1.2281890	0.4817685
C	-3.0263621	0.7557195	0.1016367
H	-3.2247088	0.9904170	1.1553184
H	-3.8342320	1.2263780	-0.4787361
C	-1.4498185	2.0384356	-2.1358426
C	-1.6920879	0.7350874	-2.9169005
H	-2.6929141	0.3183387	-2.7363444
H	-0.9369987	-0.0238950	-2.6740051
H	-1.6188692	0.9508952	-3.9947841
C	-0.0943765	2.6065951	-2.5949282
H	-0.1519013	2.8032393	-3.6779940
H	0.7231871	1.8968863	-2.4171865
H	0.1686211	3.5454618	-2.0961325
C	-2.5734994	3.0279666	-2.4884841
H	-2.4014511	4.0291291	-2.0759841
H	-3.5646057	2.6800693	-2.1635763
H	-2.6114526	3.1307761	-3.5852065
C	-1.5814058	3.1925502	0.7954720
C	-0.6801774	4.3388067	0.3013698
H	-0.9983202	4.7301576	-0.6734204
H	0.3723185	4.0362855	0.2427626
H	-0.7566097	5.1677695	1.0236254
C	-1.1891756	2.8441239	2.2431681
H	-1.2811913	3.7536299	2.8584352
H	-0.1521298	2.4900210	2.3074697
H	-1.8543726	2.0879076	2.6819120
C	-3.0391934	3.7041627	0.8109081
H	-3.0595486	4.6281110	1.4107988
H	-3.7367573	3.0029345	1.2861522
H	-3.4231607	3.9551245	-0.1841187
C	-1.5812820	-3.1937002	-0.7947571
C	-0.6792194	-4.3396979	-0.3015788
H	-0.7561434	-5.1686763	-1.0237643
H	-0.9962563	-4.7311510	0.6735304
H	0.3732460	-4.0368682	-0.2440373
C	-1.1906199	-2.8451448	-2.2428452
H	-1.2829866	-3.7546726	-2.8580272
H	-0.1537457	-2.4907307	-2.3081944
H	-1.8564865	-2.0891235	-2.6809074
C	-3.0389355	-3.7057346	-0.8087226
H	-3.7371839	-3.0046996	-1.2832458
H	-3.4218198	-3.9568273	0.1866879
H	-3.0596319	-4.6296774	-1.4086104
C	-1.4470612	-2.0395674	2.1364370
C	-1.6889344	-0.7362967	2.9177488
H	-2.6900696	-0.3198513	2.7382098
H	-0.9343220	0.0229177	2.6740941
H	-1.6145574	-0.9520885	3.9955563
C	-2.5700926	-3.0294351	2.4901992
H	-2.6069163	-3.1322597	3.5869588
H	-2.3981586	-4.0305442	2.0775229
H	-3.5616270	-2.6818326	2.1662852
C	-0.0909913	-2.6073279	2.5941568
H	0.7261810	-1.8973717	2.4156082
H	0.1717888	-3.5461080	2.0950835
H	-0.1473734	-2.8040065	3.6772763

E(BP86/def2-TZVP) = -3497.56850288254
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -3496.21865852635
First ten Excitations energies and properties at B3LYP/def2-TZVPP//BP86/def2-TZVP level
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Excitation Energy / Hartree Oscillator strength /mixed representation
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0.1470154518761122 0.1380127590846019E-02
0.1343654818284145 0.8774571520044821E-03
0.1271392898952463 0.3498747631403288E-01
0.1188713315573613 0.5446596382428056E-03
0.1077503825400238 0.5759913235661873E-02
0.7857848474738593E-01 0.5447199603200466E-02
0.7788900044583977E-01 0.7788491977785910E-03
0.7128483105011359E-01 0.2168544759154822E-02
0.6538965904592708E-01 0.3294976733796676E-02
0.6200288281195186E-01 0.1488911622702000E-02

NidtbpeI2 O structure

Ni	9.6136778	1.1438993	6.1538019
I	8.0487685	1.9382545	4.2908750
I	8.1227518	2.1943910	7.9495249
C	11.9550166	-1.0160014	6.6349736
C	12.6285867	0.0678859	5.7909157
P	10.5252232	-0.2711402	7.5887802
P	11.3359405	0.9677483	4.7770379
C	9.3909231	-1.8024226	7.8954249
C	8.9244393	-2.2996984	6.5129482
C	8.1204526	-1.4610101	8.6936771
C	10.1592180	-2.9330460	8.6046366

C	11.3522991	0.3022114	9.2550728
C	10.3657467	0.2543643	10.4361256
C	11.8073617	1.7611788	9.0754368
C	12.5872355	-0.5462455	9.6158083
C	11.2667441	-0.0636468	3.1276051
C	12.6034691	-0.7673927	2.8226737
C	10.1825265	-1.1428902	3.2939716
C	10.8872084	0.8082426	1.9167388
C	12.1736256	2.6781362	4.4636505
C	13.5536275	2.5109078	3.8008852
C	12.3532334	3.3490563	5.8397748
C	11.3062052	3.6279047	3.6190315
H	12.6756063	-1.5115067	7.2981462
H	11.5337724	-1.7941239	5.9844015
H	13.1003297	0.8154518	6.4426081
H	13.4232558	-0.3522639	5.1612345
H	8.4510451	-1.4966588	5.9306450
H	8.1771006	-3.0944011	6.6642441
H	9.7375369	-2.7341589	5.9173776
H	7.5319625	-0.6744294	8.2059392
H	8.3249895	-1.1393118	9.7188973
H	7.5014829	-2.3713557	8.7466782
H	11.0753704	-3.2237431	8.0714875
H	9.5110176	-3.8232838	8.6483354
H	10.4238676	-2.6745545	9.6379596
H	9.4431856	0.8078722	10.2201322
H	10.8514458	0.7307892	11.3032814
H	10.1142428	-0.7727075	10.7298563
H	12.5781866	1.8610330	8.3010017
H	12.2480848	2.1111794	10.0230795
H	10.9653529	2.4183096	8.8227037
H	13.4150250	-0.4086462	8.9066906
H	12.3694582	-1.6190888	9.6952474
H	12.9526587	-0.2126806	10.6002943
H	12.5096578	-1.2652159	1.8442160
H	12.8445614	-1.5500571	3.5550259
H	13.4535404	-0.0762424	2.7567055
H	10.1076137	-1.7136061	2.3540483
H	9.2014349	-0.6997664	3.5079044
H	10.4290036	-1.8566936	4.0899044
H	10.7194009	0.1396683	1.0566909
H	11.6878766	1.5037869	1.6346393
H	9.9613992	1.3704220	2.0926587
H	13.4806707	2.1368555	2.7716280
H	14.2196048	1.8455898	4.3682299
H	14.0415400	3.4979829	3.7539043
H	12.7134132	4.3774984	5.6799994
H	13.0971571	2.8435005	6.4687600
H	11.4043481	3.4049566	6.3916973
H	11.1491203	3.2773509	2.5948529
H	11.8255623	4.5983841	3.5636046
H	10.3211897	3.7917436	4.0727084

E(BP86/def2-TZVP) = -3497.56903726276
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -3496.21951548756
First ten Excitations energies and properties at B3LYP/def2-TZVPP//BP86/def2-TZVP level

Excitation Energy / Hartree	Oscillator strength /mixed representation
0.1467994741905383	0.6358269330584271E-02
0.1411615611975419	0.157740725946857 4E-02
0.1266428051180372	0.2651433651726903E-01
0.1172772097066606	0.1261421668192507E-02
0.1076045456808013	0.1024291580221196E-01
0.8019586517074000E-01	0.1129685593601043E-02
0.7832039843796543E-01	0.4775192583774746E-02
0.6983259601796918E-01	0.4295730949619200E-02
0.6428414729622968E-01	0.2619965852894413E-02
0.5852774279897418E-01	0.1918600936276193E-02

NidppeCl2

P	-0.2119096	1.5083793	0.0308628
C	0.0343303	2.4411232	1.5940481
C	1.1631672	3.2613945	1.7689059
C	1.3696863	3.9298691	2.9764405
C	0.4530416	3.7849293	4.0223759
C	-0.6731593	2.9770594	3.8529313
C	-0.8857235	2.3082702	2.6444685
H	1.8797882	3.3956229	0.9564937
H	2.2469599	4.5667579	3.0992279
H	0.6159861	4.3070105	4.9664456
H	-1.3967978	2.8682711	4.6618700
H	-1.7789871	1.7007134	2.4952120
C	-0.2989787	2.7504092	-1.3095046
C	-0.6127941	4.0925434	-1.0510564
C	-0.7121798	5.0056059	-2.1027037
C	-0.5097935	4.5877932	-3.4198821
C	-0.2153804	3.2477354	-3.6858516
C	-0.1149197	2.3322717	-2.6379418
H	-0.7913221	4.4219233	-0.0279249
H	-0.9590205	6.0466490	-1.8898730
H	-0.5925325	5.3024377	-4.2399133
H	-0.0727623	2.9102250	-4.7133111
H	0.0838192	1.2830673	-2.8642977
P	-0.1940279	-1.5169589	0.1051978
C	0.0430364	-2.2882218	-1.5478917
C	-1.0916179	-2.7650632	-2.2292470
C	-0.9581736	-3.3570367	-3.4855314
C	0.2995338	-3.4707367	-4.0853608
C	1.4295664	-2.9918414	-3.4197900
C	1.3037623	-2.4051371	-2.1572489
H	-2.0745038	-2.6601050	-1.7641021
H	-1.8463849	-3.7244212	-4.0014727
H	0.3984633	-3.9282992	-5.0708369
H	2.4152174	-3.0742403	-3.8804675
H	2.2019638	-2.0447831	-1.6549184
C	-0.2294670	-2.9012115	1.3036391
C	-0.9003871	-2.7325862	2.5243759
C	-0.8612042	-3.7405805	3.4886410
C	-0.1633174	-4.9257077	3.2392800

C	0.4951212	-5.1031214	2.0201571
C	0.4634197	-4.0951684	1.0534245
H	-1.4795205	-1.8255149	2.6990571
H	-1.3926286	-3.6055196	4.4316162
H	-0.1428742	-5.7162997	3.9908660
H	1.0301826	-6.0315867	1.8152580
H	0.9669963	-4.2469203	0.0974747
C	1.4425867	0.6772625	-0.2347413
C	1.4144399	-0.6656950	0.4940909
H	2.2857724	-1.2960742	0.2649594
H	1.4047763	-0.5200297	1.5851301
H	2.2635531	1.3210939	0.1102332
H	1.5660521	0.5343569	-1.3178873
Ni	-1.7218343	-0.0109696	0.1197509
Cl	-3.1428848	1.6822983	0.1163900
Cl	-3.2461351	-1.6012433	0.2629322

E(BP86/def2-TZVP) = -4117.73142112709
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -4116.32363612235
First ten Excitations energies and properties at B3LYP/def2-TZVPP//BP86/def2-TZVP level

Excitation Energy / Hartree	Oscillator strength /mixed representation
0.1508446576129954	0.3414351628404441E-02
0.1476686718864424	0.2675150814202296E-01
0.1459404281352299	0.1070649071716568E-02
0.1442195038571844	0.3911923156904717E-02
0.1408582141895451	0.1374618719693109E-01
0.1206260688203323	0.2572719347390185E-02
0.9729795932556654E-01	0.2080485049732102E-04
0.9327969543251213E-01	0.1729736879538099E-01
0.8844455117369354E-01	0.4012332544577611E-03
0.8756629811204078E-01	0.2315075235643589E-03

NidppeBr2

P	-0.3119726	1.4980168	-0.0548418
C	-0.0466508	2.3690019	1.5413224
C	1.0378719	3.2479674	1.7111057
C	1.2616943	3.8621270	2.9441110
C	0.4068477	3.6042456	4.0204977
C	-0.6747961	2.7363663	3.8574523
C	-0.9040170	2.1212072	2.6235224
H	1.7045403	3.4694180	0.8755623
H	2.1036708	4.5456465	3.0633986
H	0.5827825	4.0854671	4.9837577
H	-1.3509583	2.5393862	4.6904418
H	-1.7628940	1.4632077	2.4830164
C	-0.4591342	2.8003765	-1.3328664
C	-0.8437314	4.1092167	-1.0057790
C	-0.9865167	5.0710348	-2.0074881
C	-0.7579579	4.7358228	-3.3439676
C	-0.3921701	3.4294625	-3.6788725
C	-0.2474836	2.4654529	-2.6805196
H	-1.0435020	4.3738433	0.0320496
H	-1.2882795	6.0847871	-1.7406374
H	-0.8747808	5.4882547	-4.1251073
H	-0.2262051	3.1559061	-4.7217418
H	0.0109436	1.4432147	-2.9621372
P	-0.1495930	-1.5233025	0.0575263
C	0.1757103	-2.3647425	-1.5432970
C	-0.7216494	-2.2076244	-2.6099294
C	-0.4520199	-2.7967953	-3.8483365
C	0.7103101	-3.5486124	-4.0312913
C	1.6060815	-3.7160306	-2.9704178
C	1.3419825	-3.1271760	-1.7330350
H	-1.6412743	-1.6418298	-2.4534941
H	-1.1595667	-2.6713044	-4.6690110
H	0.9178603	-4.0099631	-4.9979726
H	2.5118132	-4.3091654	-3.1052552
H	2.0426078	-3.2777678	-0.9095993
C	-0.1327911	-2.8303469	1.3391413
C	0.0723792	-2.4717230	2.6817190
C	0.0505655	-3.4428572	3.6833953
C	-0.1848921	-4.7809949	3.3571125
C	-0.4068889	-5.1416229	2.0261479
C	-0.3867552	-4.1728656	1.0211485
H	0.2295262	-1.4274631	2.9572654
H	0.2102593	-3.1507573	4.7222098
H	-0.2056017	-5.5394315	4.1408999
H	-0.6076369	-6.1819115	1.7664416
H	-0.5808045	-4.4594804	-0.0119282
C	1.3596738	0.7353499	-0.3952506
C	1.4380047	-0.5865163	0.3645645
H	2.3098270	-1.1866447	0.0685541
H	1.5093002	-0.4089640	1.4473061
H	2.1686746	1.4250977	-0.1166452
H	1.4270665	0.5653576	-1.4794685
Ni	-1.7526787	-0.0940453	0.0147199
Br	-3.4111476	1.5746588	0.0520834
Br	-3.2256436	-1.9299552	0.0024171

E(BP86/def2-TZVP) = -8346.10087356987
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -8344.09285332221
First ten Excitations energies and properties at B3LYP/def2-TZVPP//BP86/def2-TZVP level

Excitation Energy / Hartree	Oscillator strength /mixed representation
0.1399740686336705	0.2258803642337868E-03
0.1363902151335096	0.1278026769909110E-02
0.1360264307605291	0.1378155162456744E-01
0.1329979367692083	0.1099663710234375E-01
0.1323514457220368	0.2916503360506778E-02
0.1035518170502461	0.1774406777330505E-02
0.9406848437972615E-01	0.5060755085225639E-05
0.9013325987465208E-01	0.1654992814488486E-01

0.8682953091366313E-01 0.4585384935494938E-03
0.8392515112320292E-01 0.3225165943057705E-03

NidppeI2

P	-0.3612947	1.5000820	-0.0665565
C	-0.0649452	2.3669116	1.5281654
C	1.0042306	3.2692557	1.6705396
C	1.2595743	3.8720742	2.9030779
C	0.4537968	3.5777506	4.0075874
C	-0.6102571	2.6836649	3.8735447
C	-0.8715279	2.0817257	2.6395141
H	1.6337617	3.5170390	0.8138752
H	2.0881671	4.5751903	3.0001381
H	0.6542894	4.0504004	4.9702671
H	-1.2479926	2.4565919	4.7288651
H	-1.7172167	1.4017595	2.5245176
C	-0.4707614	2.8045715	-1.3489432
C	-0.8235872	4.1249167	-1.0313831
C	-0.9334385	5.0853963	-2.0386315
C	-0.7052236	4.7377991	-3.3720137
C	-0.3713696	3.4207477	-3.6978700
C	-0.2577802	2.4584847	-2.6936226
H	-1.0239539	4.4004474	0.0034712
H	-1.2100304	6.1080288	-1.7784823
H	-0.7970175	5.4891619	-4.1575017
H	-0.2053185	3.1375177	-4.7381452
H	-0.0226602	1.4288814	-2.9687460
P	-0.1999387	-1.5302276	0.0764763
C	0.1545516	-2.3581838	-1.5270292
C	-0.6999270	-2.1579653	-2.6210189
C	-0.4013596	-2.7265744	-3.8623862
C	0.7484868	-3.5025909	-4.0211061
C	1.6029386	-3.7120250	-2.9339548
C	1.3100680	-3.1420554	-1.6941527
H	-1.6102981	-1.5715527	-2.4865170
H	-1.0767351	-2.5668410	-4.7039330
H	0.9784854	-3.9494951	-4.9894703
H	2.4992215	-4.3231775	-3.0502733
H	1.9792571	-3.3236021	-0.8510859
C	-0.1456226	-2.8414435	1.3555427
C	0.0578214	-2.4777804	2.6970526
C	0.0668289	-3.4487851	3.6992719
C	-0.1337144	-4.7929078	3.3746576
C	-0.3519371	-5.1597102	2.0447480
C	-0.3644599	-4.1908744	1.0396060
H	0.1892752	-1.4297560	2.9717246
H	0.2239504	-3.1519000	4.7371212
H	-0.1298491	-5.5514208	4.1586228
H	-0.5251231	-6.2051642	1.7859281
H	-0.5562047	-4.4837478	0.0078677
C	1.3060125	0.7228669	-0.4027593
C	1.3821349	-0.5817281	0.3830043
H	2.2556350	-1.1876533	0.1041352
H	1.4447466	-0.3833213	1.4626242
H	2.1157485	1.4177000	-0.1392770
H	1.3695645	0.5309974	-1.4834980
Ni	-1.8185775	-0.0961670	0.0209186
I	-3.6337139	1.6835000	0.0408472
I	-3.4367108	-2.0568124	0.0346450

E(BP86/def2-TZVP) = -3792.92711233241
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -3791.41816273834
First ten Excitations energies and properties at B3LYP/def2-TZVPP//BP86/def2-TZVP level
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Excitation Energy / Hartree Oscillator strength /mixed representation
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0.1246581610393522 0.5544866240059260E-02
0.1239285539422299 0.1502252742240789E-02
0.1183235097057002 0.4335297776694266E-02
0.1177278088110805 0.5527218583615714E-02
0.1147300179008480 0.3243404800326609E-02
0.9008426910861347E-01 0.6391649971242576E-03
0.8502600493870328E-01 0.1392958077174081E-01
0.8396037175586017E-01 0.1516269367377145E-02
0.8156122031859595E-01 0.1495620296186506E-02
0.7799320163079386E-01 0.1518059240607488E-03

NidpppCl2

P	-0.4261322	1.6076637	0.0161294
C	1.2146647	2.3962316	-0.2901036
C	1.5680127	2.7407942	-1.6076518
C	2.7981453	3.3432187	-1.8737324
C	3.7014808	3.5987337	-0.8383607
C	3.3642863	3.2522720	0.4709483
C	2.1294942	2.6573484	0.7446162
H	0.8665562	2.5331759	-2.4181076
H	3.0521015	3.6088721	-2.9009911
H	4.6654026	4.0634653	-1.0511797
H	4.0617786	3.4441971	1.2877551
H	1.8932311	2.4036014	1.7773920
C	-1.6430314	2.9839216	0.0647444
C	-1.2499499	4.2908644	0.3837434
C	-2.2080745	5.3001717	0.5165990
C	-3.5621084	5.0098210	0.3395623
C	-3.9578336	3.7073555	0.0197303
C	-3.0041578	2.6994943	-0.1235708
H	-0.1931584	4.5287549	0.5135433
H	-1.8911331	6.3168795	0.7539859
H	-4.3084680	5.7993367	0.4389514
H	-5.0127104	3.4783076	-0.1379855
H	-3.3095765	1.6947619	-0.4183080
P	-0.2611383	-1.6669989	-0.0695707
C	1.4459742	-2.3129412	-0.2885639
C	1.9438998	-3.3451072	0.5259829
C	3.2601022	-3.7870535	0.3826683
C	4.0967479	-3.1981447	-0.5700189

C	3.6093984	-2.1728818	-1.3830479
C	2.2900528	-1.7342375	-1.2475030
H	1.3010919	-3.8237284	1.2668660
H	3.6313836	-4.5944544	1.0156475
H	5.1259381	-3.5431523	-0.6803808
H	4.2542272	-1.7139726	-2.1335666
H	1.8981623	-0.9545915	-1.9011196
C	-1.4022621	-3.1025251	-0.1778224
C	-1.0163221	-4.3191414	-0.7583249
C	-1.9199432	-5.3807275	-0.8345077
C	-3.2206755	-5.2371958	-0.3461008
C	-3.6184692	-4.0217017	0.2158488
C	-2.7155640	-2.9606185	0.2986886
H	-0.0131269	-4.4313764	-1.1677137
H	-1.6069497	-6.3208777	-1.2909526
H	-3.9264739	-6.0662201	-0.4135580
H	-4.6372526	-3.8940904	0.5845114
H	-3.0513317	-2.0094738	0.7160526
C	-0.4012904	1.1891677	1.8230527
C	-0.3111122	-1.3554173	1.7648239
H	0.1351451	-2.2317487	2.2563139
H	-1.3699628	-1.3333647	2.0638340
H	-1.4607937	1.0697116	2.1006458
H	-0.0481275	2.0755360	2.3707273
C	0.3846105	-0.0675577	2.2147331
H	1.4121655	-0.0299216	1.8192461
H	0.4815384	-0.0891012	3.3122727
Ni	-0.7448494	-0.0141301	-1.3829913
Cl	-1.3799207	1.5218081	-2.8345933
Cl	-0.7136919	-1.6030128	-2.9192893

E(BP86/def2-TZVP) = -4157.05135588768
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -4155.61603057375
First ten Excitations energies and properties at B3LYP/def2-TZVPP//BP86/def2-TZVP level

Excitation Energy / Hartree	Oscillator strength /mixed representation
0.1547808020425263	0.1805394940161265E-01
0.1528299493776693	0.4531626714122904E-02
0.1493891277535880	0.9645392149499306E-02
0.1479794022581065	0.1938798811300370E-02
0.1444468046121122	0.8850693202325021E-02
0.1162601118782734	0.4224126274582672E-02
0.9291112782304442E-01	0.7483225867790002E-02
0.8954730462710590E-01	0.2163071603741987E-04
0.8542004804466014E-01	0.6615419039948931E-03
0.8239038712956427E-01	0.2511328443295159E-02

NidpppBr2

P	-0.4760272	1.6034679	0.0064449
C	1.1881606	2.3369880	-0.3113661
C	1.5697777	2.6123207	-1.6370452
C	2.8187923	3.1708404	-1.9120714
C	3.7134720	3.4499005	-0.8755710
C	3.3482242	3.1728061	0.4429259
C	2.0947388	2.6227699	0.7242515
H	0.8750907	2.3921191	-2.4500342
H	3.0933568	3.3834542	-2.9463079
H	4.6922129	3.8795974	-1.0942032
H	4.0385207	3.3846902	1.2608891
H	1.8362437	2.4241882	1.7637661
C	-1.6415743	3.0234512	0.0968136
C	-1.1896360	4.3365617	0.2809489
C	-2.1073388	5.3788462	0.4451152
C	-3.4780026	5.1161871	0.4357778
C	-3.9330903	3.8063536	0.2529660
C	-3.0214136	2.7659842	0.0779554
H	-0.1206959	4.5528637	0.2820330
H	-1.7450959	6.3997058	0.5759260
H	-4.1925795	5.9311525	0.5597091
H	-5.0033006	3.5964255	0.2273514
H	-3.3808127	1.7529393	-0.1099287
P	-0.2961312	-1.6664399	-0.1053710
C	1.4342059	-2.2612647	-0.2896512
C	1.9439717	-3.2852082	0.5281654
C	3.2768858	-3.6839208	0.4149703
C	4.1189849	-3.0588797	-0.5093770
C	3.6210473	-2.0396156	-1.3234953
C	2.2852398	-1.6448803	-1.2183396
H	1.2985031	-3.7904351	1.2486478
H	3.6570302	-4.4857705	1.0497411
H	5.1610623	-3.3702769	-0.5961425
H	4.2705059	-1.5512065	-2.0509949
H	1.8877593	-0.8678189	-1.8717391
C	-1.3950119	-3.1361031	-0.2152430
C	-0.9611225	-4.3624745	-0.7383845
C	-1.8369612	-5.4477552	-0.8068746
C	-3.1565933	-5.3190829	-0.3675811
C	-3.6011661	-4.0950114	0.1378725
C	-2.7263932	-3.0101499	0.2133470
H	0.0573519	-4.4650646	-1.1109883
H	-1.4868676	-6.3950989	-1.2194026
H	-3.8404641	-6.1666592	-0.4298342
H	-4.6347134	-3.9793393	0.4672267
H	-3.0975591	-2.0529946	0.5845908
C	-0.4499622	1.1764722	1.8127347
C	-0.3810226	-1.3651928	1.7304789
H	0.0459867	-2.2507548	2.2225915
H	-1.4459012	-1.3356157	2.0070003
H	-1.5106756	1.0713089	2.0916745
H	-0.0857295	2.0585293	2.3600983
C	0.3191028	-0.0890752	2.2035950
H	1.3527537	-0.0561924	1.8239079
H	0.3993292	-0.1213446	3.3022682
Ni	-0.8295651	-0.0087356	-1.4107285
Br	-1.6253174	1.6109248	-2.9241476
Br	-0.7475864	-1.6484866	-3.1069620

E(BP86/def2-TZVP) = -8385.41840328829
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) = -8383.38271514968

First ten Excitations energies and properties at
B3LYP/def2-TZVPP//BP86/def2-TZVP level

Excitation Energy Oscillator strength
/ Hartree /mixed representation

0.1398534257929142 0.3001277954306082E-02
0.1392687897060468 0.1404199641655262E-02
0.1379727387001128 0.5332363001281523E-02
0.1318018280658657 0.4345020025424272E-02
0.1295675717399386 0.4683904864148842E-02
0.9649307733215780E-01 0.3429300681678035E-02
0.8845356703616573E-01 0.6382185246478564E-02
0.8429995581883733E-01 0.1866559311013383E-03
0.8150538102380731E-01 0.6729394456432237E-03
0.7664019741428041E-01 0.2562588905519537E-02

NidpppI2

P	-0.5269806	1.5964846	-0.0036125
C	1.1397590	2.2982452	-0.3724272
C	1.4731803	2.5862783	-1.7085060
C	2.7224197	3.1202129	-2.0278469
C	3.6655189	3.3603287	-1.0249830
C	3.3483489	3.0702849	0.3033294
C	2.0945091	2.5460535	0.6286840
H	0.7435834	2.3943792	-2.4979064
H	2.9588124	3.3428638	-3.0692986
H	4.6446521	3.7699522	-1.2776107
H	4.0770245	3.2525303	1.0947046
H	1.8728269	2.3375776	1.6747913
C	-1.6459961	3.0519888	0.1428248
C	-1.1573371	4.3631527	0.2033038
C	-2.0353927	5.4318507	0.4105972
C	-3.4021093	5.1988053	0.5684783
C	-3.8945207	3.8909089	0.5105733
C	-3.0237454	2.8244040	0.2920536
H	-0.0918321	4.5568224	0.0770275
H	-1.6448584	6.4500538	0.4453628
H	-4.0856592	6.0340794	0.7271262
H	-4.9636426	3.7022137	0.6174643
H	-3.4195805	1.8108862	0.2051461
P	-0.2993559	-1.6710839	-0.1351912
C	1.4478363	-2.2403671	-0.2270560
C	1.9099295	-3.3021146	0.5704575
C	3.2554908	-3.6732882	0.5443760
C	4.1576860	-2.9811132	-0.2686347
C	3.7081819	-1.9203922	-1.0577848
C	2.3602338	-1.5543265	-1.0414073
H	1.2178415	-3.8563080	1.2067746
H	3.5985422	-4.5058544	1.1604802
H	5.2092120	-3.2715167	-0.2877560
H	4.4052828	-1.3775821	-1.6972678
H	2.0041944	-0.7419569	-1.6755495
C	-1.3699646	-3.1600733	-0.2785105
C	-0.9079611	-4.3773762	-0.8000618
C	-1.7680900	-5.4730253	-0.8981874
C	-3.1000934	-5.3640195	-0.4921191
C	-3.5728213	-4.1493921	0.0103702
C	-2.7138507	-3.0543570	0.1162284
H	0.1207631	-4.4652097	-1.1472819
H	-1.3955292	-6.4128790	-1.3081091
H	-3.7713442	-6.2195926	-0.5778936
H	-4.6158608	-4.0486828	0.3136029
H	-3.1067869	-2.1047779	0.4841891
C	-0.4637509	1.1713385	1.8048934
C	-0.4532212	-1.3706720	1.6980253
H	-0.0675967	-2.2680824	2.2027557
H	-1.5259728	-1.3096567	1.9360286
H	-1.5202761	1.1035455	2.1098026
H	-0.0579702	2.0450512	2.3365762
C	0.2694277	-0.1152565	2.1917586
H	1.3083708	-0.1043961	1.8255487
H	0.3350772	-0.1572285	3.2911401
Ni	-0.8773972	-0.0154394	-1.4428431
I	-2.0183703	1.6241051	-3.0209431
I	-0.5508377	-1.6683761	-3.3656873

E(BP86/def2-TZVP) = -3832.24251301712
E(B3LYP/def2-TZVPP//BP86/def2-TZVP) =
-3830.70561970092
First ten Excitations energies and properties at
B3LYP/def2-TZVPP//BP86/def2-TZVP level

Excitation Energy Oscillator strength
/ Hartree /mixed representation

0.1250674579966674 0.1150985517602436E-01
0.1203317918291860 0.6276628483163012E-02
0.1192059187821592 0.3257762324778426E-03
0.1130092949634335 0.3253169151887184E-02
0.1097726840284191 0.5870027794700943E-02
0.8280542614309339E-01 0.5819945622833430E-02
0.7962402982900565E-01 0.7122341429915848E-03
0.7671993612351528E-01 0.1431971113751265E-02
0.6998150212799684E-01 0.2236529048405656E-02
0.6693101179755477E-01 0.3149187870671429E-02

Calculations on model complex NiCl2(PH3)2

Cl	0.0000000	-1.6501692	1.4577022
Cl	0.0000000	1.6501692	1.4577022
Ni	0.0000000	0.0000000	0.0000000
P	0.0000000	1.6391586	-1.3557540
P	0.0000000	-1.6391586	-1.3557540
H	-1.0936129	-2.5606071	-1.2912995
H	0.0000000	-1.4215426	-2.7864405
H	1.0936129	-2.5606071	-1.2912995

H 1.0936129 2.5606071 -1.2912995
H 0.0000000 1.4215426 -2.7864405
H -1.0936129 2.5606071 -1.2912995

Energies for singlet ground-state (RKS or RHF (reference))
E(BP86/def2-SV(P))= -3114.86383429858
E(B3LYP/def2-TZVPP//BP86/def2-SV(P)) = -3114.93943111479
E(B3LYP/def2-SV(P)//BP86/def2-SV(P)) = -3114.50084839
E(HF/def2-TZVPP//BP86/def2-SV(P)) = -3110.86903324655
E(HF/def2-SV(P)//BP86/def2-SV(P)) = -3110.07669288
E(CC2/def2-TZVPP//BP86/def2-SV(P)) = -3112.2301811584
E(CCSD/def2-TZVPP//BP86/def2-SV(P))= -3112.1269735672
E(CCSD(T)/def2-TZVPP//BP86/def2-SV(P)) = -3112.1923853463

Energies for triplet-ground-state calculation (UHF/UKS, Sz=2, <SS> ~ 2.01 +- 0.01)
E(B3LYP/def2-TZVPP//BP86/def2-SV(P)) = -3114.88513320779
E(HF/def2-TZVPP//BP86/def2-SV(P)) = -3110.90416439074
E(CCSD(T)/def2-TZVPP//BP86/def2-SV(P)) = -3112.1375870455

Relaxed potential surfaces scans

Relaxed potential surface scan of P structure of NiI2dtbpe

Combination of torsional angles = -40
E(BP86/def2-TZVP) = -3497.56230710842
I 2.0037428 -1.5869995 0.8489024
I 2.0036701 1.5869208 -0.8493848
Ni 0.1833672 -0.0000007 -0.0000903
P -1.3657278 1.5512309 0.3908683
P -1.3658601 -1.5511652 -0.3907912
C -2.9625442 -0.5851255 -0.4939943
H -3.0385840 -0.2115699 -1.5231887
H -3.8323621 -1.2379599 -0.3288411
C -2.9624355 0.5852599 0.4943423
H -3.0383159 0.2117075 1.5235498
H -3.8322539 1.2381312 0.3293373
C -1.8875444 3.0184171 -0.7705506
C -2.4181264 2.3912888 -2.0741759
H -3.3533867 1.8333966 -1.9301352
H -1.6713913 1.7337589 -2.5385055
H -2.6322271 3.2021365 -2.7882418
C -0.7233693 3.9481756 -1.1527949
H -1.1241792 4.7378247 -1.8102488
H 0.0679906 3.4135213 -1.6889102
H -0.2632267 4.4380785 -0.2883162
C -3.0057905 3.8794284 -0.1525488
H -2.6363754 4.5033339 0.6705697
H -3.8654051 3.2978491 0.2079610
H -3.3807546 4.5631412 -0.9315010
C -1.0839735 2.2063151 2.1816209
C -0.1062158 3.3937735 2.1706307
H -0.5660636 4.3065952 1.7705150
H 0.8028353 3.1731193 1.5930836
H 0.1961809 3.6073146 3.2081926
C -0.4386014 1.0569376 2.9788067
H -0.2264712 1.4146464 3.9996452
H 0.5049063 0.7152811 2.5314078
H -1.1061400 0.1893933 3.0689446
C -2.3857996 2.6115166 2.8991624
H -2.1283648 2.9075195 3.9290565
H -3.1017655 1.7818346 2.9758051
H -2.8927152 3.4623270 2.4320891
C -1.0844346 -2.2062569 -2.1815938
C -0.1067251 -3.3937566 -2.1707740
H 0.1954914 -3.6073022 -3.2083875
H -0.5665459 -4.3065619 -1.7705903
H 0.8024303 -3.1731457 -1.5933749
C -0.4391469 -1.0569047 -2.9788840
H -0.2272050 -1.4146187 -3.9997598
H 0.5044512 -0.7152914 -2.5316429
H -1.1066625 -0.1893304 -3.0689060
C -2.3863980 -2.6113989 -2.8989196
H -3.1023392 -1.7816844 -2.9754423
H -2.8932742 -3.4621869 -2.4317634
H -2.1291476 -2.9074119 -3.9288569
C -1.8875455 -3.0183268 0.7707195
C -2.4178709 -2.3911687 2.0744347
H -3.3531290 -1.8332315 1.9305541
H -1.6710231 -1.7336733 2.5386322
H -2.6318870 -3.2020035 2.7885406
C -3.0059406 -3.8792867 0.1529157
H -3.3808029 -4.5629774 0.9319363
H -2.6366986 -4.5032147 -0.6702633
H -3.8655895 -3.2976677 -0.2074483
C -0.7233495 -3.9481404 1.1527667
H 0.0681298 -3.4135222 1.6887419
H -0.2633817 -4.4380714 0.2882113
H -1.1240842 -4.7377659 1.8102949

Combination of torsional angles = -35
E(BP86/def2-TZVP) = -3497.56388476330
I 2.0074434 -1.6416033 0.7352676
I 2.0079573 1.6413642 -0.7341263
Ni 0.1831445 0.0000077 0.0002185
P -1.3624454 1.5623305 0.3443759
P -1.3625241 -1.5621041 -0.3445382
C -2.9578656 -0.5975212 -0.4787592
H -3.0299148 -0.2509763 -1.5172787
H -3.8294810 -1.2443090 -0.2997196
C -2.9579712 0.5979651 0.4779702
H -3.0304765 0.2514297 1.5164612
H -3.8294269 1.2448728 0.2985879
C -1.8906795 2.9871416 -0.8663140

C	-2.4390521	2.3196401	-2.1423761
H	-3.3775356	1.7753669	-1.9705563
H	-1.7031240	1.6396958	-2.5917891
H	-2.6531152	3.1073609	-2.8818688
C	-0.7297259	3.9007633	-1.2938335
H	-1.1397893	4.6758754	-1.9628904
H	0.0479001	3.3486803	-1.8320283
H	-0.2482357	4.4078392	-0.4512278
C	-3.0007610	3.8695959	-0.2636515
H	-2.6256347	4.5092534	0.5446426
H	-3.8622891	3.3005643	0.1119194
H	-3.3746865	4.5376788	-1.0565016
C	-1.0900131	2.2778263	2.1147717
C	-0.1579142	3.5005891	2.0714737
H	-0.6479296	4.3826729	1.6393102
H	0.7630028	3.2946539	1.5077622
H	0.1275327	3.7577372	3.1040339
C	-0.3969647	1.1715688	2.9334396
H	-0.1954840	1.5575055	3.9461801
H	0.5580938	0.8610584	2.4877974
H	-1.0279891	0.2791966	3.0427233
C	-2.4014953	2.6549120	2.8304727
H	-2.1469709	3.0066361	3.8433732
H	-3.0789361	1.7988562	2.9517934
H	-2.9507097	3.4616704	2.3332820
C	-1.0894861	-2.2776536	-2.1148177
C	-0.1575740	-3.5005448	-2.0711268
H	0.1282496	-3.7577512	-3.1035682
H	-0.6478836	-4.3825528	-1.6391419
H	0.7631466	-3.2947265	-1.5070516
C	-0.3959555	-1.1715039	-2.9332235
H	-0.1941159	-1.5574860	-3.9458753
H	0.5589647	-0.8611153	-2.4871997
H	-1.0268141	-0.2790484	-3.0427792
C	-2.4007348	-2.6545704	-2.8310357
H	-3.0780098	-1.7984238	-2.9526398
H	-2.9502580	-3.4612460	-2.3340513
H	-2.1458550	-3.0063447	-3.8438293
C	-1.8914245	-2.9868443	0.8659427
C	-2.4402102	-2.3192731	2.1417912
H	-3.3785534	-1.7748738	1.9696046
H	-1.7043679	-1.6394286	2.5914963
H	-2.6546696	-3.1069675	2.8811970
C	-3.0013851	-3.8691476	0.2628365
H	-3.3757088	-4.5371891	1.0555336
H	-2.6260253	-4.5088459	-0.5453170
H	-3.8626916	-3.2999998	-0.1130665
C	-0.7307629	-3.9006253	1.2939131
H	0.0467256	-3.3486509	1.8324176
H	-0.2490091	-4.4077609	0.4514931
H	-1.1411948	-4.6756867	1.9628026

Combination of torsional angles = -30
E(BP86/def2-TZVP) = -3497.56500189110

I	2.0150255	-1.6845152	0.6222969
I	2.0151009	1.6844905	-0.6219049
Ni	0.1846605	-0.0000153	0.0000776
P	-1.3585501	1.5733062	0.2973294
P	-1.3585052	-1.5733438	-0.2973711
C	-2.9537785	-0.6124918	-0.4587911
H	-3.0265712	-0.2991834	-1.5074134
H	-3.8255059	-1.2531082	-0.2591816
C	-2.9538408	0.6124480	0.4585415
H	-3.0267693	0.2991390	1.5071544
H	-3.8255445	1.2530610	0.2588182
C	-1.8820839	2.9476792	-0.9722827
C	-2.4264800	2.2325952	-2.2240370
H	-3.3675953	1.6985885	-2.0356172
H	-1.6911953	1.5330799	-2.6434686
H	-2.6344610	2.9916811	-2.9945536
C	-0.7198157	3.8442785	-1.4305483
H	-1.1281385	4.5941814	-2.1288061
H	0.0583143	3.2723946	-1.9468445
H	-0.2387638	4.3807723	-0.6061756
C	-2.9956485	3.8507926	-0.4075628
H	-2.6288528	4.5131868	0.3860190
H	-3.8623617	3.2941356	-0.0254951
H	-3.3597780	4.4956396	-1.2238322
C	-1.1097185	2.3582546	2.0437808
C	-0.2179769	3.6093598	1.9692973
H	-0.7294356	4.4593495	1.4993108
H	0.7175563	3.4134394	1.4271696
H	0.0420884	3.9115040	2.9964478
C	-0.3854679	1.2998167	2.8982340
H	-0.2046900	1.7199284	3.9012477
H	0.5828690	1.0126722	2.4661513
H	-0.9858435	0.3891492	3.0276918
C	-2.4355449	2.7187071	2.7421383
H	-2.1950762	3.1300276	3.7357772
H	-3.0798308	1.8448104	2.9073435
H	-3.0150543	3.4784634	2.2061327
C	-1.1094438	-2.3582990	-2.0437876
C	-0.2177123	-3.6094041	-1.9691842
H	0.0424885	-3.9115501	-2.9963000
H	-0.7292328	-4.4593931	-1.4992638
H	0.7177497	-3.4134827	-1.4269338
C	-0.3850797	-1.2998656	-2.8981500
H	-0.2041691	-1.7199825	-3.9011377
H	0.5832003	-1.0127199	-2.4659405
H	-0.9854371	-0.3891983	-3.0276921
C	-2.4351786	-2.7187521	-2.7423191
H	-3.0794411	-1.8448550	-2.9076129
H	-3.0147602	-3.4785053	-2.2063873
H	-2.1945792	-3.1300768	-3.7359246
C	-1.8822009	-2.9477087	0.9721829
C	-2.4267605	-2.2326129	2.2238594
H	-3.3678509	-1.6986073	2.0353115
H	-1.6915303	-1.5330938	2.6433805
H	-2.6348426	-2.9916914	2.9943561
C	-2.9956917	-3.8508285	0.4073276
H	-3.3599255	-4.4956684	1.2235562
H	-2.6287932	-4.5132297	-0.3862007
H	-3.8623564	-3.2941760	0.0251434
C	-0.7199906	-3.8443011	1.4306094
H	0.0580712	-3.2724102	1.9470005
H	-0.2388306	-4.3808032	0.6063054
H	-1.1284031	-4.5941968	2.1288224

Combination of torsional angles = -25
E(BP86/def2-TZVP) = -3497.56576912321

I	2.0235991	-1.7183286	0.5098261
I	2.0234537	1.7183612	-0.5102967
Ni	0.1865566	-0.0000185	-0.0000914
P	-1.3552813	1.5834289	0.2514665
P	-1.3552534	-1.5835320	-0.2514020
C	-2.9515823	-0.6281398	-0.4361689
H	-3.0288163	-0.3519847	-1.4945655
H	-3.8219768	-1.2622934	-0.2115317
C	-2.9515388	0.6279666	0.4364899
H	-3.0285895	0.3518071	1.4948988
H	-3.8219973	1.2620823	0.2119937
C	-1.8641696	2.9015684	-1.0815859
C	-2.3922163	2.1357030	-2.3099403
H	-3.3365759	1.6109846	-2.1121651
H	-1.6525828	1.4185622	-2.6898276
H	-2.5887312	2.8623539	-3.1140091
C	-0.6957247	3.7787162	-1.5607583
H	-1.0937340	4.4972321	-2.2969311
H	0.0899983	3.1858846	-2.0408676
H	-0.2266316	4.3500171	-0.7530741
C	-2.9866132	3.8248912	-0.5694474
H	-2.6357179	4.5138979	0.2083650
H	-3.8610827	3.2813136	-0.1862302
H	-3.3344661	4.4412835	-1.4142808
C	-1.1409155	2.4427505	1.9699181
C	-0.2837821	3.7158142	1.8640650
H	-0.8086319	4.5325383	1.3518144
H	0.6679899	3.5259255	1.3495993
H	-0.0550658	4.0637961	2.8842217
C	-0.3995864	1.4355579	2.8703484
H	-0.2474892	1.8932934	3.8615664
H	0.5833607	1.1658054	2.4612884
H	-0.9747370	0.5118543	3.0206731
C	-2.4843424	2.7950551	2.6392130
H	-2.2655741	3.2664235	3.6108847
H	-3.1015166	1.9109811	2.8470989
H	-3.0835331	3.5061890	2.0594544
C	-1.1411244	-2.4428527	-1.9698841
C	-0.2839198	-3.7158792	-1.8641620
H	-0.0553504	-4.0638553	-2.8843537
H	-0.8086533	-4.5326237	-1.3518251
H	0.6679257	-3.5259476	-1.3498481
C	-0.3999810	-1.4356335	-2.8704372
H	-0.2480207	-1.8933681	-3.8616767
H	0.5830190	-1.1658360	-2.4615341
H	-0.9751954	-0.5119559	-3.0206763
C	-2.4846422	-2.7952174	-2.6389649
H	-3.1018860	-1.9111703	-2.8467585
H	-3.0837117	-3.5063729	-2.0591077
H	-2.2660076	-3.2665822	-3.6106685
C	-1.8638717	-2.9016833	1.0817404
C	-2.3917522	-2.1358292	2.3101735
H	-3.3361634	-1.6111481	2.1125449
H	-1.6520854	-1.4186573	2.6899379
H	-2.5881112	-2.8624818	3.1142787
C	-2.9863595	-3.8250563	0.5697889
H	-3.3340518	-4.4414564	1.4146828
H	-2.6355600	-4.5140546	-0.2080742
H	-3.8609129	-3.2815180	0.1867073
C	-0.6953123	-3.7787779	1.5607321
H	0.0904628	-3.1859087	2.0407099
H	-0.2263250	-4.3500658	0.7529774
H	-1.0931726	-4.4973044	2.2969751

Combination of torsional angles = -20
E(BP86/def2-TZVP) = -3497.56631721773

I	2.0284797	-1.7433388	0.4008840
I	2.0285310	1.7432125	-0.4012355
Ni	0.1848227	-0.0000105	-0.0000654
P	-1.3563489	1.5927685	0.2046059
P	-1.3564676	-1.5926981	-0.2045604
C	-2.9548336	-0.6443921	-0.4107702
H	-3.0392106	-0.4098882	-1.4784154
H	-3.8226907	-1.2710507	-0.1570181
C	-2.9547474	0.6445609	0.4110036
H	-3.0390135	0.4100632	1.4786589
H	-3.8225961	1.2712726	0.1573520
C	-1.8406729	2.8479902	-1.1955697
C	-2.3421285	2.0280537	-2.3996186
H	-3.2902522	1.5115273	-2.1984516
H	-1.5943576	1.2956343	-2.7309992
H	-2.5219587	2.7179623	-3.2391770
C	-0.6615046	3.7032181	-1.6876139
H	-1.0414246	4.3846670	-2.4672536
H	0.1359778	3.0892861	-2.1197320
H	-0.2124292	4.3130670	-0.8969353
C	-2.9751931	3.7905562	-0.7494101
H	-2.6460877	4.5093033	0.0106196
H	-3.8597506	3.2609390	-0.3697561
H	-3.3003416	4.3733679	-1.6264950
C	-1.1847199	2.5318978	1.8886202
C	-0.3557802	3.8204844	1.7481386
H	-0.8864345	4.6019225	1.1891128
H	0.6128764	3.6321839	1.2664913
H	-0.1622533	4.2164701	2.7580867
C	-0.4392865	1.5802764	2.8440630
H	-0.3194986	2.0804444	3.8190301
H	0.5579899	1.3201852	2.4651992
H	-0.9960031	0.6497128	3.0195736
C	-2.5477263	2.8840952	2.5184540
H	-2.3557431	3.4156864	3.4642918
H	-3.1446021	1.9972892	2.7687564
H	-3.1566352	3.5450185	1.8910472
C	-1.1850789	-2.5318230	-1.8886027
C	-0.3562021	-3.8204616	-1.7482262
H	-0.1628034	-4.2164436	-2.7582004
H	-0.8868453	-4.6018763	-1.1891578
H	0.6125158	-3.6322261	-1.2666767
C	-0.4396858	-1.5802378	-2.8441122
H	-0.3200343	-2.0804005	-3.8190988
H	0.5576479	-1.3202171	-2.4653507
H	-0.9963598	-0.6496350	-3.0195503
C	-2.5481730	-2.8839260	-2.5183007
H	-3.1450138	-1.9970789	-2.7685402
H	-3.1570638	-3.5448102	-1.8908358
H	-2.3563209	-3.4155268	-3.4641598
C	-1.8407049	-2.8478997	1.1956682
C	-2.3419627	-2.0279381	2.3997818
H	-3.2900771	-1.5113494	2.1987319
H	-1.5941042	-1.2955693	2.7310760

H	-2.5217365	-2.7178397	3.2393580
C	-2.9753404	-3.7903917	0.7496456
H	-3.3004189	-4.3731836	1.6267698
H	-2.6463743	-4.5091590	-0.0104247
H	-3.8599107	-3.2607180	0.3701011
C	-0.6615366	-3.7032077	1.6875730
H	0.1360366	-3.0893301	2.1195998
H	-0.2125942	-4.3130856	0.8968418
H	-1.0414124	-4.3846324	2.4672557

Combination of torsional angles = -15
E(BP86/def2-TZVP) = -3497.56664805441

I	2.0308842	-1.7603363	0.2972517
I	2.0310665	1.7601695	-0.2971283
Ni	0.1810262	0.0000058	0.0000190
P	-1.3601949	1.6010705	0.1548544
P	-1.3603406	-1.6009137	-0.1548766
C	-2.9614366	-0.6613874	-0.3820514
H	-3.0547831	-0.4734336	-1.4580348
H	-3.8258071	-1.2786882	-0.0954200
C	-2.9613876	0.6616960	0.3819747
H	-3.0547878	0.4737504	1.4579550
H	-3.8256905	1.2790784	0.0953143
C	-1.8109570	2.7845594	-1.3159799
C	-2.2763857	1.9058498	-2.4922824
H	-3.2284535	1.3960880	-2.2924674
H	-1.5175136	1.1611642	-2.7656437
H	-2.4343956	2.5533123	-3.3692157
C	-0.6177777	3.6161657	-1.8146889
H	-0.9729500	4.2540823	-2.6413342
H	0.1937788	2.9823766	-2.1884020
H	-0.1949084	4.2681326	-1.0434780
C	-2.9596614	3.7438970	-0.9493474
H	-2.6571019	4.4971576	-0.2122286
H	-3.8552026	3.2288370	-0.5753103
H	-3.2574323	4.2853607	-1.8619220
C	-1.2375494	2.6262160	1.7953646
C	-0.4273662	3.9220667	1.6151243
H	-0.9548429	4.6656409	1.0040127
H	0.5581436	3.7289398	1.1720429
H	-0.2717361	4.3696885	2.6099923
C	-0.5032614	1.7347906	2.8148643
H	-0.4146031	2.2845515	3.7660974
H	0.5063156	1.4717445	2.4729086
H	-1.0526630	0.8067887	3.0235772
C	-2.6209677	2.9885507	2.3741988
H	-2.4587657	3.5784927	3.2904888
H	-3.2079051	2.1075188	2.6645530
H	-3.2272785	3.6003104	1.6962513
C	-1.2377408	-2.6260674	-1.7953875
C	-0.4276924	-3.9220004	-1.6151319
H	-0.2720733	-4.3696277	-2.6099992
H	-0.9552636	-4.6655285	-1.0040463
H	0.5578216	-3.7289759	-1.1720158
C	-0.5033312	-1.7347114	-2.8148600
H	-0.4146978	-2.2844772	-3.7660926
H	0.5062611	-1.4717678	-2.4728710
H	-1.0526332	-0.8066537	-3.0235865
C	-2.6211753	-2.9882590	-2.3742723
H	-3.2080132	-2.1071658	-2.6646421
H	-3.2275719	-3.5999611	-1.6963501
H	-2.4590008	-3.5782120	-3.2905602
C	-1.8112651	-2.7843508	1.3159500
C	-2.2766429	-1.9055836	2.4922296
H	-3.2286528	-1.3957272	2.2923791
H	-1.5177044	-1.1609719	2.7656082
H	-2.4347464	-2.5530219	3.3691639
C	-2.9600534	-3.7435792	0.9492934
H	-3.2579059	-4.2850022	1.8618657
H	-2.6575460	-4.4968789	0.2121938
H	-3.8555323	-3.2284355	0.5752227
C	-0.6181810	-3.6160664	1.8147058
H	0.1934260	-2.9823508	2.1884349
H	-0.1953517	-4.2680847	1.0435169
H	-0.9734399	-4.2539372	2.6413492

Combination of torsional angles = -10
E(BP86/def2-TZVP) = -3497.56691707805

I	2.0338893	-1.7715163	0.1964192
I	2.0339538	1.7714610	-0.1961182
Ni	0.1797480	-0.0000042	0.0000590
P	-1.3617968	1.6075033	0.1040156
P	-1.3618227	-1.6074763	-0.1040648
C	-2.9663723	-0.6782290	-0.3508466
H	-3.0703981	-0.5399578	-1.4333620
H	-3.8262777	-1.2843215	-0.0289060
C	-2.9663949	0.6782960	0.3506218
H	-3.0705420	0.5400279	1.4331258
H	-3.8262507	1.2844094	0.0285869
C	-1.7710256	2.7106065	-1.4382453
C	-2.1915596	1.7691898	-2.5820173
H	-3.1471134	1.2637882	-2.3877165
H	-1.4194128	1.0168965	-2.7887487
H	-2.3230975	2.3686375	-3.4966874
C	-0.5622077	3.5189650	-1.9378351
H	-0.8873166	4.1074201	-2.8120810
H	0.2645215	2.8689239	-2.2448513
H	-0.1705385	4.2153903	-1.1894112
C	-2.9350346	3.6814443	-1.1623970
H	-2.6628069	4.4728137	-0.4540204
H	-3.8414476	3.1803920	-0.7953788
H	-3.2019194	4.1741005	-2.1114245
C	-1.2923589	2.7220493	1.6912002
C	-0.4925000	4.0178316	1.4675111
H	-1.0085657	4.7201549	0.8004788
H	0.5096002	3.8154747	1.0688453
H	-0.3770333	4.5200188	2.4416304
C	-0.5822993	1.8957783	2.7798691
H	-0.5225877	2.5001760	3.6996123
H	0.4374240	1.6203270	2.4809611
H	-1.1344502	0.9790839	3.0273847
C	-2.6961192	3.1010345	2.2084823
H	-2.5655611	3.7471384	3.0912901
H	-3.2820052	2.2325324	2.5358665
H	-3.2893976	3.6638244	1.4784989
C	-1.2922149	-2.7220016	-1.6912586
C	-0.4923913	-4.0177948	-1.4675051
H	-0.3768087	-4.5199573	-2.4416236
H	-1.0085418	-4.7201325	-0.8005550
H	0.5096618	-3.8154540	-1.0687122

C	-0.5820115	-1.8957163	-2.7798217
H	-0.5221943	-2.5000944	-3.6995709
H	0.4376785	-1.6202844	-2.4807816
H	-1.1341203	-0.9790090	-3.0273847
C	-2.6959152	-3.1009556	-2.2087284
H	-3.2817471	-2.2324380	-2.5361682
H	-3.2892950	-3.6637536	-1.4788353
H	-2.5652533	-3.7470408	-3.0915346
C	-1.7712463	-2.7105766	1.4381534
C	-2.1918873	-1.7691536	2.5818794
H	-3.1474090	-1.2637320	2.3874734
H	-1.4197477	-1.0168775	2.7886974
H	-2.3235392	-2.3686002	3.4965338
C	-2.9352480	-3.6813904	1.1621899
H	-3.2022453	-4.1740305	2.1111942
H	-2.6629633	-4.4727735	0.4538520
H	-3.8416105	-3.1803213	0.7950705
C	-0.5625041	-3.5189585	1.9378873
H	0.2642023	-2.8689337	2.2449986
H	-0.1707617	-4.2153941	1.1895123
H	-0.8877280	-4.1074039	2.8120971

Combination of torsional angles = -5
E(BP86/def2-TZVP) = -3497.56712491024

I	2.0383117	-1.7779499	0.0979372
I	2.0382841	1.7779483	-0.0979547
Ni	0.1818424	-0.0000148	-0.0000024
P	-1.3602262	1.6113882	0.0519154
P	-1.3601943	-1.6114481	-0.0519245
C	-2.9690076	-0.6942337	-0.3173495
H	-3.0852993	-0.6081565	-1.4040920
H	-3.8234054	-1.2871249	0.0418052
C	-2.9690228	0.6941426	0.3173314
H	-3.0853191	0.6080632	1.4040732
H	-3.8234301	1.2870174	-0.0418281
C	-1.7219926	2.6272961	-1.5587415
C	-2.0954557	1.6222084	-2.6635339
H	-3.0541649	1.1203678	-2.4754996
H	-1.3114441	0.8662171	-2.7993840
H	-2.1977870	2.1694616	-3.6140126
C	-0.4960728	3.4112620	-2.0561292
H	-0.7867290	3.9454458	-2.9760709
H	0.3440112	2.7481641	-2.2911391
H	-0.1367600	4.1525877	-1.3351547
C	-2.8983593	3.6053122	-1.3792385
H	-2.6562273	4.4348674	-0.7044490
H	-3.8159029	3.1188205	-1.0201419
H	-3.1314911	4.0450779	-2.3625230
C	-1.3440585	2.8146007	1.5770027
C	-0.5474720	4.1039787	1.3078600
H	-1.0463151	4.7624302	0.5852759
H	0.4694883	3.8903516	0.9562329
H	-0.4711297	4.6610379	2.2556845
C	-0.6673081	2.0568245	2.7341923
H	-0.6350072	2.7160486	3.6168323
H	0.3608667	1.7658147	2.4830453
H	-1.2283972	1.1570828	3.0205388
C	-2.7661799	3.2130144	2.0264798
H	-2.6663353	3.9119415	2.8722560
H	-3.3575983	2.3619969	2.3877043
H	-3.3392613	3.7270291	1.2461303
C	-1.3439829	-2.8146473	-1.5770216
C	-0.5473641	-4.1040071	-1.3078870
H	-0.4709929	-4.6610497	-2.2557189
H	-1.0461984	-4.7624835	-0.5853201
H	0.4695858	-3.8903568	-0.9562428
C	-0.6672340	-2.0568392	-2.7341910
H	-0.6349064	-2.7160496	-3.6168403
H	0.3609309	-1.7658101	-2.4830255
H	-1.2283392	-1.1571053	-3.0205315
C	-2.7660888	-3.2130874	-2.0265256
H	-3.3575209	-2.3620784	-2.3877480
H	-3.3391707	-3.7271252	-1.2461922
H	-2.6662155	-3.9120009	-2.8723097
C	-1.7219568	-2.6273666	1.5587294
C	-2.0954465	-1.6222870	2.6635190
H	-3.0541606	-1.1204595	2.4754747
H	-1.3114471	-0.8662855	2.7993794
H	-2.1977809	-2.1695437	3.6139954
C	-2.8983081	-3.6053999	1.3792198
H	-3.1314412	-4.0451661	2.3625037
H	-2.6561592	-4.4349535	0.7044351
H	-3.8158559	-3.1189224	1.0201150
C	-0.4960314	-3.4113131	2.0561334
H	0.3440384	-2.7482022	2.2911561
H	-0.1366966	-4.1526325	1.3351640
H	-0.7866923	-3.9455023	2.9760706

Combination of torsional angles = 0
E(BP86/def2-TZVP) = -3497.56743375391

I	2.0363572	-1.7802894	-0.0015292
I	2.0361431	1.7805898	0.0017590
Ni	0.1799493	0.0000391	0.0000415
P	-1.3627602	1.6124664	0.0014750
P	-1.3625782	-1.6125620	-0.0015030
C	-2.9763686	-0.7085777	-0.2834514
H	-3.1060392	-0.6747030	-1.3717241
H	-3.8243069	-1.2867844	0.1130926
C	-2.9764684	0.7083000	0.2833108
H	-3.1062103	0.6744101	1.3715748
H	-3.8244448	1.2864113	-0.1132915
C	-1.6721066	2.5378181	-1.6713407
C	-1.9977134	1.4707046	-2.7318180
H	-2.9602416	0.9731110	-2.5518453
H	-1.2050997	0.7139754	-2.7935370
H	-2.0664955	1.9629709	-3.7148652
C	-0.4280839	3.2975939	-2.1620990
H	-0.6802512	3.7747647	-3.1237021
H	0.4229291	2.6257795	-2.3219108
H	-0.1017968	4.0822652	-1.4719946
C	-2.8573506	3.5177529	-1.5913281
H	-2.6446615	4.3843512	-0.9541418
H	-3.7860641	3.0457388	-1.2414702
H	-3.0543010	3.9018456	-2.6053882
C	-1.3985099	2.8993470	1.4583207
C	-0.5981097	4.1766903	1.1460456
H	-1.0738385	4.7903580	0.3703831
H	0.4318321	3.9506358	0.8442304
H	-0.5595336	4.7863136	2.0633501
C	-0.7633971	2.2109832	2.6803568

H	-0.7586416	2.9218319	3.5225252
H	0.2719327	1.9051409	2.4815932
H	-1.3373922	1.3312424	3.0010789
C	-2.8365848	3.3175303	1.8344998
H	-2.7665591	4.0651682	2.6406678
H	-3.4388329	2.4873249	2.2248220
H	-3.3833663	3.7832077	1.0064199
C	-1.3980900	-2.8994565	-1.4583424
C	-0.5975747	-4.1767105	-1.1459993
H	-0.5588827	-4.7863475	-2.0632899
H	-1.0732839	-4.7904129	-0.3703521
H	0.4323260	-3.9505433	-0.8441291
C	-0.7629755	-2.2110385	-2.6803471
H	-0.7580873	-2.9218991	-3.5225046
H	0.2723077	-1.9050790	-2.4815222
H	-1.3370476	-1.3313663	-3.0011186
C	-2.8360952	-3.3178023	-1.8346061
H	-3.4384052	-2.4876713	-2.2249903
H	-3.3828824	-3.7835157	-1.0065502
H	-2.7659366	-4.0654542	-2.6407496
C	-1.6719295	-2.5379474	1.6712929
C	-1.9977358	-1.4708739	2.7317501
H	-2.9603144	-0.9733994	2.5517167
H	-1.2052195	-0.7140465	2.7935199
H	-2.0665189	-1.9631495	3.7147927
C	-2.8570480	-3.5180277	1.5911989
H	-3.0540172	-3.9021480	2.6052451
H	-2.6442110	-4.3845975	0.9540230
H	-3.7857962	-3.0461256	1.2412820
C	-0.4278452	-3.2975724	2.1621301
H	0.4230757	-2.6256537	2.3219955
H	-0.1014183	-4.0822029	1.4720447
H	-0.6800145	-3.7747750	3.1237171

Combination of torsional angles = 5
E(BP86/def2-TZVP) = -3497.56769971210

I	2.0338993	-1.7784044	-0.1048436
I	2.0341221	1.7781372	0.1044874
Ni	0.1795622	-0.0000241	-0.0000689
P	-1.3637603	1.6108520	-0.0458187
P	-1.3639492	-1.6107149	0.0458609
C	-2.9830281	-0.7204674	-0.2500481
H	-3.1268159	-0.7369186	-1.3371574
H	-3.8236805	-1.2829296	0.1829952
C	-2.9829125	0.7208017	0.2502775
H	-3.1265739	0.7372711	1.3374034
H	-3.8235465	1.2833656	-0.1826701
C	-1.6193896	2.4468957	-1.7714217
C	-1.9047205	1.3233245	-2.7838282
H	-2.8725612	0.8332965	-2.6111515
H	-1.1097588	0.5664448	-2.7742870
H	-1.9385601	1.7609091	-3.7942228
C	-0.3557156	3.1798554	-2.2535873
H	-0.5670908	3.6005226	-3.2506400
H	0.5008129	2.5012352	-2.3393997
H	-0.0579338	4.0036369	-1.5969467
C	-2.8066987	3.4268816	-1.7866987
H	-2.6179543	4.3266692	-1.1891444
H	-3.7466713	2.9709371	-1.4454266
H	-2.9677058	3.7560341	-2.8260981
C	-1.4456928	2.9731351	1.3401956
C	-0.6357739	4.2341563	0.9881531
H	-1.0857298	4.8044622	0.1654691
H	0.4040472	3.9954374	0.7343229
H	-0.6295270	4.8916089	1.8726552
C	-0.8557776	2.3521125	2.6194525
H	-0.8765209	3.1090553	3.4201185
H	0.1845670	2.0338756	2.4733842
H	-1.4446655	1.4935254	2.9692298
C	-2.8957614	3.4100314	1.6434092
H	-2.8518619	4.2005514	2.4095111
H	-3.5122298	2.6023020	2.0577534
H	-3.4133389	3.8299597	0.7731901
C	-1.4462022	-2.9729907	-1.3401429
C	-0.6363951	-4.2341084	-0.9881894
H	-0.6303260	-4.8915627	-1.8726916
H	-1.0863277	-4.8043593	-0.1654547
H	0.4034828	-3.9955137	-0.7344757
C	-0.8563548	-2.3520414	-2.6194665
H	-0.8772778	-3.1089832	-3.4201288
H	0.1840440	-2.0339288	-2.4735143
H	-1.4451787	-1.4933844	-2.9691802
C	-2.8963565	-3.4097158	-1.6431950
H	-3.5127745	-2.6019156	-2.0574754
H	-3.4138883	-3.8295787	-0.7729172
H	-2.8526352	-4.2002447	-2.4092980
C	-1.6194793	-2.4467274	1.7714949
C	-1.9045520	-1.3231214	2.7839353
H	-2.8723531	-0.8329748	2.6113738
H	-1.1094987	-0.5663391	2.7742993
H	-1.9383250	-1.7607017	3.7943341
C	-2.8069078	-3.4265665	1.7869124
H	-2.9678324	-3.7556991	2.8263309
H	-2.6183455	-4.3263774	1.1893358
H	-3.7468643	-2.9705059	1.4457519
C	-0.3558412	-3.1798442	2.2535147
H	0.5007819	-2.5013309	2.3392272
H	-0.0582385	-4.0036637	1.5968408
H	-0.5671537	-3.6004838	3.2505924

Combination of torsional angles = 10
E(BP86/def2-TZVP) = -3497.56800840822

I	2.0269688	-1.7717825	-0.2011747
I	2.0270814	1.7716786	0.2013764
Ni	0.1758915	0.0000139	0.0000361
P	-1.3685405	1.6062136	-0.0994826
P	-1.3686637	-1.6060739	0.0994494
C	-2.9934916	-0.7321598	-0.2134517
H	-3.1519751	-0.8036459	-1.2965140
H	-3.8259129	-1.2753015	0.2584620
C	-2.9934530	0.7324173	0.2133078
H	-3.1520051	0.8039148	1.2963594
H	-3.8258028	1.2756194	-0.2586624
C	-1.5705004	2.3461759	-1.8729687
C	-1.8277510	1.1680564	-2.8290905
H	-2.8024000	0.6906500	-2.6585695
H	-1.0367025	0.4108627	-2.7510846
H	-1.8286759	1.5475470	-3.8633128
C	-0.2847193	3.0443076	-2.3491959
H	-0.4541856	3.4054247	-3.3770207

H	0.5702327	2.3580885	-2.3609988
H	-0.0075049	3.9048356	-1.7317206
C	-2.7512329	3.3274624	-1.9826781
H	-2.5778810	4.2591392	-1.4311157
H	-3.7034900	2.8934776	-1.6464670
H	-2.8774740	3.5974544	-3.0437175
C	-1.4908040	3.0423976	1.2072373
C	-0.6640856	4.2805317	0.8149689
H	-1.0827695	4.8048284	-0.0535765
H	0.3832144	4.0265297	0.6122793
H	-0.6871497	4.9862305	1.6612139
C	-0.9509429	2.4917376	2.5397048
H	-0.9950351	3.2931842	3.2947438
H	0.0920707	2.1617608	2.4490122
H	-1.5576341	1.6573008	2.9165237
C	-2.9487474	3.4996563	1.4343831
H	-2.9272998	4.3304753	2.1576092
H	-3.5836881	2.7178478	1.8698553
H	-3.4330946	3.8737151	0.5250777
C	-1.4909441	-3.0422495	-1.2072782
C	-0.6643426	-4.2804433	-0.8149527
H	-0.6874033	-4.9861427	-1.6611973
H	-1.0831218	-4.8047069	0.0535669
H	0.3829629	-4.0265178	-0.6121951
C	-0.9509541	-2.4916299	-2.5397103
H	-0.9950530	-3.2930745	-3.2947511
H	0.0920770	-2.1617277	-2.4489482
H	-1.5575605	-1.6571504	-2.9165715
C	-2.9489058	-3.4994025	-1.4345198
H	-3.5837608	-2.7175486	-1.8700354
H	-3.4333405	-3.8734244	-0.5252457
H	-2.9274707	-4.3302244	-2.1577429
C	-1.5707995	-2.3460241	1.8729204
C	-1.8280299	-1.1678881	2.8290274
H	-2.8026319	-0.6904094	2.6584401
H	-1.0369203	-0.4107523	2.7510788
H	-1.8290547	-1.5473815	3.8632486
C	-2.7516110	-3.3272250	1.9825450
H	-2.8779449	-3.5972116	3.0435747
H	-2.5782887	-4.2589123	1.4309910
H	-3.7038132	-2.8931696	1.6462697
C	-0.2851023	-3.0442517	2.3492338
H	0.5698992	-2.3580954	2.3610978
H	-0.0079085	-3.9047979	1.7317745
H	-0.4546657	-3.4053599	3.3770457

Combination of torsional angles = 15

E(BP86/def2-TZVP) = -3497.56827947608

I	2.0214823	-1.7611420	-0.2968969
I	2.0213794	1.7612117	0.2972741
Ni	0.1755377	0.0000008	0.0000720
P	-1.3700493	1.5987418	-0.1548843
P	-1.3700089	-1.5987978	0.1548348
C	-3.0004824	-0.7423004	-0.1758644
H	-3.1730765	-0.8692150	-1.2519006
H	-3.8245078	-1.2634938	0.3341082
C	-3.0005322	0.7421841	0.1756114
H	-3.1732657	0.8690923	1.2516261
H	-3.8245133	1.2633469	-0.3344641
C	-1.5205178	2.2426880	-1.9681884
C	-1.7612685	1.0160227	-2.8655767
H	-2.7438898	0.5551866	-2.6942616
H	-0.9788993	0.2586761	-2.7253246
H	-1.7326761	1.3384353	-3.9186279
C	-0.2112173	2.9011404	-2.4378930
H	-0.3392367	3.2038005	-3.4902051
H	0.6361210	2.2075250	-2.3792311
H	0.0529125	3.7935236	-1.8610577
C	-2.6875442	3.2257772	-2.1671027
H	-2.5221479	4.1851861	-1.6627294
H	-3.6528719	2.8174279	-1.8356265
H	-2.7805287	3.4374944	-3.2447105
C	-1.5254921	3.1026887	1.0691860
C	-0.6774888	4.3136200	0.6390974
H	-1.0636768	4.7925449	-0.2697972
H	0.3741855	4.0438072	0.4857163
H	-0.7236308	5.0640584	1.4449612
C	-1.0365733	2.6223376	2.4477872
H	-1.1024277	3.4640012	3.1560049
H	0.0072180	2.2842732	2.4120569
H	-1.6611955	1.8122523	2.8478420
C	-2.9873101	3.5788173	1.2215088
H	-2.9843759	4.4462359	1.9007620
H	-3.6420772	2.8242136	1.6751804
H	-3.4378331	3.9074154	0.2780185
C	-1.5252420	-3.1027480	-1.0692588
C	-0.6772468	-4.3136493	-0.6390697
H	-0.7232596	-5.0640857	-1.4449429
H	-1.0635305	-4.7925933	0.2697741
H	0.3743981	-4.0437977	-0.4855557
C	-1.0361681	-2.6223745	-2.4477971
H	-1.1019020	-3.4640383	-3.1560257
H	0.0076061	-2.2842711	-2.4119346
H	-1.6607702	-1.8123113	-2.8479279
C	-2.9870230	-3.5789308	-1.2217689
H	-3.6417605	-2.8243501	-1.6755212
H	-3.4376537	-3.9075489	-0.2783372
H	-2.9839701	-4.4463471	-1.9010246
C	-1.5206790	-2.2427478	1.9681215
C	-1.7615854	-1.0160899	2.8654778
H	-2.7442023	-0.5552900	2.6940405
H	-0.9792264	-0.2587151	2.7253214
H	-1.7331115	-1.3384998	3.9185330
C	-2.6876944	-3.2258787	2.1668949
H	-2.7808041	-3.4375955	3.2444919
H	-2.5222009	-4.1852833	1.6625455
H	-3.6529959	-2.8175657	1.8352980
C	-0.2114125	-2.9011505	2.4379910
H	0.6359072	-2.2075036	2.3794335
H	0.0528227	-3.7935250	1.8611908
H	-0.3395521	-3.2038132	3.4902878

Combination of torsional angles = 20

E(BP86/def2-TZVP) = -3497.56846293868

I	2.0170692	-1.7451278	-0.3961365
I	2.0169951	1.7451942	0.3960511
Ni	0.1775545	-0.0000128	-0.0000122
P	-1.3692098	1.5888150	-0.2087712
P	-1.3691169	-1.5889240	0.2087959
C	-3.0054105	-0.7503816	-0.1382595

H	-3.1924062	-0.9315281	-1.2043131
H	-3.8205010	-1.2477106	0.4087189
C	-3.0054472	0.7501838	0.1383345
H	-3.1924197	0.9313197	1.2043940
H	-3.8205816	1.2474685	-0.4086185
C	-1.4715048	2.1412653	-2.0533498
C	-1.7097363	0.8738391	-2.8927546
H	-2.7021918	0.4352814	-2.7186174
H	-0.9413948	0.1142965	-2.6976490
H	-1.6552577	1.1420520	-3.9599061
C	-0.1370062	2.7536781	-2.5156616
H	-0.2255907	3.0018945	-3.5860394
H	0.6959281	2.0506116	-2.3929558
H	0.1238869	3.6713843	-1.9781376
C	-2.6168779	3.1294498	-2.3336743
H	-2.4500524	4.1114843	-1.8754900
H	-3.5962314	2.7516741	-2.0067285
H	-2.6791785	3.2858336	-3.4229106
C	-1.5493559	3.1516695	0.9343159
C	-0.6735910	4.3309046	0.4730378
H	-1.0227363	4.7660588	-0.4721297
H	0.3797064	4.0435515	0.3706830
H	-0.7386820	5.1223202	1.2373157
C	-1.1134098	2.7368578	2.3515498
H	-1.1945753	3.6141135	3.0134504
H	-0.0725110	2.3887134	2.3692329
H	-1.7601665	1.9540222	2.7704755
C	-3.0104373	3.6476881	1.0135010
H	-3.0215002	4.5447075	1.6531133
H	-3.6884011	2.9201513	1.4772879
H	-3.4246303	3.9376326	0.0413043
C	-1.5492102	-3.1517832	-0.9342937
C	-0.6733649	-4.3309728	-0.4730519
H	-0.7384329	-5.1223846	-1.2373358
H	-1.0224581	-4.7661563	0.4721210
H	0.3799191	-4.0435609	-0.3707248
C	-1.1133272	-2.7369367	-2.3515366
H	-1.1944624	-3.6141918	-3.0134417
H	-0.0724482	-2.3887341	-2.3692461
H	-1.7601391	-1.9541337	-2.7704381
C	-3.0102665	-3.6478813	-1.0134433
H	-3.6882827	-2.9203780	-1.4772060
H	-3.4244175	-3.9378565	-0.0412382
H	-3.0212973	-4.5448960	-1.6530627
C	-1.4713264	-2.1413771	2.0533795
C	-1.7096030	-0.8739617	2.8927872
H	-2.7020877	-0.4354590	2.7186775
H	-0.9413087	-0.1143777	2.6976566
H	-1.6550782	-1.1421680	3.9599380
C	-2.6166375	-3.1296220	2.3337443
H	-2.6788967	-3.2860022	3.4229836
H	-2.4497728	-4.1116503	1.8755616
H	-3.5960213	-2.7519013	2.0068259
C	-0.1367802	-2.7537126	2.5156566
H	0.6961106	-2.0505992	2.3929250
H	0.1241504	-3.6714059	1.9781296
H	-0.2253210	-3.0019294	3.5860381

Combination of torsional angles = 25
E(BP86/def2-TZVP) = -3497.56850075804

I	2.0105137	-1.7224827	-0.5017962
I	2.0106816	1.7223915	0.5012923
Ni	0.1787875	-0.0000037	-0.0000899
P	-1.3689583	1.5773887	-0.2587164
P	-1.3689790	-1.5773301	0.2588160
C	-3.0109799	-0.7562087	-0.1023900
H	-3.2119762	-0.9881447	-1.1562129
H	-3.8170897	-1.2288401	0.4788422
C	-3.0109275	0.7563373	0.1027935
H	-3.2117181	0.9882827	1.1566535
H	-3.8171246	1.2290035	-0.4782893
C	-1.4262219	2.0457794	-2.1266761
C	-1.6700243	0.7457992	-2.9128276
H	-2.6724527	0.3312080	-2.7360833
H	-0.9176158	-0.0160801	-2.6707424
H	-1.5936010	0.9651428	-3.9897775
C	-0.0669038	2.6108873	-2.5782378
H	-0.1189616	2.8113137	-3.6608749
H	0.7474526	1.8977229	-2.3993388
H	0.1970686	3.5472208	-2.0751528
C	-2.5453854	3.0399996	-2.4803149
H	-2.3718265	4.0393126	-2.0640049
H	-3.5387350	2.6940477	-2.1601743
H	-2.5789186	3.1463694	-3.5768457
C	-1.5670228	3.1902501	0.8076839
C	-0.6606002	4.3359413	0.3218620
H	-0.9727448	4.7310952	-0.6533296
H	0.3914782	4.0310683	0.2677485
H	-0.7386855	5.1628380	1.0463054
C	-1.1829915	2.8362631	2.2562520
H	-1.2764405	3.7439802	2.8739375
H	-0.1469584	2.4799978	2.3248006
H	-1.8519525	2.0799790	2.6891437
C	-3.0238265	3.7047739	0.8176288
H	-3.0454968	4.6261358	1.4214501
H	-3.7252146	3.0028261	1.2861642
H	-3.4020998	3.9608117	-0.1782521
C	-1.5673046	-3.1901869	-0.8075403
C	-0.6608389	-4.3359082	-0.3218701
H	-0.7390907	-5.1628118	-1.0462876
H	-0.9728201	-4.7310358	0.6533851
H	0.3912616	-4.0310764	-0.2679541
C	-1.1835249	-2.8362266	-2.2561819
H	-1.2771207	-3.7439456	-2.8738422
H	-0.1474909	-2.4800007	-2.3249236
H	-1.8525368	-2.0799216	-2.6889575
C	-3.0241298	-3.7046544	-0.8172081
H	-3.7255784	-3.0026844	-1.2856194
H	-3.4022266	-3.9606678	0.1787466
H	-3.0459484	-4.6260217	-1.4210159
C	-1.4259145	-2.0457328	2.1267809
C	-1.6695170	-0.7457515	2.9129936
H	-2.6719624	-0.3311186	2.7364440
H	-0.9171243	0.0161013	2.6707755
H	-1.5928988	-0.9651109	3.9899264
C	-2.5450517	-3.0399147	2.4806104
H	-2.5783859	-3.1463023	3.5771455
H	-2.3716087	-4.0392274	2.0642502
H	-3.5384468	-2.6939184	2.1606593
C	-0.0665362	-2.6109063	2.5780782

H	0.7478175	-1.8977745	2.3990367
H	0.1973006	-3.5472437	2.0749281
H	-0.1183987	-2.8113478	3.6607218

Combination of torsional angles = 30
E(BP86/def2-TZVP) = -3497.56845428927

I	1.9996404	-1.6922512	-0.6113504
I	1.9998034	1.6920993	0.6111852
Ni	0.1765333	-0.0000077	-0.0000286
P	-1.3721515	1.5636020	-0.3068372
P	-1.3722493	-1.5635020	0.3068743
C	-3.0201814	-0.7604795	-0.0675235
H	-3.2350016	-1.0413564	-1.1068044
H	-3.8169203	-1.2072314	0.5462635
C	-3.0201199	0.7607015	0.0676639
H	-3.2348539	1.0415948	1.1069581
H	-3.8168640	1.2075129	-0.5460732
C	-1.3882820	1.9534518	-2.1924569
C	-1.6474758	0.6279449	-2.9292948
H	-2.6601024	0.2402545	-2.7486750
H	-0.9130413	-0.1377202	-2.6479744
H	-1.5540737	0.8028156	-4.0130485
C	-0.0045348	2.4675411	-2.6321244
H	-0.0236659	2.6251280	-3.7228205
H	0.7868903	1.7421731	-2.4040671
H	0.2696134	3.4170621	-2.1597507
C	-2.4758831	2.9565206	-2.6122647
H	-2.2886985	3.9686969	-2.2348779
H	-3.4833051	2.6457576	-2.2998986
H	-2.4834212	3.0164761	-3.7128168
C	-1.5806022	3.2190467	0.6867482
C	-0.6379636	4.3273390	0.1838702
H	-0.9100157	4.6854451	-0.8172750
H	0.4095437	4.0020490	0.1785525
H	-0.7236145	5.1859801	0.8694672
C	-1.2497907	2.9202723	2.1608513
H	-1.3497421	3.8545698	2.7364105
H	-0.2218556	2.5535616	2.2788927
H	-1.9440591	2.1924451	2.6028027
C	-3.0287695	3.7541334	0.6291848
H	-3.0575013	4.6946994	1.2024355
H	-3.7557965	3.0769392	1.0953235
H	-3.3691165	3.9828645	-0.3865733
C	-1.5808842	-3.2189361	-0.6866882
C	-0.6382961	-4.3272918	-0.1838555
H	-0.7240542	-5.1859359	-0.8694354
H	-0.9103116	-4.6853639	0.8173123
H	0.4092356	-4.0020793	-0.1786084
C	-1.2501434	-2.9201992	-2.1608152
H	-1.3501995	-3.8544947	-2.7363593
H	-0.2221888	-2.5535650	-2.2789248
H	-1.9443862	-2.1923253	-2.6027296
C	-3.0290866	-3.7539164	-0.6290237
H	-3.7560948	-3.0766753	-1.0951234
H	-3.3693835	-3.9826097	0.3867601
H	-3.0579244	-4.6944877	-1.2022604
C	-1.3882890	-1.9533592	2.1924917
C	-1.6473382	-0.6278386	2.9293566
H	-2.6599481	-0.2400729	2.7488058
H	-0.9128661	0.1377753	2.6479945
H	-1.5538783	-0.8027245	4.0131028
C	-2.4759365	-2.9563538	2.6123563
H	-2.4834088	-3.0163234	3.7129081
H	-2.2888499	-3.9685390	2.2349436
H	-3.4833558	-2.6455133	2.3000584
C	-0.0045523	-2.4675576	2.6320638
H	0.7869131	-1.7422475	2.4039618
H	0.2694927	-3.4170951	2.1596622
H	-0.0236239	-2.6251543	3.7227595

Combination of torsional angles = 35
E(BP86/def2-TZVP) = -3497.56814085214

I	1.9860054	-1.6548458	-0.7220054
I	1.9858340	1.6548737	0.7224428
Ni	0.1726938	-0.0000154	0.0000717
P	-1.3770352	1.5473243	-0.3561653
P	-1.3770385	-1.5474089	0.3560590
C	-3.0307123	-0.7634277	-0.0330741
H	-3.2580077	-1.0919340	-1.0557740
H	-3.8185164	-1.1828246	0.6108721
C	-3.0307442	0.7632842	0.0326996
H	-3.2582171	1.0917825	1.0553628
H	-3.8184587	1.1826533	-0.6113741
C	-1.3582206	1.8606056	-2.2553547
C	-1.6413647	0.5146876	-2.9446269
H	-2.6643439	0.1573366	-2.7588492
H	-0.9268349	-0.2560923	-2.6290840
H	-1.5351650	0.6471770	-4.0332113
C	0.0482490	2.3203570	-2.6845094
H	0.0569193	2.4382638	-3.7802782
H	0.8136623	1.5813224	-2.4137489
H	0.3388246	3.2789182	-2.2406126
C	-2.4108419	2.8736904	-2.7352313
H	-2.2047954	3.8951800	-2.3947565
H	-3.4315477	2.6005393	-2.4307690
H	-2.3960080	2.8894760	-3.8372488
C	-1.5881337	3.2411502	0.5657050
C	-0.6080404	4.3090192	0.0474964
H	-0.8409720	4.6298988	-0.9758303
H	0.4323083	3.9630639	0.0889872
H	-0.6956352	5.1973121	0.6939154
C	-1.3063338	2.9968992	2.0600748
H	-1.4080440	3.9554872	2.5938731
H	-0.2883235	2.6203661	2.2240769
H	-2.0255031	2.2987678	2.5102685
C	-3.0245595	3.7965976	0.4453303
H	-3.0569837	4.7535758	0.9906392
H	-3.7763323	3.1434202	0.9068231
H	-3.3288899	4.0006696	-0.5867069
C	-1.5879243	-3.2412459	-0.5658385
C	-0.6078757	-4.3090743	-0.0474625
H	-0.6953310	-5.1973750	-0.6938895
H	-0.8409626	-4.6299553	0.9758286
H	0.4324667	-3.9630797	-0.0887854
C	-1.3058886	-2.9969919	-2.0601635
H	-1.4074748	-3.9555866	-2.5939735
H	-0.2878657	-2.6204208	-2.2240005
H	-2.0250106	-2.2988903	-2.5104790
C	-3.0243486	-3.7967469	-0.4456939
H	-3.7760713	-3.1436002	-0.9073116

H	-3.3288383	-4.0008254	0.5862952
H	-3.0566483	-4.7537291	-0.9910033
C	-1.3585206	-1.8606894	2.2552507
C	-1.6418247	-0.5147822	2.9444787
H	-2.6647866	-0.1574677	2.7585356
H	-0.9272715	0.2560239	2.6290529
H	-1.5357971	-0.6472694	4.0330802
C	-2.4111837	-2.8738134	2.7349529
H	-2.3965289	-2.8896021	3.8369727
H	-2.2050448	-3.8952946	2.3945082
H	-3.4318496	-2.6006981	2.4303247
C	0.0478954	-2.3203930	2.6846321
H	0.8133272	-1.5813320	2.4139957
H	0.3385752	-3.2789441	2.2407811
H	0.0563929	-2.4383008	3.7804020

Combination of torsional angles = 40
E(BP86/def2-TZVP) = -3497.56751188079

I	1.9745515	-1.6105344	-0.8333947
I	1.9743597	1.6106711	0.8338085
Ni	0.1723229	0.0000279	0.0000772
P	-1.3782517	1.5287406	-0.4075289
P	-1.3782435	-1.5287519	0.4074631
C	-3.0374251	-0.7646214	0.0022657
H	-3.2762496	-1.1405066	-1.0014585
H	-3.8167925	-1.1543218	0.6745674
C	-3.0374572	0.7645397	-0.0025628
H	-3.2764372	1.1404149	1.0011281
H	-3.8167476	1.1542067	-0.6749730
C	-1.3306949	1.7686743	-2.3167313
C	-1.6404203	0.4060350	-2.9599212
H	-2.6722170	0.0783352	-2.7673765
H	-0.9443959	-0.3684059	-2.6144183
H	-1.5262085	0.4981956	-4.0518481
C	0.0945578	2.1764210	-2.7379031
H	0.1249977	2.2555945	-3.8367246
H	0.8352063	1.4265212	-2.4292768
H	0.4025344	3.1424705	-2.3224049
C	-2.3490242	2.7895757	-2.8504528
H	-2.1212987	3.8177225	-2.5457944
H	-3.3809471	2.5541315	-2.5523467
H	-2.3168416	2.7626348	-3.9519005
C	-1.5852710	3.2559993	0.4461787
C	-0.5650162	4.2799909	-0.0823924
H	-0.7587402	4.5652492	-1.1242510
H	0.4649928	3.9113826	0.0048629
H	-0.6488260	5.1950785	0.5259905
C	-1.3509857	3.0630967	1.9563842
H	-1.4482998	4.0434930	2.4498810
H	-0.3456746	2.6744058	2.1644392
H	-2.0968066	2.3972496	2.4122305
C	-3.0063322	3.8336657	0.2658420
H	-3.0396444	4.8033602	0.7882404
H	-3.7836552	3.2035038	0.7173388
H	-3.2739585	4.0186025	-0.7795848
C	-1.5850703	-3.2560190	-0.4462744
C	-0.5648477	-4.2799679	0.0824413
H	-0.6485342	-5.1950595	-0.5259526
H	-0.7587064	-4.5652331	1.1242730
H	0.4651584	-3.9113173	-0.0046695
C	-1.3505803	-3.0631064	-1.9564468
H	-1.4477839	-4.0435067	-2.4499575
H	-0.3452563	-2.6743731	-2.1643603
H	-2.0963651	-2.3972905	-2.4123980
C	-3.0061327	-3.8337444	-0.2661366
H	-3.7834186	-3.2036151	-0.7177425
H	-3.2738975	-4.0186921	0.7792529
H	-3.0393312	-4.8034406	-0.7885393
C	-1.3309452	-1.7686903	2.3166711
C	-1.6408182	-0.4060672	2.9598245
H	-2.6726013	-0.0784090	2.7671358
H	-0.9447772	0.3684047	2.6144247
H	-1.5267574	-0.4982294	4.0517671
C	-2.3493072	-2.7896375	2.8502422
H	-2.3172823	-2.7627017	3.9516946
H	-2.1214950	-3.8177730	2.5456101
H	-3.3811976	-2.5542352	2.5519907
C	0.0942650	-2.1763809	2.7380409
H	0.8349260	-1.4264485	2.4295238
H	0.4023398	-3.1424149	2.3225794
H	0.1245535	-2.2555606	3.8368661

Combination of torsional angles = 45
E(BP86/def2-TZVP) = -3497.56640105759

I	1.9666039	-1.5552510	-0.9498806
I	1.9665839	1.5553164	0.9500694
Ni	0.1755067	0.0000499	0.0000467
P	-1.3760904	1.5095491	-0.4561419
P	-1.3761400	-1.5094234	0.4561512
C	-3.0398033	-0.7642398	0.0341209
H	-3.2869069	-1.1818228	-0.9510625
H	-3.8128309	-1.1258427	0.7291016
C	-3.0397890	0.7643928	-0.0342036
H	-3.2869400	1.1819797	0.9509663
H	-3.8127725	1.1260083	-0.7292268
C	-1.3102125	1.6885668	-2.3715782
C	-1.6426244	0.3137907	-2.9761217
H	-2.6798245	0.0088464	-2.7746436
H	-0.9589051	-0.4615637	-2.6097309
H	-1.5273545	0.3737721	-4.0701695
C	0.1269019	2.0566305	-2.7899453
H	0.1703242	2.1014279	-3.8902500
H	0.8500391	1.3019016	-2.4518479
H	0.4477108	3.0297401	-2.4012167
C	-2.3028510	2.7130161	-2.9451644
H	-2.0550961	3.7453284	-2.6717726
H	-3.3418331	2.5090279	-2.6485004
H	-2.2622296	2.6499081	-4.0448577
C	-1.5724529	3.2628691	0.3411902
C	-0.5149523	4.2447439	-0.1934675
H	-0.6773458	4.5028513	-1.2477060
H	0.5031514	3.8527925	-0.0710011
H	-0.5871418	5.1798186	0.3852160
C	-1.3764382	3.1121724	1.8616958
H	-1.4657119	4.1094129	2.3218461
H	-0.3836400	2.7120621	2.1052921
H	-2.1453405	2.4755899	2.3210186
C	-2.9769070	3.8629880	0.1127119
H	-3.0078549	4.8407275	0.6201406
H	-3.7768746	3.2523380	0.5517774

H	-3.2130146	4.0365768	-0.9419224
C	-1.5724846	-3.2627398	-0.3411949
C	-0.5150278	-4.2446325	0.1935168
H	-0.5871986	-5.1797033	-0.3851753
H	-0.6774835	-4.5027429	1.2477449
H	0.5030883	-3.8526951	0.0711089
C	-1.3763819	-3.1120416	-1.8616889
H	-1.4656446	-4.1092794	-2.3218473
H	-0.3835640	-2.7119454	-2.1052278
H	-2.1452487	-2.4754461	-2.3210530
C	-2.9769608	-3.8628393	-0.1128002
H	-3.7768941	-3.2521756	-0.5519094
H	-3.2131320	-4.0364295	0.9418192
H	-3.0078936	-4.8405760	-0.6202353
C	-1.3103695	-1.6884360	2.3715923
C	-1.6427936	-0.3136524	2.9761118
H	-2.6799779	-0.0086930	2.7745753
H	-0.9590422	0.4616899	2.6097555
H	-1.5275850	-0.3736311	4.0701662
C	-2.3030545	-2.7128666	2.9451315
H	-2.2624918	-2.6497515	4.0448265
H	-2.0553003	-3.7451844	2.6717606
H	-3.3420175	-2.5088647	2.6484098
C	0.1267168	-2.0565178	2.7900400
H	0.8498829	-1.3018002	2.4519791
H	0.4475339	-3.0296332	2.4013332
H	0.1700781	-2.1013109	3.8903473

Combination of torsional angles = 50
E(BP86/def2-TZVP) = -3497.56456911680

I	1.9592820	-1.4837125	-1.0727043
I	1.9591684	1.4838010	1.0730553
Ni	0.1771555	0.0000617	0.0000573
P	-1.3762648	1.4911078	-0.4983055
P	-1.3763609	-1.4909526	0.4982163
C	-3.0436188	-0.7629791	0.0607097
H	-3.2964408	-1.2150530	-0.9077205
H	-3.8119632	-1.1001018	0.7730020
C	-3.0435948	0.7631692	-0.0610162
H	-3.2965334	1.2152485	0.9073811
H	-3.8118394	1.1003078	-0.7734085
C	-1.3034010	1.6279495	-2.4173329
C	-1.6517733	0.2452406	-2.9937086
H	-2.6905106	-0.0464657	-2.7803723
H	-0.9722818	-0.5287241	-2.6176096
H	-1.5428171	0.2840408	-4.0893444
C	0.1379619	1.9730313	-2.8407314
H	0.1840500	1.9908864	-3.9416919
H	0.8539095	1.2196428	-2.4844547
H	0.4650951	2.9531966	-2.4756534
C	-2.2826135	2.6527479	-3.0129444
H	-2.0172634	3.6873392	-2.7657305
H	-3.3239854	2.4726332	-2.7094821
H	-2.2449156	2.5618439	-4.1107859
C	-1.5567465	3.2614496	0.2612464
C	-0.4637203	4.2046097	-0.2709694
H	-0.5995480	4.4467876	-1.3327892
H	0.5411098	3.7872712	-0.1220228
H	-0.5191948	5.1521587	0.2888355
C	-1.3924270	3.1371274	1.7878896
H	-1.4678162	4.1455840	2.2255183
H	-0.4133329	2.7211948	2.0589104
H	-2.1838265	2.5277899	2.2458834
C	-2.9431546	3.8874608	-0.0033490
H	-2.9695070	4.8661781	0.5025410
H	-3.7645974	3.2912959	0.4160394
H	-3.1500144	4.0638028	-1.0633602
C	-1.5567812	-3.2612917	-0.2613561
C	-0.4638464	-4.2044746	0.2710070
H	-0.5192678	-5.1520239	-0.2888027
H	-0.5998200	-4.4466466	1.3328095
H	0.5410128	-3.7871591	0.1221922
C	-1.3922579	-3.1369773	-1.7879780
H	-1.4676122	-4.1454334	-2.2256139
H	-0.4131188	-2.7210674	-2.0588710
H	-2.1835834	-2.5276232	-2.2460774
C	-2.9432378	-3.8872712	0.0030597
H	-3.7646121	-3.2910911	-0.4164411
H	-3.1502415	-4.0636020	1.0630447
H	-2.9695446	-4.8659911	-0.5028277
C	-1.3037504	-1.6277980	2.4172526
C	-1.6521672	-0.2450826	2.9935859
H	-2.6908695	0.0466482	2.7801131
H	-0.9726081	0.5288675	2.6175789
H	-1.5433568	-0.2838885	4.0892360
C	-2.2830636	-2.6525765	3.0127327
H	-2.2455062	-2.5616782	4.1105794
H	-2.0177054	-3.6871729	2.7655486
H	-3.3243919	-2.4724365	2.7091359
C	0.1375495	-1.9729137	2.8408377
H	0.8535606	-1.2195404	2.4846563
H	0.4647078	-2.9530853	2.4757992
H	0.1834939	-1.9907730	3.9418040

Relaxed potential surface scan of O structure of NiI2dtbpe

Combination of torsional angles = -10
E(BP86/def2-TZVP) = -3497.56316027117

Ni	-0.2873592	0.0010209	-0.0003097
I	-2.1145664	0.3786790	-1.7614064
I	-2.1152067	-0.3726625	1.7609157
C	2.8609762	-0.3272806	0.6871761
C	2.8613043	0.3252068	-0.6875506
P	1.2523145	-0.0567661	1.6067885
P	1.2524944	0.0565093	-1.6072890
C	1.4398207	-1.4753975	2.9377692
C	1.1723086	-2.7985255	2.1958816
C	0.4660434	-1.4208610	4.1307265
C	2.8717437	-1.4914969	3.5114503
C	1.4195865	1.6918014	2.4312754
C	0.7072799	1.7614864	3.7927375
C	0.7243548	2.6965402	1.4951838
C	2.8887669	2.1109980	2.6123966
C	1.4174688	-1.6922304	-2.4316316
C	2.8860779	-2.1122229	-2.6154387
C	0.7235473	-2.6962870	-1.4938374
C	0.7023783	-1.7619474	-3.7916543
C	1.4415163	1.4750865	-2.9380346

C	2.8741961	1.4920663	-3.5098119
C	1.1724809	2.7980119	-2.1963575
C	0.4695480	1.4196902	-4.1324436
H	3.7210037	0.0138159	1.2788906
H	2.9602653	-1.4175123	0.5845817
H	2.9615011	1.4153661	-0.5848734
H	3.7210659	-0.0165424	-1.2792911
H	0.1598772	-2.8208504	1.7708349
H	1.2572867	-3.6270476	2.9167295
H	1.8999421	-2.9968422	1.3972519
H	-0.5760423	-1.3074118	3.8127354
H	0.7091140	-0.6232781	4.8390627
H	0.5577233	-2.3756938	4.6735327
H	3.6465579	-1.6654423	2.7544894
H	2.9383387	-2.3169369	4.2383347
H	3.1123807	-0.5670318	4.0537701
H	-0.3117165	1.3547007	3.7472372
H	0.6333623	2.8214757	4.0847106
H	1.2669101	1.2451644	4.5818900
H	1.1901899	2.7357717	0.5047258
H	0.7966590	3.7032572	1.9391476
H	-0.3390424	2.4546851	1.3622063
H	3.4221732	2.2073312	1.6564174
H	3.4530412	1.4230168	3.2562468
H	2.9106534	3.1016548	3.0944161
H	2.9065813	-3.1030022	-3.0972718
H	3.4212513	-2.2085762	-1.6604459
H	3.4494611	-1.4246689	-3.2605201
H	0.7939504	-3.7031051	-1.9378723
H	-0.3393463	-2.4535182	-1.3584083
H	1.1916963	-2.7358666	-0.5044952
H	0.6263630	-2.8220461	-4.0826696
H	1.2611906	-1.2470286	-4.5822657
H	-0.3159394	-1.3536269	-3.7445516
H	3.1163704	0.5675506	-4.0513573
H	3.6478628	1.6671029	-2.7519325
H	2.9410022	2.3171974	-4.2370270
H	1.2587764	3.6267393	-2.9168181
H	1.8986889	2.9960489	-1.3963433
H	0.1592950	2.8201371	-1.7731037
H	0.7162261	0.6238646	-4.8415624
H	0.5592222	2.3755545	-4.6737482
H	-0.5727185	1.3027964	-3.8162599

Combination of torsional angles = -5
E(BP86/def2-TZVP) = -3497.56405558067

Ni	-0.2825986	0.0006769	-0.0000619
I	-2.1098351	0.2615270	-1.7834856
I	-2.1099069	-0.2583098	1.7835746
C	2.8608713	-0.3496774	0.6759492
C	2.8611269	0.3480286	-0.6763818
P	1.2549516	-0.0924879	1.6051443
P	1.2548789	0.0923460	-1.6054183
C	1.4204175	-1.5630111	2.8801699
C	1.1661213	-2.8560087	2.0823165
C	0.4250277	-1.5608459	4.0558150
C	2.8431880	-1.5975254	3.4752077
C	1.4557533	1.6213462	2.4956906
C	0.7852825	1.6412142	3.8796921
C	0.7445561	2.6692329	1.6209800
C	2.9331951	2.0216228	2.6534559
C	1.4539624	-1.6216815	-2.4959625
C	2.9310073	-2.0233124	-2.6539887
C	0.7419675	-2.6689008	-1.6210994
C	0.7832108	-1.6409603	-3.8798361
C	1.4215963	1.5627138	-2.8804573
C	2.8443863	1.5960460	-3.4755084
C	1.1683900	2.8559205	-2.0825954
C	0.4262065	1.5613654	-4.0561074
H	3.7248595	-0.0342520	1.2758196
H	2.9517654	-1.4364280	0.5371260
H	2.9530330	1.4346958	-0.5375665
H	3.7247638	0.0318097	-1.2763410
H	0.1617240	-2.8602784	1.6379885
H	1.2358400	-3.7119807	2.7720279
H	1.9073086	-3.0257300	1.2897867
H	-0.6133406	-1.4672886	3.7200295
H	0.6295048	-0.7723003	4.7857406
H	0.5334119	-2.5249214	4.5790245
H	3.6303292	-1.7317618	2.7228317
H	2.9048983	-2.4544274	4.1651466
H	3.0692053	-0.6966965	4.0618773
H	-0.2449641	1.2634726	3.8433602
H	0.7485877	2.6870396	4.2252231
H	1.3536347	1.0722049	4.6257524
H	1.1799853	2.7404218	0.6182889
H	0.8437826	3.6572671	2.1002276
H	-0.3250297	2.4440277	1.5134447
H	3.4418820	2.1538081	1.6884003
H	3.5086145	1.3038020	3.2535096
H	2.9755617	2.9914014	3.1748542
H	2.9723931	-2.9931339	-3.1753862
H	3.4397462	-2.1559534	-1.6890227
H	3.5069752	-1.3060226	-3.2541523
H	0.8401785	-3.6570300	-2.1003597
H	-0.3273883	-2.4427018	-1.5133494
H	1.1775350	-2.7404902	-0.6184974
H	0.7454206	-2.6867672	-4.2253064
H	1.3519856	-1.0725497	-4.6260289
H	-0.2466557	-1.2621991	-3.8433368
H	3.0696597	0.6950115	-4.0621498
H	3.6316483	1.7296715	-2.7231505
H	2.9067805	2.4528720	-4.1654798
H	1.2388955	3.7118488	-2.7722806
H	1.9096928	3.0249624	-1.2900275
H	0.1639800	2.8610591	-1.6383064
H	0.6301704	0.7727596	-4.7861146
H	0.5352544	2.5254220	-4.5792135
H	-0.6122334	1.4684840	-3.7203532

Combination of torsional angles = 0
E(BP86/def2-TZVP) = -3497.56496248745

Ni	-0.2778766	0.0000730	0.0000010
I	-2.1034498	0.1407804	-1.7992026
I	-2.1031727	-0.1401091	1.7995300
C	2.8620297	-0.3713322	0.6642143
C	2.8620200	0.3705434	-0.6647935
P	1.2587913	-0.1252072	1.6020798
P	1.2585358	0.1249072	-1.6023649
C	1.3947686	-1.6433609	2.8207319

C	1.1627386	-2.9067472	1.9700055
C	0.3665586	-1.6884149	3.9661217
C	2.8025900	-1.6970182	3.4485192
C	1.4967995	1.5499122	2.5578341
C	0.8441011	1.5264130	3.9503531
C	0.7967973	2.6450722	1.7336719
C	2.9828419	1.9185891	2.7150526
C	1.4958677	-1.5502743	-2.5581791
C	2.9817711	-1.9193896	-2.7156857
C	0.7957004	-2.6452382	-1.7338957
C	0.8429091	-1.5265662	-3.9505723
C	1.3947427	1.6430213	-2.8210379
C	2.8024454	1.6962159	-3.4491295
C	1.1633103	2.9064892	-1.9702668
C	0.3662945	1.6884143	-3.9662020
H	3.7300021	-0.0819879	1.2712155
H	2.9439626	-1.4534188	0.4898080
H	2.9443182	1.4526041	-0.4904020
H	3.7297922	0.0809315	-1.2719540
H	0.1748973	-2.8901996	1.4902397
H	1.2024610	-3.7858753	2.6323916
H	1.9303860	-3.0553609	1.1989876
H	-0.6634276	-1.6232619	3.5993386
H	0.5186085	-0.9023521	4.7110532
H	0.4909851	-2.6553893	4.4805488
H	3.6083789	-1.7843715	2.7088646
H	2.8572423	-2.5880238	4.0944633
H	3.0054732	-0.8256882	4.0858422
H	-0.1988512	1.1864456	3.9086745
H	0.8481940	2.5553061	4.3453100
H	1.4010917	0.9033462	4.6613830
H	1.2255773	2.7493080	0.7307964
H	0.9186341	3.6106449	2.2517637
H	-0.2773398	2.4430730	1.6276476
H	3.4833728	2.0830787	1.7507364
H	3.5527440	1.1676287	3.2786714
H	3.0460944	2.8651315	3.2754873
H	3.0446376	-2.8659446	-3.2761421
H	3.4824352	-2.0840374	-1.7514654
H	3.5517894	-1.1685919	-3.2794031
H	0.9171553	-3.6108408	-2.2520206
H	-0.2783569	-2.4429238	-1.6276655
H	1.2246374	-2.7496117	-0.7311017
H	0.8466377	-2.5554532	-4.3455493
H	1.3999365	-0.9036422	-4.6616986
H	-0.1999403	-1.1863086	-3.9086849
H	3.0048942	0.8248336	-4.0865188
H	3.6084231	1.7832758	-2.7096455
H	2.8572609	2.5872198	-4.0950619
H	1.2031641	3.7856001	-2.6326668
H	1.9311782	3.0548632	-1.1994219
H	0.1755709	2.8902628	-1.4902812
H	0.5178941	0.9022781	-4.7111482
H	0.4909511	2.6553319	-4.4806800
H	-0.6636321	1.6236377	-3.5991872

Combination of torsional angles = 5
E(BP86/def2-TZVP) = -3497.56589277584

Ni	-0.2716970	0.0001863	0.0001097
I	-2.0939139	0.0220270	-1.8075409
I	-2.0933161	-0.0209053	1.8083691
C	2.8651616	-0.3947583	0.6509272
C	2.8650989	0.3938480	-0.6517880
P	1.2649041	-0.1589073	1.5972717
P	1.2644225	0.1586356	-1.5975839
C	1.3635114	-1.7211699	2.7578886
C	1.1587195	-2.9543174	1.8568703
C	0.2943600	-1.8055692	3.8621616
C	2.7508452	-1.7992722	3.4267566
C	1.5427447	1.4724358	2.6184825
C	0.8854119	1.4122335	4.0079821
C	0.8782776	2.6188539	1.8359661
C	3.0375953	1.7956152	2.7947058
C	1.5412520	-1.4728248	-2.6188797
C	3.0359136	-1.7966127	-2.7955740
C	0.8765592	-2.6189710	-1.8361549
C	0.8835039	-1.4123480	-4.0081697
C	1.3632636	1.7208488	-2.7582468
C	2.7504087	1.7984076	-3.4275664
C	1.1592405	2.9540767	-1.8571609
C	0.2937899	1.8056603	-3.8621753
H	3.7374325	-0.1344261	1.2646977
H	2.9364762	-1.4705755	0.4385790
H	2.9369151	1.4696363	-0.4394651
H	3.7370573	0.1331661	-1.2658543
H	0.1957151	-2.9112263	1.3304679
H	1.1556140	-3.8536302	2.4927539
H	1.9612074	-3.0896803	1.1198657
H	-0.7215354	-1.7666234	3.4545773
H	0.3892684	-1.0207362	4.6176104
H	0.4265076	-2.7730534	4.3738910
H	3.5794273	-1.8369711	2.7079877
H	2.7952882	-2.7252382	4.0223868
H	2.9253333	-0.9638867	4.1179713
H	-0.1702518	1.1175494	3.9481222
H	0.9304052	2.4212049	4.4492364
H	1.4138777	0.7353527	4.6912918
H	1.3215064	2.7552701	0.8430992
H	1.0190609	3.5578533	2.3962121
H	-0.1992827	2.4487767	1.7114574
H	3.5447880	1.9900723	1.8394959
H	3.5872545	1.0073417	3.3263559
H	3.1219424	2.7151599	3.3957731
H	3.1196951	-2.7161944	-3.3966647
H	3.5433306	-1.9912713	-1.8405241
H	3.5857242	-1.0085631	-3.3274004
H	1.0167857	-3.5580285	-2.3964438
H	-0.2008928	-2.4484547	-1.7113128
H	1.3200395	-2.7555665	-0.8434253
H	0.9279368	-2.4213363	-4.4494415
H	1.4120345	-0.7356833	-4.6916442
H	-0.1720176	-1.1172252	-3.9479725
H	2.9243609	0.9629295	-4.1188050
H	3.5792383	1.8358283	-2.7090686
H	2.7950003	2.7243335	-4.0232479
H	1.1562860	3.8533935	-2.4930402
H	1.9620157	3.0891198	-1.1204117
H	0.1963891	2.9113615	-1.3304480
H	0.3881674	1.0208003	-4.6176628
H	0.4261362	2.7731009	-4.3739360

H -0.7219909 1.7670899 -3.4542694

Combination of torsional angles = 10
E(BP86/def2-TZVP) = -3497.56682258019
Ni -0.2623623 0.0001934 0.0001558
I -2.0800203 -0.0993789 -1.8087217
I -2.0792033 0.1005351 1.8098100
C 2.8713054 -0.4181681 0.6367722
C 2.8712106 0.4171975 -0.6378142
P 1.2744718 -0.1915490 1.5913462
P 1.2738646 0.1912738 -1.5916973
C 1.3285207 -1.7943755 2.6920356
C 1.1390969 -2.9935601 1.7427842
C 0.2216666 -1.9031829 3.7557481
C 2.6950284 -1.9116649 3.3964144
C 1.5918645 1.3920717 2.6764881
C 0.9221911 1.2990004 4.0586112
C 0.9715318 2.5886668 1.9342013
C 3.0943651 1.6633524 2.8765410
C 1.5900929 -1.3924823 -2.6769806
C 3.0923868 -1.6644199 -2.8776895
C 0.9695631 -2.5888081 -1.9344253
C 0.9198538 -1.2991161 -4.0588095
C 1.3281332 1.7940792 -2.6924088
C 2.6943776 1.9107625 -3.3973985
C 1.1396671 2.9933482 -1.7430728
C 0.2208510 1.9033841 -3.7556250
H 3.7480265 -0.1884396 1.2562590
H 2.9306289 -1.4862921 0.3861870
H 2.9311057 1.4852955 -0.3872542
H 3.7475648 0.1870899 -1.2576796
H 0.2016588 -2.9142213 1.1758540
H 1.0899374 -3.9121125 2.3484953
H 1.9708516 -3.1223149 1.0379226
H -0.7788852 -1.8603273 3.3117358
H 0.2827555 -1.1308917 4.5274249
H 0.3387111 -2.8794355 4.2543780
H 3.5431680 -1.9133639 2.6993392
H 2.7218675 -2.8678471 3.9434244
H 2.8512791 -1.1140541 4.1347018
H -0.1439881 1.0509152 3.9791828
H 1.0051427 2.2855174 4.5431207
H 1.4170679 0.5724451 4.7156229
H 1.4350274 2.7542728 0.9549683
H 1.1303869 3.4986960 2.5357427
H -0.1082501 2.4549729 1.7875537
H 3.6139637 1.8857032 1.9341986
H 3.6177200 0.8375428 3.3766016
H 3.1994406 2.5529991 3.5179581
H 3.1967931 -2.5541111 -3.5191543
H 3.6122979 -1.8870008 -1.9355738
H 3.6158855 -0.8388382 -3.3779754
H 1.1277674 -3.4989067 -2.5360333
H -0.1100981 -2.4546492 -1.7873137
H 1.4334077 -2.7546117 -0.9553906
H 1.0021598 -2.2856683 -4.5433577
H 1.4147585 -0.5727759 -4.7160376
H -0.1461815 -1.0505645 -3.9789098
H 2.8499411 1.1130876 -4.1357612
H 3.5428296 1.9120766 -2.7007028
H 2.7213994 2.8669369 -3.9444134
H 1.0906427 3.9119216 -2.3487629
H 1.9717951 3.1217357 -1.0385845
H 0.2024487 2.9144252 -1.1757222
H 0.2812368 1.1310576 -4.5273215
H 0.3381195 2.8795784 -4.2543166
H -0.7795203 1.8609924 -3.3111621

Combination of torsional angles = 15
E(BP86/def2-TZVP) = -3497.56766331673
Ni -0.2496317 0.0001714 0.0001267
I -2.0615494 -0.2257379 -1.8018258
I -2.0606772 0.2268403 1.8028607
C 2.8811925 -0.4397821 0.6228336
C 2.8810998 0.4388480 -0.6239412
P 1.2875995 -0.2213636 1.5845996
P 1.2869997 0.2210759 -1.5850128
C 1.2902014 -1.8619769 2.6223530
C 1.1060706 -3.0223632 1.6248001
C 0.1484732 -1.9835732 3.6466835
C 2.6349075 -2.0313224 3.3566499
C 1.6434576 1.3099183 2.7328146
C 0.9547365 1.1860443 4.1034758
C 1.0748942 2.5557608 2.0314149
C 3.1516672 1.5232948 2.9604025
C 1.6417299 -1.3103482 -2.7333835
C 3.1497530 -1.5243386 -2.9616265
C 1.0729588 -2.5559592 -2.0317412
C 0.9524633 -1.1861817 -4.1037436
C 1.2898123 1.8616810 -2.6227767
C 2.6342697 2.0304818 -3.3576533
C 1.1065714 3.0221485 -1.6251521
C 0.1476943 1.9837217 -3.6466205
H 3.7619154 -0.2394276 1.2466709
H 2.9287274 -1.4993833 0.3366012
H 2.9291887 1.4984299 -0.3377301
H 3.7614708 0.2381372 -1.2481615
H 0.1951674 -2.8977037 1.0235897
H 1.0079761 -3.9591052 2.1956319
H 1.9620324 -3.1499295 0.9494662
H -0.8363604 -1.9122909 3.1715532
H 0.1941861 -1.2333557 4.4409052
H 0.2335605 -2.9751291 4.1209061
H 3.5006686 -2.0084855 2.6814498
H 2.6371435 -3.0138432 3.8556037
H 2.7809022 -1.2731738 4.1371993
H -0.1193562 0.9846332 4.0029413
H 1.0715134 2.1474238 4.6297688
H 1.4126043 0.4135393 4.7343469
H 1.5642723 2.7484739 1.0696717
H 1.2503044 3.4337390 2.6744244
H -0.0053366 2.4631022 1.8594501
H 3.6883314 1.7727535 2.0345822
H 3.6437262 0.6597578 3.4271826
H 3.2764303 2.3791006 3.6430147
H 3.2738726 -2.3801949 -3.6442928
H 3.6867168 -1.7740145 -2.0360388
H 3.6419601 -0.6610012 -3.4286199
H 1.2477364 -3.4340089 -2.6748252
H -0.0071604 -2.4628597 -1.8593146

H 1.5626682 -2.7488716 -1.0702065
H 1.0686197 -2.1476035 -4.6300968
H 1.4103695 -0.4138565 -4.7348074
H -0.1215035 -0.9843348 -4.0027389
H 2.7796283 1.2722641 -4.1382546
H 3.5003114 2.0073108 -2.6828245
H 2.6366808 3.0129943 -3.8566221
H 1.0086065 3.9589258 -2.1959478
H 1.9628729 3.1493783 -0.9501847
H 0.1958769 2.8978560 -1.0235501
H 0.1927726 1.2334795 -4.4408557
H 0.2329713 2.9752401 -4.1208868
H -0.8369645 1.9128327 -3.1710695

Combination of torsional angles = 20
E(BP86/def2-TZVP) = -3497.56835162211
Ni -0.2337306 0.0001179 0.0000828
I -2.0383633 -0.3540623 -1.7861744
I -2.0374703 0.3549457 1.7871136
C 2.8950729 -0.4598623 0.6090772
C 2.8949795 0.4589586 -0.6102606
P 1.3040337 -0.2513586 1.5768609
P 1.3034445 0.2510434 -1.5773544
C 1.2513622 -1.9262143 2.5495067
C 1.0690907 -3.0448198 1.5048584
C 0.0759698 -2.0527488 3.5341675
C 2.5718552 -2.1539967 3.3105596
C 1.6946646 1.2235041 2.7867455
C 0.9779327 1.0728652 4.1405510
C 1.1861369 2.5159498 2.1247661
C 3.2053975 1.3735354 3.0477545
C 1.6930129 -1.2239499 -2.7874210
C 3.2035759 -1.3745172 -3.0491019
C 1.1843213 -2.5162203 -2.1252250
C 0.9757321 -1.0730465 -4.1409063
C 1.2509551 1.9259235 -2.5499665
C 2.5711870 2.1532230 -3.3116152
C 1.0695693 3.0445929 -1.5052322
C 0.0751610 2.0528929 -3.5340912
H 3.7788612 -0.2864196 1.2364813
H 2.9328142 -1.5102069 0.2895632
H 2.9332495 1.5092892 -0.2907631
H 3.7784320 0.2851887 -1.2380472
H 0.1840687 -2.8725798 0.8769831
H 0.9250084 -3.9977920 2.0377592
H 1.9443878 -3.1726148 0.8549816
H -0.8915437 -1.9387191 3.0318269
H 0.1153809 -1.3307919 4.3545861
H 0.1194989 -3.0617054 3.9760451
H 3.4551429 -2.1131929 2.6587839
H 2.5456353 -3.1593635 3.7610595
H 2.7094652 -1.4366963 4.1301006
H -0.1012059 0.9181679 4.0151286
H 1.1230787 2.0073378 4.7067206
H 1.3945709 0.2586405 4.7470155
H 1.7071394 2.7310549 1.1842879
H 1.3757678 3.3600594 2.8077438
H 0.1079510 2.4688383 1.9241978
H 3.7654118 1.6486398 2.1433252
H 3.6608447 0.4730886 3.4804029
H 3.3465060 2.1916915 3.7720791
H 3.3440715 -2.1927178 -3.7734953
H 3.7638922 -1.6498283 -2.1449227
H 3.6591526 -0.4742296 -3.4819451
H 1.3733437 -3.3603911 -2.8082957
H 0.1062428 -2.4687264 -1.9241709
H 1.7056708 -2.7315203 -1.1849838
H 1.1202957 -2.0075650 -4.7071489
H 1.3923877 -0.2589640 -4.7475501
H -0.1032954 -0.9179684 -4.0150011
H 2.7081584 1.4358824 -4.1312278
H 3.4547543 2.1120814 -2.6602399
H 2.5451379 3.1586056 -3.7620900
H 0.9255957 3.9976194 -2.0380654
H 1.9452091 3.1720660 -0.8557528
H 0.1847693 2.8726777 -0.8769557
H 0.1139232 1.3309123 -4.3545193
H 0.1188689 3.0618288 -3.9759984
H -0.8921656 1.9392339 -3.0313068

Combination of torsional angles = 25
E(BP86/def2-TZVP) = -3497.56886922960
Ni -0.2147728 0.0000898 0.0000674
I -2.0110205 -0.4838000 -1.7613260
I -2.0100350 0.4845789 1.7623066
C 2.9133161 -0.4779892 0.5959054
C 2.9132094 0.4770837 -0.5972216
P 1.3236491 -0.2821502 1.5679973
P 1.3230177 0.2818155 -1.5685686
C 1.2140327 -1.9875773 2.4728988
C 1.0342344 -3.0618616 1.3821863
C 0.0052594 -2.1135146 3.4163566
C 2.5069535 -2.2768710 3.2590139
C 1.7433545 1.1329250 2.8382083
C 0.9931915 0.9585737 4.1711295
C 1.2983059 2.4678014 2.2157060
C 3.2528230 1.2175460 3.1352138
C 1.7416396 -1.1333863 -2.8389957
C 3.2509339 -1.2184997 -3.1367428
C 1.2964636 -2.4681237 -2.2162853
C 0.9908776 -0.9587810 -4.1715466
C 1.2135566 1.9872899 -2.4733969
C 2.5061698 2.2761263 -3.2601847
C 1.0347181 3.0616348 -1.3825866
C 0.0043291 2.1136652 -3.4162142
H 3.7988874 -0.3276655 1.2266303
H 2.9444431 -1.5187605 0.2461962
H 2.9448762 1.5178433 -0.2475268
H 3.7984311 0.3264404 -1.2283610
H 0.1747190 -2.8419836 0.7336619
H 0.8479228 -4.0291405 1.8746799
H 1.9257990 -3.1894577 0.7549325
H -0.9421418 -1.9487372 2.8896404
H 0.0415356 -1.4239865 4.2644940
H 0.0018072 -3.1390655 3.8202822
H 3.4082896 -2.2237156 2.6328185
H 2.4495873 -3.3011849 3.6614782
H 2.6356683 -1.6005858 4.1139624
H -0.0880850 0.8497030 4.0192274
H 1.1611416 1.8648091 4.7755880

H	1.3668683	0.1069265	4.7537188
H	1.8524092	2.7006979	1.2983197
H	1.5003657	3.2769701	2.9363024
H	0.2246682	2.4684158	1.9874007
H	3.8400066	1.5167397	2.2561019
H	3.6693987	0.2827554	3.5324206
H	3.4058149	1.9951355	3.9006610
H	3.4032935	-1.9961268	-3.9022778
H	3.8384476	-1.5179025	-2.2579230
H	3.6676244	-0.2838408	-3.5341379
H	1.4978901	-3.2773496	-2.9369946
H	0.2229418	-2.4683858	-1.9874358
H	1.8509562	-2.7012164	-1.2991837
H	1.1582393	-1.8650636	-4.7760975
H	1.3645405	-0.1072480	-4.7543122
H	-0.0902884	-0.8495642	-4.0191096
H	2.6341891	1.5998151	-4.1152167
H	3.4078136	2.2226248	-2.6344613
H	2.4489689	3.3004711	-3.6625939
H	0.8484771	4.0289787	-1.8749794
H	1.9266668	3.1889227	-0.7558150
H	0.1754753	2.8420562	-0.7336007
H	0.0398862	1.4241001	-4.2643515
H	0.0010508	3.1392073	-3.8201637
H	-0.9428530	1.9492615	-2.8889869

Combination of torsional angles = 30
E(BP86/def2-TZVP) = -3497.56904066769

Ni	-0.1927836	0.0000658	0.0000671
I	-1.9799983	-0.6138857	-1.7265435
I	-1.9789023	0.6145608	1.7276178
C	2.9363159	-0.4936580	0.5839533
C	2.9361868	0.4927465	-0.5854238
P	1.3461677	-0.3147569	1.5578060
P	1.3454742	0.3144037	-1.5584542
C	1.1800618	-2.0474186	2.3928597
C	1.0088305	-3.0772375	1.2586797
C	-0.0634315	-2.1693178	3.2909708
C	2.4405226	-2.3974425	3.2055343
C	1.7872648	1.0371508	2.8872995
C	0.9951711	0.8436131	4.1932240
C	1.4112887	2.4102123	2.3031239
C	3.2905478	1.0534812	3.2260226
C	1.7854289	-1.0376229	-2.8882022
C	3.2885191	-1.0544070	-3.2277582
C	1.4093590	-2.4105756	-2.3038294
C	0.9926675	-0.8438282	-4.1936837
C	1.1795093	2.0471271	-2.3934036
C	2.4396029	2.3966937	-3.2068433
C	1.0093424	3.0770217	-1.2591333
C	-0.0644881	2.1694611	-3.2907562
H	3.8219626	-0.3610373	1.2184426
H	2.9655151	-1.5251807	0.2080370
H	2.9659454	1.5242571	-0.2095190
H	3.8214590	0.3598158	-1.2203715
H	0.1738839	-2.8145375	0.5938794
H	0.7871822	-4.0569938	1.7102369
H	1.9154198	-3.2017811	0.6527511
H	-0.9866371	-1.9520780	2.7402300
H	-0.0332994	-1.5138192	4.1660452
H	-0.1154220	-3.2086061	3.6540714
H	3.3616571	-2.3355202	2.6091624
H	2.3509995	-3.4369939	3.5603426
H	2.5557568	-1.7616796	4.0927642
H	-0.0848322	0.7798388	4.0099171
H	1.1787649	1.7210688	4.8344682
H	1.3225965	-0.0411803	4.7538824
H	2.0011592	2.6549093	1.4109964
H	1.6239926	3.1838801	3.0587409
H	0.3452858	2.4616747	2.0468430
H	3.9104823	1.3740865	2.3775469
H	3.6651083	0.0871592	3.5874968
H	3.4491817	1.7881008	4.0317389
H	3.4464814	-1.7890593	-4.0335763
H	3.9088243	-1.3752199	-2.3796324
H	3.6631770	-0.0881936	-3.5894207
H	1.6213909	-3.1842999	-3.0595773
H	0.3434873	-2.4617113	-2.0469406
H	1.9996663	-2.6554677	-1.4120441
H	1.1756538	-1.7213215	-4.8350497
H	1.3200337	0.0408839	-4.7545056
H	-0.0872150	-0.7797477	-4.0097747
H	2.5540596	1.7609057	-4.0941554
H	3.3610774	2.3344161	-2.6110326
H	2.3502520	3.4362857	-3.5615764
H	0.7877430	4.0568456	-1.7105678
H	1.9163591	3.2012701	-0.6537823
H	0.1747240	2.8146201	-0.5938043
H	-0.0351642	1.5138824	-4.1657984
H	-0.1162885	3.2087437	-3.6539008
H	-0.9874385	1.9526296	-2.7394276

Combination of torsional angles = 35
E(BP86/def2-TZVP) = -3497.56889939572

Ni	-0.1696701	0.0000585	0.0000657
I	-1.9469924	-0.7414188	-1.6827719
I	-1.9457625	0.7421146	1.6839422
C	2.9625608	-0.5078824	0.5724868
C	2.9624004	0.5069793	-0.5741599
P	1.3699916	-0.3517653	1.5455315
P	1.3692160	0.3513994	-1.5462814
C	1.1520525	-2.1084339	2.3097889
C	1.0019549	-3.0967684	1.1364858
C	-0.1285397	-2.2257670	3.1555557
C	2.3743220	-2.5133259	3.1538462
C	1.8232513	0.9352047	2.9321513
C	0.9837278	0.7270035	4.2059329
C	1.5174122	2.3407447	2.3850020
C	3.3152888	0.8837816	3.3157234
C	1.8212512	-0.9357012	-2.9331773
C	3.3130740	-0.8847385	-3.3176459
C	1.5153064	-2.3411497	-2.3858499
C	0.9810258	-0.7272347	-4.2064525
C	1.1513960	2.1081421	-2.3103983
C	2.3732630	2.5126222	-3.1552353
C	1.0023792	3.0965349	-1.1370075
C	-0.1296980	2.2258962	-3.1553466
H	3.8464811	-0.3884716	1.2119762
H	2.9946716	-1.5301065	0.1725657
H	2.9950898	1.5291913	-0.1742555

H	3.8459092	0.3872689	-1.2141616
H	0.1918313	-2.7997334	0.4555109
H	0.7525973	-4.0874116	1.5481929
H	1.9254031	-3.2144172	0.5549681
H	-1.0231312	-1.9624015	2.5778474
H	-0.1138648	-1.6013929	4.0536737
H	-0.2251099	-3.2746677	3.4794264
H	3.3176313	-2.4442550	2.5935452
H	2.2544362	-3.5645838	3.4622820
H	2.4675467	-1.9159004	4.0696980
H	-0.0916426	0.7086329	3.9880722
H	1.1773744	1.5751222	4.8826942
H	1.2620515	-0.1874141	4.7452424
H	2.1425908	2.5917848	1.5185557
H	1.7384324	3.0798356	3.1721645
H	0.4617548	2.4428665	2.1025501
H	3.9711927	1.2214533	2.5016861
H	3.6472392	-0.1096577	3.6429347
H	3.4729425	1.5757741	4.1585465
H	3.4700051	-1.5767709	-4.1605709
H	3.9693619	-1.2226241	-2.5040072
H	3.6451384	0.1086002	-3.6450458
H	1.7356241	-3.0803053	-3.1731485
H	0.4597880	-2.4429455	-2.1027631
H	2.1409294	-2.5923876	-1.5197818
H	1.1740126	-1.5754027	-4.8833402
H	1.2592972	0.1871063	-4.7459197
H	-0.0942078	-0.7085449	-3.9879446
H	2.4656987	1.9151729	-4.0711512
H	3.3169067	2.4432242	-2.5955373
H	2.2535393	3.5639238	-3.4635854
H	0.7530708	4.0872543	-1.5485608
H	1.9262458	3.2138942	-0.5560955
H	0.1926024	2.7997680	-0.4555036
H	-0.1158265	1.6014761	-4.0534458
H	-0.2261042	3.2748175	-3.4792001
H	-1.0240098	1.9628724	-2.5770502

Combination of torsional angles = 40

E(BP86/def2-TZVP) = -3497.56830260670

Ni	-0.1466979	0.0000776	0.0000745
I	-1.9141498	-0.8658831	-1.6299038
I	-1.9127608	0.8666449	1.6312302
C	2.9906149	-0.5213913	0.5609263
C	2.9904291	0.5204507	-0.5628368
P	1.3940429	-0.3933219	1.5306236
P	1.3931755	0.3929459	-1.5314835
C	1.1305752	-2.1708982	2.2240617
C	1.0190370	-3.1228071	1.0170959
C	-0.1907823	-2.2841413	3.0063474
C	2.3070160	-2.6223784	3.1080142
C	1.8504655	0.8280932	2.9719547
C	0.9609033	0.6081829	4.2093733
C	1.6125438	2.2610646	2.4628598
C	3.3268695	0.7117410	3.4005266
C	1.8482221	-0.8286217	-2.9731186
C	3.3243769	-0.7127662	-3.4026830
C	1.6101596	-2.2615148	-2.4638664
C	0.9579011	-0.6084099	-4.2099378
C	1.1298741	2.1706129	-2.2247497
C	2.3058642	2.6216609	-3.1095222
C	1.0195120	3.1225784	-1.0177205
C	-0.1919839	2.2843163	-3.0061232
H	3.8712500	-0.4122522	1.2068417
H	3.0293264	-1.5338935	0.1379757
H	3.0297768	1.5329380	-0.1399103
H	3.8705999	0.4109994	-1.2093318
H	0.2387736	-2.7989684	0.3139173
H	0.7449608	-4.1222379	1.3901294
H	1.9644120	-3.2326451	0.4699396
H	-1.0515944	-1.9888006	2.3934596
H	-0.2066395	-1.6812637	3.9192614
H	-0.3237741	-3.3381007	3.2990872
H	3.2753946	-2.5473028	2.5926045
H	2.1596437	-3.6821944	3.3721719
H	2.3668086	-2.0595290	4.0480297
H	-0.1064869	0.6358529	3.9555556
H	1.1598172	1.4259688	4.9210244
H	1.1881613	-0.3329807	4.7261378
H	2.2705722	2.5159030	1.6217948
H	1.8397354	2.9657146	3.2793074
H	0.5691779	2.4123072	2.1576523
H	4.0192159	1.0613024	2.6225170
H	3.6177311	-0.3038850	3.6961256
H	3.4782037	1.3638048	4.2757483
H	3.4749032	-1.3648831	-4.2780042
H	4.0171291	-1.0625584	-2.6251385
H	3.6153816	0.3027609	-3.6984804
H	1.8365582	-2.9662385	-3.2804705
H	0.5669497	-2.4124060	-2.1579524
H	2.2686722	-2.5165803	-1.6232496
H	1.1560696	-1.4262548	-4.9217290
H	1.1851187	0.3326837	-4.7268484
H	-0.1093267	-0.6357322	-3.9554020
H	2.3648028	2.0587820	-4.0495740
H	3.2745731	2.5462397	-2.5947833
H	2.1586913	3.6815278	-3.3735864
H	0.7455197	4.1220978	-1.3905773
H	1.9653091	3.2320985	-0.4712306
H	0.2396282	2.7990219	-0.3139910
H	-0.2087014	1.6814051	-3.9190004
H	-0.3247864	3.3383129	-3.2988153
H	-1.0524789	1.9893209	-2.3926247

Combination of torsional angles = 45

E(BP86/def2-TZVP) = -3497.56715894427

Ni	-0.1243434	0.0001104	0.0000781
I	-1.8822951	-0.9868562	-1.5680153
I	-1.8807107	0.9877640	1.5695064
C	3.0198417	-0.5340868	0.5494173
C	3.0196351	0.5330751	-0.5516190
P	1.4176970	-0.4392087	1.5127679
P	1.4167339	0.4388209	-1.5137697
C	1.1165684	-2.2354904	2.1370087
C	1.0592893	-3.1575548	0.9037966
C	-0.2467701	-2.3456123	2.8456088
C	2.2400092	-2.7251543	3.0679122
C	1.8678013	0.7178956	3.0051973
C	0.9236304	0.4917088	4.2002404
C	1.6975712	2.1731693	2.5328058

C	3.3233465	0.5388682	3.4817694
C	1.8652577	-0.7184654	-3.0065337
C	3.3205102	-0.5400096	-3.4842132
C	1.6948174	-2.1736704	-2.5340066
C	0.9202680	-0.4919211	-4.2008623
C	1.1158443	2.2352161	-2.1377925
C	2.2387599	2.7244237	-3.0695692
C	1.0598818	3.1573195	-0.9045484
C	-0.2479974	2.3458660	-2.8453414
H	3.8954332	-0.4322673	1.2035395
H	3.0689814	-1.5365472	0.1046979
H	3.0694919	1.5355151	-0.1069344
H	3.8946972	0.4309185	-1.2063963
H	0.3121886	-2.8157585	0.1739868
H	0.7657541	-4.1642240	1.2408966
H	2.0294708	-3.2582169	0.3994533
H	-1.0693295	-2.0336152	2.1895571
H	-0.3062166	-1.7530319	3.7637371
H	-0.4073518	-3.4014070	3.1169327
H	3.2346543	-2.6453803	2.6056438
H	2.0687106	-3.7909657	3.2902943
H	2.2559450	-2.1925585	4.0268756
H	-0.1314723	0.5659576	3.9066413
H	1.1216075	1.2793488	4.9453463
H	1.0967887	-0.4726626	4.6946357
H	2.3889729	2.4284041	1.7187515
H	1.9266065	2.8443689	3.3764748
H	0.6693772	2.3720950	2.2044767
H	4.0538794	0.8913620	2.7408983
H	3.5725119	-0.4940502	3.7528865
H	3.4632314	1.1573434	4.3829242
H	3.4594710	-1.1585559	-4.3854623
H	4.0514698	-0.8927726	-2.7438912
H	3.5698691	0.4928069	-3.7555392
H	1.9229376	-2.8449625	-3.3778498
H	0.6667978	-2.3721887	-2.2048863
H	2.3867450	-2.4291767	-1.7204847
H	1.1173812	-1.2796385	-4.9461156
H	1.0934171	0.4723827	-4.6953922
H	-0.1346401	-0.5657682	-3.9064635
H	2.2537416	2.1918132	-4.0285397
H	3.2337300	2.6442570	-2.6080692
H	2.0677142	3.7903013	-3.2918285
H	0.7664682	4.1640958	-1.2414338
H	2.0304956	3.2576178	-0.4009647
H	0.3132202	2.8158197	-0.1741505
H	-0.3084008	1.7532643	-3.7633937
H	-0.4083553	3.4017136	-3.1165930
H	-1.0701751	2.0342382	-2.1886362

Combination of torsional angles = 50

E(BP86/def2-TZVP) = -3497.56542743895

Ni	-0.1053993	0.0001771	0.0000971
I	-1.8545853	-1.1045609	-1.4968527
I	-1.8526990	1.1057793	1.4985997
C	3.0469236	-0.5467312	0.5372451
C	3.0467075	0.5455668	-0.5398218
P	1.4384427	-0.4881838	1.4918826
P	1.4373665	0.4877771	-1.4930532
C	1.1100918	-2.3007948	2.0521843
C	1.1142213	-3.1989597	0.8007553
C	-0.2905139	-2.4102273	2.6857964
C	2.1795038	-2.8198462	3.0294397
C	1.8742697	0.6099822	3.0294859
C	0.8783257	0.3794907	4.1808359
C	1.7624439	2.0818713	2.5918877
C	3.3067630	0.3774311	3.5510657
C	1.8713088	-0.6106116	-3.0310288
C	3.3034550	-0.3787606	-3.5538718
C	1.7591498	-2.0824438	-2.5933253
C	0.8744613	-0.3796423	-4.1815018
C	1.1094036	2.3005364	-2.0530947
C	2.1781892	2.8190438	-3.0313235
C	1.1150974	3.1987244	-0.8016878
C	-0.2917160	2.4106377	-2.6854530
H	3.9163941	-0.4516758	1.2008043
H	3.1083315	-1.5383619	0.0707396
H	3.1089796	1.5371668	-0.0733662
H	3.9155548	0.4501100	-1.2041388
H	0.3996477	-2.8470468	0.0444437
H	0.8086322	-4.2121923	1.1060472
H	2.1081032	-3.2883566	0.3418628
H	-1.0742997	-2.0912459	1.9865500
H	-0.3968721	-1.8220273	3.6028279
H	-0.4710568	-3.4667136	2.9413441
H	3.1974747	-2.7369940	2.6216217
H	1.9893222	-3.8894789	3.2151815
H	2.1484279	-2.3118624	4.0010393
H	-0.1619915	0.4958170	3.8494568
H	1.0696770	1.1389505	4.9562660
H	1.0014256	-0.6036591	4.6525819
H	2.4847386	2.3373840	1.8049425
H	1.9874253	2.7229086	3.4597620
H	0.7502600	2.3211306	2.2417133
H	4.0719315	0.7247183	2.8434048
H	3.5180513	-0.6672585	3.8068883
H	3.4332888	0.9723946	4.4699033
H	3.4288869	-0.9738036	-4.4728082
H	4.0690780	-0.7264025	-2.8468766
H	3.5150206	0.6658220	-3.8099008
H	1.9830494	-2.7235949	-3.4613954
H	0.7471585	-2.3212059	-2.2422556
H	2.4820143	-2.3383069	-1.8070179
H	1.0647619	-1.1391963	-4.9570983
H	0.9976164	0.6034469	-4.6533594
H	-0.1656197	-0.4954666	-3.8492044
H	2.1459901	2.3110544	-4.0028834
H	3.1964859	2.7357043	-2.6244204
H	1.9883620	3.8887652	-3.2169183
H	0.8097112	4.2120955	-1.1067219
H	2.1094393	3.2876585	-0.3437025
H	0.4010456	2.8471654	-0.0447190
H	-0.3991915	1.8224466	-3.6023608
H	-0.4719628	3.4672017	-2.9408889
H	-1.0750315	2.0920777	-1.9854879

Relaxed potential surface scan of P structure of NiCl2dtbpe

Combination of torsional angles = -40

E(BP86/def2-TZVP) = -3822.37097513709

Cl	2.5228075	-1.2440507	1.0068220
Cl	2.5359380	1.2441497	-0.9728705
Ni	0.9898116	-0.0000221	0.0066591
P	-0.5398918	1.5661901	0.1045642
P	-0.5385190	-1.5662032	-0.1116458
C	-2.1564955	-0.6711511	-0.3864264
H	-2.2480886	-0.5055352	-1.4680229
H	-3.0118810	-1.2946864	-0.0860585
C	-2.1613601	0.6711939	0.3580287
H	-2.2671163	0.5055658	1.4383294
H	-3.0127190	1.2947631	0.0464862
C	-0.9679327	2.8010372	-1.3214945
C	-1.5419760	1.9651850	-2.4815417
H	-2.5016882	1.4907754	-2.2341341
H	-0.8322506	1.1968196	-2.8128435
H	-1.7238748	2.6362912	-3.3356626
C	0.2676991	3.5444510	-1.8592998
H	-0.0553320	4.1667303	-2.7104742
H	1.0452310	2.8497184	-2.1950704
H	0.7195433	4.2095383	-1.1156765
C	-2.0266518	3.8371735	-0.9007771
H	-1.6211845	4.5806195	-0.2036871
H	-2.9251192	3.3897957	-0.4523821
H	-2.3505060	4.3830552	-1.8019139
C	-0.2170166	2.5256212	1.7389216
C	0.8437306	3.6149577	1.5014848
H	0.4460094	4.4630609	0.9293896
H	1.7265040	3.2181389	0.9802200
H	1.1703631	4.0037456	2.4790043
C	0.3503657	1.5147038	2.7546097
H	0.6057347	2.0586944	3.6785988
H	1.2558728	1.0111876	2.3884412
H	-0.3858426	0.7456541	3.0241348
C	-1.4902971	3.1458691	2.3445669
H	-1.2212078	3.6040754	3.3100500
H	-2.2657217	2.3953095	2.5524224
H	-1.9294945	3.9314204	1.7209348
C	-0.1940408	-2.5255159	-1.7416675
C	0.8634840	-3.6148522	-1.4902391
H	1.2031030	-4.0035464	-2.4633584
H	0.4582012	-4.4630099	-0.9235605
H	1.7392371	-3.2180602	-0.9572340
C	0.3867583	-1.5145791	-2.7497244
H	0.6543519	-2.0585615	-3.6702484
H	1.2873394	-1.0110738	-2.3715738
H	-0.3457910	-0.7455087	-3.0289820
C	-1.4591830	-3.1457466	-2.3641349
H	-2.2317720	-2.3951738	-2.5822270
H	-1.9066034	-3.9313050	-1.7463870
H	-1.1773276	-3.6039437	-3.3259752
C	-0.9854218	-2.8011731	1.3085174
C	-1.5745001	-1.9653465	2.4610278
H	-2.5308092	-1.4907615	2.2010981
H	-0.8690502	-1.1971280	2.8016860
H	-1.7676850	-2.6364997	3.3126297
C	-2.0386632	-3.8371435	0.8738805
H	-2.3743498	-4.3830593	1.7706568
H	-1.6241976	-4.5805886	0.1820987
H	-2.9311348	-3.3896308	0.4138046
C	0.2429695	-3.5447862	1.8624070
H	1.0161990	-2.8501733	2.2082431
H	0.7043307	-4.2099994	1.1247606
H	-0.0912213	-4.1669591	2.7093359

Combination of torsional angles = -35

E(BP86/def2-TZVP) = -3822.37354396726

Cl	2.5280370	-1.3313116	0.8752752
Cl	2.5334334	1.3313944	-0.8591878
Ni	0.9901567	0.0000203	0.0032144
P	-0.5344139	1.5680093	0.0970148
P	-0.5337629	-1.5680040	-0.1001551
C	-2.1512839	-0.6722602	-0.3767605
H	-2.2433755	-0.5094951	-1.4585066
H	-3.0077157	-1.2935422	-0.0745842
C	-2.1535928	0.6722297	0.3635571
H	-2.2523683	0.5094609	1.4447112
H	-3.0081521	1.2934959	0.0560867
C	-0.9734767	2.7838763	-1.3421459
C	-1.5711219	1.9405970	-2.4849299
H	-2.5334958	1.4811390	-2.2207016
H	-0.8754861	1.1590856	-2.8160591
H	-1.7547060	2.6034522	-3.3451036
C	0.2572001	3.5144896	-1.9074940
H	-0.0797805	4.1435867	-2.7482873
H	1.0173337	2.8121324	-2.2653618
H	0.7378907	4.1692099	-1.1730316
C	-2.0208720	3.8295316	-0.9160286
H	-1.6060009	4.5711977	-0.2225947
H	-2.9191400	3.3885064	-0.4610209
H	-2.3474186	4.3757782	-1.8159419
C	-0.2146591	2.5487234	1.7198604
C	0.8064337	3.6714909	1.4654954
H	0.3779855	4.4997476	0.8863814
H	1.6992954	3.2974010	0.9449603
H	1.1229108	4.0814083	2.4378381
C	0.4027100	1.5587733	2.7274098
H	0.6491740	2.1097733	3.6497298
H	1.3225325	1.0933198	2.3469780
H	-0.2982685	0.7597052	3.0033771
C	-1.4974798	3.1311315	2.3427745
H	-1.2256535	3.6174605	3.2935869
H	-2.2392478	2.3562153	2.5812447
H	-1.9794907	3.8877964	1.7145675
C	-0.2038032	-2.5486646	-1.7209956
C	0.8157002	-3.6714117	-1.4602413
H	1.1383044	-4.0812913	-2.4305837
H	0.3836346	-4.4996979	-0.8838641
H	1.7052566	-3.2973111	-0.9340836
C	0.4198637	-1.5587009	-2.7246429
H	0.6721093	-2.1096953	-3.6454008
H	1.3372792	-1.0932404	-2.3384504
H	-0.2793732	-0.7596331	-3.0049996
C	-1.4826741	-3.1310870	-2.3519554
H	-2.2229163	-2.3561705	-2.5951111
H	-1.9686317	-3.8877327	-1.7267739
H	-1.2048681	-3.6174448	-3.3010240
C	-0.9817835	-2.7839372	1.3361904
C	-1.5864713	-1.9406903	2.4752917
H	-2.5471555	-1.4811566	2.2051148

H	-0.8928543	-1.1592455	2.8107867
H	-1.7754379	-2.6035854	3.3342678
C	-2.0265447	-3.8295479	0.9035466
H	-2.3586731	-4.3758231	1.8013973
H	-1.6074089	-4.5711990	0.2126630
H	-2.9219694	-3.3884865	0.4430036
C	0.2453475	-3.5146078	1.9091281
H	1.0032897	-2.8122871	2.2716946
H	0.7305388	-4.1693442	1.1776454
H	-0.0968488	-4.1436946	2.7478185

Combination of torsional angles = -30
E(BP86/def2-TZVP) = -3822.37573324925

Cl	2.5248560	-1.4040153	0.7791795
Cl	2.5457090	1.4045402	-0.7050542
Ni	0.9933976	0.0000345	0.0149879
P	-0.5277002	1.5707857	0.0815275
P	-0.5250257	-1.5708916	-0.0949261
C	-2.1393013	-0.6754865	-0.3934627
H	-2.2205001	-0.5217672	-1.4771960
H	-2.9994518	-1.2936168	-0.0952964
C	-2.1495502	0.6752127	0.3347105
H	-2.2608861	0.5214798	1.4157510
H	-3.0011221	1.2932642	0.0126685
C	-0.9461816	2.7621987	-1.3836541
C	-1.5316886	1.9045055	-2.5219408
H	-2.4996367	1.4532784	-2.2641985
H	-0.8355719	1.1148344	-2.8322505
H	-1.7004176	2.5553080	-3.3942728
C	0.2921606	3.4830895	-1.9442500
H	-0.0353412	4.1068946	-2.7927510
H	1.0516697	2.7748994	-2.2914485
H	0.7712714	4.1399327	-1.2108079
C	-1.9985712	3.8139429	-0.9851150
H	-1.5964559	4.5598939	-0.2888886
H	-2.9060694	3.3771579	-0.5446096
H	-2.3071310	4.3538656	-1.8951018
C	-0.2466278	2.5789768	1.6959720
C	0.7441937	3.7294454	1.4457852
H	0.3032748	4.5367967	0.8468347
H	1.6578522	3.3742497	0.9493873
H	1.0270314	4.1615529	2.4190077
C	0.3895812	1.6141299	2.7161630
H	0.6073610	2.1759745	3.6391901
H	1.3287084	1.1798999	2.3466043
H	-0.2873706	0.7928338	2.9867306
C	-1.5511643	3.1318737	2.3008484
H	-1.3000529	3.6477496	3.2416865
H	-2.2688086	2.3391082	2.5534194
H	-2.0541949	3.8587210	1.6537445
C	-0.1981354	-2.5786396	-1.7010156
C	0.7854723	-3.7289416	-1.4231210
H	1.0960295	-4.1606162	-2.3880480
H	0.3278380	-4.5366284	-0.8373094
H	1.6845354	-3.3737328	-0.9007668
C	0.4664667	-1.6134767	-2.7026239
H	0.7104507	-2.1751401	-3.6191826
H	1.3946158	-1.1790131	-2.3065633
H	-0.2027841	-0.7923357	-2.9921734
C	-1.4848842	-3.1317102	-2.3426722
H	-2.1951549	-2.3390285	-2.6154934
H	-2.0059672	-3.8586256	-1.7100976
H	-1.2071048	-3.6475566	-3.2760064
C	-0.9846239	-2.7627158	1.3575534
C	-1.6011591	-1.9050741	2.4793958
H	-2.5612717	-1.4531734	2.1949157
H	-0.9134713	-1.1159466	2.8092725
H	-1.7945420	-2.5560746	3.3464446
C	-2.0259408	-3.8138939	0.9295179
H	-2.3600707	-4.3538519	1.8304056
H	-1.6048483	-4.5599057	0.2446492
H	-2.9205994	-3.3766694	0.4638905
C	0.2372992	-3.4843782	1.9521820
H	0.9871824	-2.7766713	2.3206638
H	0.7363396	-4.1412037	1.2321465
H	-0.1140142	-4.1083051	2.7910078

Combination of torsional angles = -25
E(BP86/def2-TZVP) = -3822.37752418460

Cl	2.5394899	-1.4637912	0.6141043
Cl	2.5390460	1.4638563	-0.6158428
Ni	0.9954207	0.0000155	-0.0003526
P	-0.5205808	1.5741886	0.0782418
P	-0.5206022	-1.5741881	-0.0779225
C	-2.1396660	-0.6796234	-0.3549422
H	-2.2399405	-0.5387385	-1.4386200
H	-2.9947315	-1.2940428	-0.0350550
C	-2.1394424	0.6795934	0.3563494
H	-2.2389912	0.5387059	1.4400940
H	-2.9947336	1.2939953	0.0370335
C	-0.9472412	2.7369477	-1.4067679
C	-1.5368272	1.8599692	-2.5279561
H	-2.5039561	1.4137880	-2.2587186
H	-0.8423296	1.0645426	-2.8269110
H	-1.7085217	2.4955189	-3.4108912
C	0.2883788	3.4489206	-1.9841614
H	-0.0430509	4.0597315	-2.8405567
H	1.0456640	2.7353930	-2.3253508
H	0.7722679	4.1155783	-1.2629249
C	-2.0005593	3.7930374	-1.0219707
H	-1.6016236	4.5472696	-0.3330278
H	-2.9083973	3.3596162	-0.5788717
H	-2.3081780	4.3220609	-1.9386237
C	-0.2457983	2.6148959	1.6749935
C	0.7106974	3.7900388	1.4059611
H	0.2478405	4.5746553	0.7935899
H	1.6346669	3.4522996	0.9175209
H	0.9781736	4.2458971	2.3727799
C	0.4253702	1.6799283	2.7004022
H	0.6324744	2.2563815	3.6168605
H	1.3745795	1.2731025	2.3261963
H	-0.2242824	0.8408422	2.9830420
C	-1.5591775	3.1427703	2.2837631
H	-1.3115272	3.6911445	3.2069282
H	-2.2488791	2.3360826	2.5674344
H	-2.0927538	3.8367759	1.6247674
C	-0.2468852	-2.6148877	-1.6748641
C	0.7098266	-3.7900061	-1.4064946
H	0.9766529	-4.2458511	-2.3734994
H	0.2474121	-4.5746390	-0.7938110

H	1.6341217	-3.4522450	-0.9186852
C	0.4235586	-1.6798977	-2.7007258
H	0.6300596	-2.2563423	-3.6173256
H	1.3730092	-1.2730439	-2.3271625
H	-0.2263116	-0.8408313	-2.9829229
C	-1.5606650	-3.1427897	-2.2827459
H	-2.2505866	-2.3361173	-2.5659269
H	-2.0937683	-3.8368269	-1.6234022
H	-1.3136297	-3.6911344	-3.2060934
C	-0.9462321	-2.7369415	1.4073891
C	-1.5350936	-1.8599644	2.5289581
H	-2.5024194	-1.4138220	2.2603638
H	-0.8404236	-1.0645074	2.8274314
H	-1.7061707	-2.4955045	3.4120201
C	-1.9997771	-3.7930708	1.0233228
H	-2.3067648	-4.3220820	1.9401944
H	-1.6012813	-4.5473074	0.3341311
H	-2.9079242	-3.3596853	0.5808231
C	0.2897975	-3.4488628	1.9839699
H	1.0472863	-2.7353034	2.3246402
H	0.7732273	-4.1155170	1.2624228
H	-0.0410395	-4.0596696	2.8405975

Combination of torsional angles = -20
E(BP86/def2-TZVP) = -3822.37896190904

Cl	2.5409406	-1.5092055	0.4947728
Cl	2.5425170	1.5094255	-0.4858762
Ni	0.9957818	0.0000579	0.0018177
P	-0.5174503	1.5779136	0.0633594
P	-0.5171000	-1.5779263	-0.0648608
C	-2.1371574	-0.6856784	-0.3468549
H	-2.2412293	-0.5635076	-1.4322865
H	-2.9910054	-1.2951393	-0.0142826
C	-2.1383625	0.6855261	0.3399102
H	-2.2460423	0.5633467	1.4249876
H	-2.9911477	1.2949165	0.0044886
C	-0.9204766	2.7042448	-1.4549440
C	-1.4862515	1.8013071	-2.5674357
H	-2.4572994	1.3587443	-2.3064807
H	-0.7844056	1.0012374	-2.8347954
H	-1.6425782	2.4165154	-3.4674742
C	0.3254708	3.4054866	-2.0230067
H	0.0112867	3.9946074	-2.9007974
H	1.0910863	2.6859257	-2.3317626
H	0.7931174	4.0897917	-1.3076932
C	-1.9847739	3.7646698	-1.1146439
H	-1.6059963	4.5321733	-0.4291743
H	-2.9020810	3.3356606	-0.6870186
H	-2.2712932	4.2763405	-2.0478110
C	-0.2825642	2.6594405	1.6414565
C	0.6478614	3.8542812	1.3666978
H	0.1788702	4.6132419	0.7274053
H	1.5909732	3.5303249	0.9074949
H	0.8800895	4.3375820	2.3293746
C	0.3962869	1.7608959	2.6936747
H	0.5744671	2.3581360	3.6028484
H	1.3610247	1.3744523	2.3388789
H	-0.2359638	0.9103736	2.9815500
C	-1.6164471	3.1693818	2.2211634
H	-1.3927086	3.7537564	3.1281552
H	-2.2869571	2.3540926	2.5248884
H	-2.1620731	3.8273556	1.5352782
C	-0.2767650	-2.6593985	-1.6421808
C	0.6528311	-3.8541667	-1.3643088
H	0.8883660	-4.3374100	-2.3262108
H	0.1817395	-4.6131964	-0.7266441
H	1.5943489	-3.5301446	-0.9018955
C	0.4055745	-1.7607648	-2.6920638
H	0.5868933	-2.3579658	-3.6006429
H	1.3690658	-1.3742422	-2.3339862
H	-0.2257746	-0.9102949	-2.9820641
C	-1.6086232	-3.1694413	-2.2264350
H	-2.2781598	-2.3542023	-2.5324290
H	-2.1565276	-3.8274727	-1.5424256
H	-1.3817446	-3.7537828	-3.1326679
C	-0.9251716	-2.7043203	1.4520466
C	-1.4947647	-1.8014469	2.5626416
H	-2.4649456	-1.3589291	2.2984083
H	-0.7938729	-1.0013472	2.8324036
H	-1.6541094	-2.4166921	3.4621251
C	-1.9882392	-3.7648088	1.1081166
H	-2.2778890	-4.2765182	2.0402952
H	-1.6070873	-4.5322712	0.4239180
H	-2.9041205	-3.3358558	0.6773892
C	0.3188914	-3.4054987	2.0243028
H	1.0834046	-2.6858989	2.3356895
H	0.7890133	-4.0897359	1.3105489
H	0.0017729	-3.9946820	2.9009951

Combination of torsional angles = -15
E(BP86/def2-TZVP) = -3822.38005377159

Cl	2.5464035	-1.5425483	0.3700965
Cl	2.5469018	1.5427715	-0.3656519
Ni	0.9986987	0.0000488	0.0009133
P	-0.5123900	1.5815421	0.0472603
P	-0.5121853	-1.5815627	-0.0479795
C	-2.1348232	-0.6929047	-0.3296816
H	-2.2480238	-0.5942776	-1.4164967
H	-2.9853666	-1.2962100	0.0222288
C	-2.1354175	0.6927544	0.3262783
H	-2.2503911	0.5941173	1.4129060
H	-2.9854310	1.2959929	-0.0270266
C	-0.8883551	2.6650844	-1.5075879
C	-1.4250273	1.7307971	-2.6080996
H	-2.3992845	1.2899096	-2.3564038
H	-0.7133156	0.9280530	-2.8380924
H	-1.5647844	2.3212328	-3.5272735
C	0.3692366	3.3545450	-2.0643322
H	0.0761454	3.9154117	-2.9675005
H	1.1450866	2.6292905	-2.3321020
H	0.8160099	4.0617801	-1.3581072
C	-1.9646929	3.7290239	-1.2205319
H	-1.6084094	4.5141469	-0.5431693
H	-2.8913617	3.3052774	-0.8080637
H	-2.2283670	4.2172463	-2.1727796
C	-0.3180112	2.7098198	1.6002072
C	0.5926041	3.9174560	1.3139769
H	0.1231589	4.6488465	0.6437876
H	1.5529717	3.6018934	0.8869958
H	0.7901121	4.4311172	2.2687121

C	0.3586874	1.8520219	2.6868011
H	0.5110374	2.4757863	3.5827134
H	1.3355917	1.4753852	2.3563646
H	-0.2639845	0.9987182	2.9869977
C	-1.6709786	3.2107043	2.1435199
H	-1.4719289	3.8317860	3.0316335
H	-2.3286813	2.3931345	2.4678598
H	-2.2205580	3.8323454	1.4273245
C	-0.3151160	-2.7098021	-1.6006160
C	0.5951306	-3.9173605	-1.3128870
H	0.7942720	-4.4309906	-2.2672995
H	0.1246366	-4.6488032	-0.6434905
H	1.5547575	-3.6017183	-0.8843031
C	0.3633186	-1.8519287	-2.6860675
H	0.5172347	-2.4756717	-3.5817273
H	1.3396285	-1.4751942	-2.3539917
H	-0.2589374	-0.9986891	-2.9873049
C	-1.6671274	-3.2108003	-2.1461972
H	-2.3243599	-2.3932845	-2.4716229
H	-2.2178474	-3.8325031	-1.4309330
H	-1.4665348	-3.8318492	-3.0339866
C	-0.8906609	-2.6651554	1.5062210
C	-1.4292656	-1.7309279	2.6058393
H	-2.4031385	-1.2901279	2.3525108
H	-0.7180162	-0.9281192	2.8370343
H	-1.5705113	-2.3213866	3.5247705
C	-1.9664185	-3.7291892	1.2173413
H	-2.2316499	-4.2174483	2.1691375
H	-1.6089232	-4.5142707	0.5405691
H	-2.8924310	-3.3055235	0.8033190
C	0.3660541	-3.3545136	2.0650675
H	1.1413839	-2.6291948	2.3341647
H	0.8140855	-4.0616861	1.3595768
H	0.0714926	-3.9154334	2.9677241

Combination of torsional angles = -10

E(BP86/def2-TZVP) = -3822.38081606749

Cl	2.5515362	-1.5662108	0.2402697
Cl	2.5511841	1.5661601	-0.2443819
Ni	1.0019002	-0.0000124	-0.0008349
P	-0.5076016	1.5846315	0.0348151
P	-0.5076746	-1.5846390	-0.0340925
C	-2.1337540	-0.6997347	-0.3107391
H	-2.2585522	-0.6247519	-1.3981527
H	-2.9797240	-1.2968896	0.0622425
C	-2.1332540	0.6997487	0.3140375
H	-2.2563445	0.6247685	1.4016463
H	-2.9798013	1.2969134	-0.0576150
C	-0.8505572	2.6257454	-1.5548838
C	-1.3521779	1.6600334	-2.6442087
H	-2.3292552	1.2180471	-2.4055664
H	-0.6286106	0.8575689	-2.8338428
H	-1.4727540	2.2252880	-3.5817852
C	0.4204339	3.3047998	-2.0940261
H	0.1531032	3.8360959	-3.0226335
H	1.2072689	2.5757225	-2.3162713
H	0.8424222	4.0355257	-1.3965803
C	-1.9391638	3.6909641	-1.3255357
H	-1.6075452	4.4942140	-0.6570873
H	-2.8755328	3.2716878	-0.9307093
H	-2.1770517	4.1544414	-2.2967340
C	-0.3558956	2.7579223	1.5611956
C	0.5423424	3.9727307	1.2650807
H	0.0792870	4.6778050	0.5631092
H	1.5186481	3.6619866	0.8732642
H	0.7047542	4.5153160	2.2104312
C	0.3072957	1.9394468	2.6853425
H	0.4362431	2.5906564	3.5651943
H	1.2937354	1.5640382	2.3837336
H	-0.3143414	1.0902431	2.9988791
C	-1.7269060	3.2558742	2.0614923
H	-1.5536113	3.9095156	2.9314211
H	-2.3791609	2.4404638	2.4014396
H	-2.2713912	3.8450708	1.3145064
C	-0.3584154	-2.7579341	-1.5607112
C	0.5402749	-3.9727548	-1.2660227
H	0.7011842	-4.5153393	-2.2116308
H	0.0783213	-4.6778264	-0.5633225
H	1.5172040	-3.6620256	-0.8757500
C	0.3029999	-1.9394697	-2.6859120
H	0.4305385	-2.5906812	-3.5659675
H	1.2899242	-1.5640751	-2.3858724
H	-0.3191211	-1.0902558	-2.9984591
C	-1.7302277	-3.2558686	-2.0588260
H	-2.3830150	-2.4404506	-2.3977329
H	-2.2735289	-3.8450600	-1.3109746
H	-1.5583283	-3.9095095	-2.9290321
C	-0.8481099	-2.6257442	1.5561555
C	-1.3479373	-1.6600103	2.6462851
H	-2.3253798	-1.2179828	2.4092177
H	-0.6240298	-0.8575771	2.8347514
H	-1.4670269	-2.2252565	3.5840569
C	-1.9371229	-3.6909217	1.3285564
H	-2.1734702	-4.1543879	2.3001360
H	-1.6066059	-4.4941854	0.6595792
H	-2.8741087	-3.2716124	0.9352310
C	0.4237169	-3.3048489	2.0932596
H	1.2109375	-2.5758034	2.3142393
H	0.8445539	-4.0355963	1.3951415
H	0.1578533	-3.8361294	3.0222971

Combination of torsional angles = -5

E(BP86/def2-TZVP) = -3822.38131948851

Cl	2.5519526	-1.5796504	0.1173676
Cl	2.5519167	1.5797280	-0.1174398
Ni	1.0014469	0.0000227	-0.0000149
P	-0.5076714	1.5868191	0.0209085
P	-0.5076466	-1.5867986	-0.0208944
C	-2.1371669	-0.7068013	-0.2954349
H	-2.2721978	-0.6573655	-1.3831451
H	-2.9784543	-1.2972488	0.0983678
C	-2.1371703	0.7067942	0.2954923
H	-2.2721708	0.6573554	1.3832060
H	-2.9784785	1.2972277	-0.0982869
C	-0.8080146	2.5830283	-1.6041346
C	-1.2689013	1.5845681	-2.6812765
H	-2.2493514	1.1409417	-2.4598163
H	-0.5334072	0.7836296	-2.8251203
H	-1.3652071	2.1227025	-3.6374866
C	0.4792812	3.2506429	-2.1188389

H	0.2444933	3.7498450	-3.0735998
H	1.2764468	2.5184330	-2.2887970
H	0.8728654	4.0058521	-1.4309713
C	-1.9073550	3.6489584	-1.4402207
H	-1.6022860	4.4712974	-0.7824995
H	-2.8547733	3.2351843	-1.0663829
H	-2.1142870	4.0852877	-2.4308823
C	-0.4037216	2.8053544	1.5174940
C	0.4908970	4.0212588	1.2139713
H	0.0428359	4.7006166	0.4777791
H	1.4822195	3.7106754	0.8627998
H	0.6165943	4.5926979	2.1478797
C	0.2317581	2.0257345	2.6840947
H	0.3370997	2.7056026	3.5451418
H	1.2261799	1.6439838	2.4192842
H	-0.3976399	1.1868167	3.0095138
C	-1.7922742	3.3070875	1.9640403
H	-1.6471035	3.9904666	2.8160641
H	-2.4473259	2.4982048	2.3137189
H	-2.3209510	3.8669958	1.1838980
C	-0.4037241	-2.8053392	-1.5174761
C	0.4909296	-4.0212225	-1.2139738
H	0.6166010	-4.5926713	-2.1478796
H	0.0429106	-4.7005793	-0.4777549
H	1.4822593	-3.7106156	-0.8628448
C	0.2316954	-2.0257135	-2.6841060
H	0.3370245	-2.7055868	-3.5451505
H	1.2261170	-1.6439356	-2.4193339
H	-0.3977352	-1.1868148	-3.0095108
C	-1.7922823	-3.3071061	-1.9639657
H	-2.4473680	-2.4982398	-2.3136182
H	-2.3209134	-3.8670267	-1.1838014
H	-1.6471292	-3.9904823	-2.8159947
C	-0.8079266	-2.5830125	1.6041557
C	-1.2688170	-1.5845663	2.6813093
H	-2.2492868	-1.1409713	2.4598743
H	-0.5333449	-0.7836044	2.8251346
H	-1.3650809	-2.1227036	3.6375219
C	-1.9072397	-3.6489738	1.4402642
H	-2.1141366	-4.0853114	2.4309294
H	-1.6021618	-4.4713022	0.7825340
H	-2.8546779	-3.2352257	1.0664487
C	0.4794011	-3.2505915	2.1188252
H	1.2765493	-2.5183593	2.2887666
H	0.8729906	-4.0057849	1.4309435
H	0.2446522	-3.7498054	3.0735895

Combination of torsional angles = 0
E(BP86/def2-TZVP) = -3822.38165037234

Cl	2.5500865	-1.5836505	0.0015851
Cl	2.5500645	1.5836823	-0.0009618
Ni	0.9993463	0.0000048	0.0001260
P	-0.5101403	1.5876664	-0.0013307
P	-0.5101282	-1.5876693	0.0012227
C	-2.1438527	-0.7152449	-0.2740853
H	-2.2909910	-0.6984937	-1.3613302
H	-2.9791969	-1.2962257	0.1456759
C	-2.1439225	0.7152300	0.2735943
H	-2.2913137	0.6984776	1.3608050
H	-2.9791735	1.2962043	-0.1463615
C	-0.7645948	2.5274183	-1.6655967
C	-1.1868941	1.4899182	-2.7208794
H	-2.1716233	1.0485660	-2.5138850
H	-0.4433151	0.6888192	-2.8119467
H	-1.2559861	1.9932883	-3.6981910
C	0.5400790	3.1777473	-2.1588820
H	0.3406307	3.6378051	-3.1408626
H	1.3439023	2.4412984	-2.2704831
H	0.9071489	3.9608191	-1.4877290
C	-1.8699836	3.5954388	-1.5754003
H	-1.5887311	4.4408719	-0.9366367
H	-2.8284783	3.1915436	-1.2192326
H	-2.0448377	3.9967553	-2.5868403
C	-0.4515899	2.8590624	1.4545931
C	0.4462592	4.0689528	1.1362076
H	0.0185511	4.7184854	0.3619705
H	1.4500210	3.7525697	0.8291326
H	0.5376247	4.6745363	2.0524462
C	0.1484048	2.1246657	2.6680772
H	0.2319790	2.8378696	3.5041219
H	1.1487010	1.7314409	2.4457441
H	-0.4936304	1.3015761	3.0088549
C	-1.8546709	3.3718234	1.8402961
H	-1.7360945	4.0873394	2.6697487
H	-2.5180015	2.5747593	2.2010705
H	-2.3613020	3.9003249	1.0244713
C	-0.4512285	-2.8590590	-1.4546930
C	0.4465537	-4.0689460	-1.1361058
H	0.5381374	-4.6745223	-2.0523274
H	0.0186686	-4.7184868	-0.3619737
H	1.4502415	-3.7525586	-0.8287939
C	0.1490456	-2.1246519	-2.6680326
H	0.2328231	-2.8378513	-3.5040607
H	1.1492862	-1.7314194	-2.4454622
H	-0.4929163	-1.3015662	-3.0089580
C	-1.8542156	-3.3718259	-1.8407291
H	-2.5174665	-2.5747632	-2.2016534
H	-2.3610350	-3.9003366	-1.0250274
H	-1.7354400	-4.0873350	-2.6701590
C	-0.7649738	-2.5274248	1.6654272
C	-1.1875335	-1.4899276	2.7206086
H	-2.1722171	-1.0485840	2.5133790
H	-0.4439833	-0.6888218	2.8118522
H	-1.2568536	-1.9932975	3.6979041
C	-1.8703341	-3.5954524	1.5749669
H	-2.0454274	-3.9967694	2.5863652
H	-1.5889233	-4.4408840	0.9362711
H	-2.8287462	-3.1915636	1.2185698
C	0.5395857	-3.1777449	2.1590270
H	1.3433762	-2.4412900	2.2708252
H	0.9068249	-3.9608118	1.4879609
H	0.3399030	-3.6378072	3.1409580

Combination of torsional angles = 5
E(BP86/def2-TZVP) = -3822.38174352782

Cl	2.5488085	-1.5795424	-0.1207781
Cl	2.5488638	1.5795504	0.1186597
Ni	0.9989701	-0.0000170	-0.0004246
P	-0.5113710	1.5872010	-0.0183832
P	-0.5113643	-1.5872308	0.0187816

C	-2.1498180	-0.7223693	-0.2530888
H	-2.3103048	-0.7354782	-1.3386491
H	-2.9782055	-1.2944769	0.1918988
C	-2.1496051	0.7223564	0.2548487
H	-2.3091976	0.7354669	1.3405405
H	-2.9783541	1.2944696	-0.1894583
C	-0.7182589	2.4740142	-1.7160692
C	-1.1040636	1.4011104	-2.7492226
H	-2.0935540	0.9630814	-2.5578838
H	-0.3557969	0.6002051	-2.7887922
H	-1.1440006	1.8711579	-3.7446329
C	0.6039637	3.1074469	-2.1849155
H	0.4415875	3.5303009	-3.1900801
H	1.4113335	2.3681359	-2.2397078
H	0.9460448	3.9155339	-1.5304180
C	-1.8258168	3.5429268	-1.6970610
H	-1.5661664	4.4090724	-1.0771324
H	-2.7951140	3.1488705	-1.3593860
H	-1.9678860	3.9109836	-2.7261383
C	-0.4943308	2.9050204	1.3976292
C	0.4115308	4.1060163	1.0679639
H	0.0069318	4.7287657	0.2600209
H	1.4248683	3.7825268	0.8032260
H	0.4727260	4.7415403	1.9662752
C	0.0661067	2.2119056	2.6533518
H	0.1280944	2.9542019	3.4655514
H	1.0710587	1.8087164	2.4740761
H	-0.5898189	1.4040826	3.0041447
C	-1.9086901	3.4296970	1.7226115
H	-1.8145031	4.1732980	2.5301993
H	-2.5831904	2.6454297	2.0904567
H	-2.3901366	3.9299189	0.8743677
C	-0.4955609	-2.9050485	-1.3972513
C	0.4105124	-4.1060953	-1.0683543
H	0.4709256	-4.7416114	-1.9667243
H	0.0065504	-4.7288332	-0.2600834
H	1.4240872	-3.7826648	-0.8044565
C	0.0638461	-2.2119576	-2.6534468
H	0.1251181	-2.9542573	-3.4656977
H	1.0689648	-1.8088081	-2.4750205
H	-0.5923434	-1.4041096	-3.0036880
C	-1.9102193	-3.4296571	-1.7210402
H	-2.5849904	-2.6453582	-2.0883227
H	-2.3909774	-3.9298485	-0.8723869
H	-1.8167503	-4.1732691	-2.5287012
C	-0.7168816	-2.4740289	1.7166440
C	-1.1017498	-1.4010895	2.7501097
H	-2.0913630	-0.9629829	2.5595850
H	-0.3533866	-0.6002439	2.7890562
H	-1.1409034	-1.8711284	3.7455551
C	-1.8245296	-3.5428644	1.6985600
H	-1.9657693	-3.9109087	2.7277557
H	-1.5654528	-4.4090303	1.0784184
H	-2.7940802	-3.1487444	1.3616872
C	0.6056821	-3.1075524	2.1844038
H	1.4131534	-2.3683026	2.2385128
H	0.9471565	-3.9156811	1.5296424
H	0.4441051	-3.5303726	3.1897115

Combination of torsional angles = 10

E(BP86/def2-TZVP) = -3822.38159177604

Cl	2.5462304	-1.5660920	-0.2479863
Cl	2.5470387	1.5660365	0.2396407
Ni	0.9982559	-0.0000164	-0.0016549
P	-0.5137242	1.5854473	-0.0321605
P	-0.5136164	-1.5854726	0.0338020
C	-2.1570788	-0.7283993	-0.2322539
H	-2.3313958	-0.7687657	-1.3151863
H	-2.9777637	-1.2922111	0.2369482
C	-2.1563019	0.7283852	0.2393210
H	-2.3270619	0.7687557	1.3228188
H	-2.9785236	1.2921975	-0.2271858
C	-0.6751028	2.4248104	-1.7567847
C	-1.0353660	1.3230691	-2.7682067
H	-2.0306733	0.8924985	-2.5897842
H	-0.2884888	0.5198861	-2.7633103
H	-1.0478894	1.7634408	-3.7778564
C	0.6654916	3.0369671	-2.2022009
H	0.5395122	3.4276055	-3.2253684
H	1.4701474	2.2923176	-2.2067325
H	0.9903065	3.8643816	-1.5631649
C	-1.7772673	3.4980556	-1.8008015
H	-1.5317237	4.3810100	-1.1990765
H	-2.7573240	3.1169528	-1.4794630
H	-1.8885587	3.8363785	-2.8437809
C	-0.5312479	2.9424352	1.3466555
C	0.3883899	4.1310141	1.0099171
H	0.0098053	4.7313177	0.1728878
H	1.4079950	3.7974550	0.7850389
H	0.4249197	4.7920085	1.8910409
C	-0.0130044	2.2841310	2.6386249
H	0.0294390	3.0504184	3.4294592
H	0.9945788	1.8712722	2.5009918
H	-0.6842832	1.4909918	2.9940365
C	-1.9524974	3.4815236	1.6141016
H	-1.8784399	4.2472187	2.4029374
H	-2.6414609	2.7108110	1.9836749
H	-2.4061755	3.9597647	0.7383805
C	-0.5357150	-2.9424486	-1.3449674
C	0.3849974	-4.1310540	-1.0112803
H	0.4186215	-4.7920247	-1.8925380
H	0.0091418	-4.7313707	-0.1730304
H	1.4053424	-3.7975261	-0.7897367
C	-0.0217282	-2.2841361	-2.6386323
H	0.0181483	-3.0504240	-3.4295999
H	0.9862873	-1.8712432	-2.5043072
H	-0.6941968	-1.4910237	-2.9918463
C	-1.9578507	-3.4815102	-1.6077261
H	-2.6480279	-2.7107809	-1.9749951
H	-2.4086332	-3.9597694	-0.7305194
H	-1.8864161	-4.2471847	-2.3968236
C	-0.6693082	-2.4248192	1.7589569
C	-1.0260548	-1.3230206	2.7715638
H	-2.0218930	-0.8923186	2.5964569
H	-0.2790908	-0.5199379	2.7641675
H	-1.0352711	-1.7633833	3.7812533
C	-1.7714418	-3.4979385	1.8066445
H	-1.8793091	-3.8362426	2.8499891
H	-1.5279901	-4.3809252	1.2041136
H	-2.7525187	-3.1167351	1.4885522

C	0.6726849	-3.0371349	2.1999185
H	1.4774503	-2.2925931	2.2017436
H	0.9952545	-3.8646182	1.5598364
H	0.5500629	-3.4277200	3.2235143

Combination of torsional angles = 15
E(BP86/def2-TZVP) = -3822.38123706278

Cl	2.5398903	-1.5432728	-0.3706532
Cl	2.5406941	1.5431927	0.3652891
Ni	0.9941170	-0.0000228	-0.0010598
P	-0.5201445	1.5824860	-0.0471626
P	-0.5200857	-1.5824907	0.0482106
C	-2.1680943	-0.7338684	-0.2157757
H	-2.3539286	-0.8009296	-1.2956442
H	-2.9816129	-1.2891151	0.2756217
C	-2.1676265	0.7339094	0.2202331
H	-2.3512383	0.8009775	1.3004807
H	-2.9821413	1.2891755	-0.2694908
C	-0.6349922	2.3764684	-1.7951544
C	-0.9792272	1.2505081	-2.7849493
H	-1.9821002	0.8325849	-2.6183282
H	-0.2395783	0.4418944	-2.7396964
H	-0.9641872	1.6630776	-3.8062864
C	0.7257232	2.9612933	-2.2168451
H	0.6365551	3.3235869	-3.2541299
H	1.5213401	2.2076714	-2.1759278
H	1.0406314	3.8031356	-1.5917216
C	-1.7242472	3.4583602	-1.8983502
H	-1.4863939	4.3554656	-1.3147525
H	-2.7159899	3.0945918	-1.5928766
H	-1.8046736	3.7684811	-2.9528795
C	-0.5681245	2.9750948	1.2945487
C	0.3706909	4.1475548	0.9540605
H	0.0221520	4.7275071	0.0900637
H	1.3939989	3.8007498	0.7696362
H	0.3858537	4.8321044	1.8176672
C	-0.0959392	2.3486119	2.6195727
H	-0.0720471	3.1363388	3.3897987
H	0.9124243	1.9258127	2.5242976
H	-0.7842695	1.5704620	2.9757459
C	-1.9927323	3.5311932	1.5038723
H	-1.9366093	4.3157422	2.2755009
H	-2.6990194	2.7750758	1.8708641
H	-2.4152553	3.9908852	0.6030986
C	-0.5709082	-2.9751123	-1.2933861
C	0.3685555	-4.1476155	-0.9548429
H	0.3819108	-4.8321563	-1.8184869
H	0.0217670	-4.7275629	-0.0901383
H	1.3922564	-3.8008602	-0.7725217
C	-0.1014533	-2.3486566	-2.6193929
H	-0.0791967	-3.1363872	-3.3896645
H	0.9071237	-1.9259001	-2.5262153
H	-0.7904895	-1.5704784	-2.9741364
C	-1.9959737	-3.5311490	-1.4997395
H	-2.7029882	-2.7750073	-1.8652792
H	-2.4166443	-3.9908015	-0.5980788
H	-1.9414900	-4.3157160	-2.2714670
C	-0.6313237	-2.3764375	1.7964514
C	-0.9733853	-1.2504290	2.7869441
H	-1.9765647	-0.8324146	2.6224115
H	-0.2337584	-0.4418857	2.7401313
H	-0.9562515	-1.6629844	3.8082545
C	-1.7204488	-3.4582382	1.9019501
H	-1.7986966	-3.7683298	2.9566519
H	-1.4838892	-4.3553765	1.3178761
H	-2.7127995	-3.0943977	1.5985416
C	0.7302245	-2.9613639	2.2153014
H	1.5258212	-2.2078155	2.1726751
H	1.0437372	-3.8032657	1.5895579
H	0.6432085	-3.3236003	3.2527892

Combination of torsional angles = 20
E(BP86/def2-TZVP) = -3822.38061865134

Cl	2.5408599	-1.5118183	-0.4463230
Cl	2.5248959	1.5118527	0.5288907
Ni	0.9899273	0.0000262	0.0161318
P	-0.5256603	1.5782601	-0.0759108
P	-0.5278242	-1.5781995	0.0589000
C	-2.1759014	-0.7395367	-0.2333910
H	-2.3552834	-0.8362335	-1.3122704
H	-2.9903245	-1.2842731	0.2682020
C	-2.1823051	0.7395761	0.1629995
H	-2.3963636	0.8362867	1.2355454
H	-2.9801202	1.2843254	-0.3645881
C	-0.5665243	2.3233486	-1.8472024
C	-0.8889044	1.1744519	-2.8175437
H	-1.9029680	0.7742616	-2.6759775
H	-0.1627315	0.3580275	-2.7223964
H	-0.8311117	1.5577455	-3.8487580
C	0.8214281	2.8737699	-2.2255352
H	0.7844399	3.2089334	-3.2749690
H	1.6006784	2.1075528	-2.1308062
H	1.1244864	3.7268131	-1.6096516
C	-1.6331829	3.4175067	-2.0254870
H	-1.4053754	4.3279890	-1.4588893
H	-2.6416920	3.0764206	-1.7499539
H	-1.6665978	3.6974011	-3.0909743
C	-0.6192813	3.0074354	1.2233135
C	0.3491849	4.1586856	0.8936050
H	0.0484825	4.7171658	-0.0019342
H	1.3754715	3.7947377	0.7673781
H	0.3334909	4.8680384	1.7369654
C	-0.2176298	2.4144710	2.5865321
H	-0.2219200	3.2240908	3.3340476
H	0.7898859	1.9804935	2.5510462
H	-0.9303592	1.6534417	2.9318117
C	-2.0455240	3.5840163	1.3505113
H	-2.0165693	4.3866833	2.1048385
H	-2.7772324	2.8446626	1.7016180
H	-2.4194625	4.0258352	0.4199568
C	-0.5792371	-3.0072050	-1.2428225
C	0.3779360	-4.1585285	-0.8818499
H	0.3896015	-4.8678527	-1.7252897
H	0.0482688	-4.7169798	0.0034444
H	1.3996045	-3.7946406	-0.7223538
C	-0.1333460	-2.4142112	-2.5922043
H	-0.1132255	-3.2238037	-3.3394817
H	0.8724672	-1.9802004	-2.5238751
H	-0.8344712	-1.6532053	-2.9605472
C	-2.0005942	-3.5836906	-1.4164588

H	-2.7204195	-2.8442499	-1.7911287
H	-2.4046573	-4.0255921	-0.4986258
H	-1.9471446	-4.3862963	-2.1695207
C	-0.6261446	-2.3235573	1.8278568
C	-0.9802052	-1.1748989	2.7873806
H	-1.9891818	-0.7748480	2.6128897
H	-0.2514351	-0.3583387	2.7161559
H	-0.9560158	-1.5583908	3.8198487
C	-1.6978607	-3.4179163	1.9711048
H	-1.7658280	-3.6981052	3.0348671
H	-1.4516285	-4.3281988	1.4119594
H	-2.6969272	-3.0768799	1.6630479
C	0.7488429	-2.8738094	2.2511801
H	1.5306422	-2.1074412	2.1820623
H	1.0720204	-3.7266891	1.6453768
H	0.6776875	-3.2091539	3.2987917

Combination of torsional angles = 25
E(BP86/def2-TZVP) = -3822.37975497964

Cl	2.5283807	-1.4697585	-0.6096496
Cl	2.5280583	1.4697715	0.6109064
Ni	0.9889085	0.0000004	0.0002404
P	-0.5307811	1.5729640	-0.0847762
P	-0.5308104	-1.5729774	0.0844833
C	-2.1882249	-0.7443413	-0.1807325
H	-2.3962687	-0.8680813	-1.2518442
H	-2.9866701	-1.2790539	0.3561184
C	-2.1883230	0.7443137	0.1795897
H	-2.3969169	0.8680517	1.2505943
H	-2.9864973	1.2790190	-0.3576698
C	-0.5599499	2.2756418	-1.8725857
C	-0.9040372	1.1109951	-2.8160971
H	-1.9251187	0.7327819	-2.6637318
H	-0.1926516	0.2839926	-2.7033752
H	-0.8412307	1.4696461	-3.8558693
C	0.8423800	2.7863636	-2.2552448
H	0.8189698	3.1023274	-3.3109390
H	1.6024879	2.0029483	-2.1432990
H	1.1631461	3.6432577	-1.6536321
C	-1.6028611	3.3868456	-2.0811694
H	-1.3586728	4.3061976	-1.5362285
H	-2.6188106	3.0724645	-1.8011044
H	-1.6271017	3.6409478	-3.1533656
C	-0.6196726	3.0322751	1.1791948
C	0.3717036	4.1589045	0.8329963
H	0.0919670	4.6990599	-0.0803804
H	1.3934075	3.7747520	0.7298445
H	0.3577958	4.8899083	1.6576896
C	-0.2439030	2.4670578	2.5615583
H	-0.2472192	3.2950086	3.2886960
H	0.7585150	2.0201576	2.5495914
H	-0.9710658	1.7241010	2.9162926
C	-2.0387189	3.6320447	1.2758249
H	-2.0082220	4.4474038	2.0163947
H	-2.7857407	2.9093839	1.6296662
H	-2.3935278	4.0625559	0.3327615
C	-0.6190301	-3.0322988	-1.1795268
C	0.3721851	-4.1589092	-0.8328056
H	0.3587172	-4.8899198	-1.6575004
H	0.0919839	-4.6990615	0.0804313
H	1.3938302	-3.7747381	-0.7291267
C	-0.2425502	-2.4670887	-2.5617000
H	-0.2454763	-3.2950467	-3.2888317
H	0.7598561	-2.0201732	-2.5492167
H	-0.9695395	-1.7241454	-2.9168191
C	-2.0380168	-3.6320917	-1.2768899
H	-2.7848659	-2.9094447	-1.6311244
H	-2.3933086	-4.0626024	-0.3340074
H	-2.0071224	-4.4474559	-2.0174383
C	-0.5608899	-2.2756500	1.8722825
C	-0.9054761	-1.1110036	2.8156128
H	-1.9264826	-0.7328010	2.6627189
H	-0.1940404	-0.2839947	2.7032574
H	-0.8432040	-1.4696522	3.8554179
C	-1.6038953	-3.3868653	2.0803352
H	-1.6286847	-3.6409630	3.1525201
H	-1.3594161	-4.3062175	1.5355236
H	-2.6197046	-3.0724968	1.7997460
C	0.8412495	-2.7863549	2.2556629
H	1.6014070	-2.0029313	2.1441023
H	1.1623336	-3.6432493	1.6542179
H	0.8173021	-3.1023136	3.3113465

Combination of torsional angles = 30
E(BP86/def2-TZVP) = -3822.37860083248

Cl	2.5212212	-1.4142788	-0.7359483
Cl	2.5197389	1.4142411	0.7410284
Ni	0.9858437	-0.0000041	0.0009713
P	-0.5368591	1.5671486	-0.0965833
P	-0.5370496	-1.5671563	0.0954237
C	-2.1991124	-0.7479090	-0.1680078
H	-2.4171282	-0.8934203	-1.2345331
H	-2.9902094	-1.2745538	0.3873829
C	-2.1994503	0.7478973	0.1634834
H	-2.4196277	0.8934098	1.2295654
H	-2.9894214	1.2745414	-0.3935085
C	-0.5293782	2.2374394	-1.8966147
C	-0.8874117	1.0651077	-2.8250606
H	-1.9179383	0.7109571	-2.6775134
H	-0.1946421	0.2257191	-2.6917789
H	-0.8063337	1.4057305	-3.8696354
C	0.8924796	2.7064605	-2.2618631
H	0.8958891	3.0113838	-3.3210005
H	1.6286515	1.9029598	-2.1303017
H	1.2266636	3.5607157	-1.6635490
C	-1.5415250	3.3690876	-2.1420477
H	-1.2847939	4.2924088	-1.6098382
H	-2.5689772	3.0832153	-1.8736061
H	-1.5419730	3.6037164	-3.2189626
C	-0.6357717	3.0483986	1.1387096
C	0.3869728	4.1482897	0.7979967
H	0.1437571	4.6751672	-0.1333958
H	1.4033232	3.7417279	0.7312887
H	0.3661697	4.8960912	1.6073293
C	-0.3072497	2.5028125	2.5409991
H	-0.3176999	3.3444921	3.2521207
H	0.6883864	2.0414476	2.5646770
H	-1.0554598	1.7778835	2.8895423
C	-2.0462513	3.6734222	1.1875344
H	-2.0235056	4.4953407	1.9211445

H	-2.8151898	2.9664450	1.5261657
H	-2.3663197	4.1002972	0.2307167
C	-0.6334550	-3.0484013	-1.1400727
C	0.3885851	-4.1482999	-0.7972769
H	0.3694260	-4.8960986	-1.6066519
H	0.1434675	-4.6751768	0.1336167
H	1.4048000	-3.7417449	-0.7284967
C	-0.3020670	-2.5028223	-2.5416898
H	-0.3110613	-3.3445046	-3.2528277
H	0.6936161	-2.0414568	-2.5633353
H	-1.0495642	-1.7778962	-2.8917646
C	-2.0438352	-3.6734176	-1.1917775
H	-2.8120745	-2.9664384	-1.5319852
H	-2.3658616	-4.1002864	-0.2356143
H	-2.0195934	-4.4953411	-1.9253347
C	-0.5332184	-2.2374516	1.8954644
C	-0.8930939	-1.0651117	2.8231875
H	-1.9233063	-0.7109239	2.6735510
H	-0.2000247	-0.2257480	2.6913190
H	-0.8141507	-1.4057453	3.8679223
C	-1.5458937	-3.3690706	2.1388429
H	-1.5485345	-3.6037017	3.2157541
H	-1.2881099	-4.2923984	1.6071537
H	-2.5727905	-3.0831684	1.8683165
C	0.8878853	-2.7065136	2.2635897
H	1.6243490	-1.9030382	2.1335068
H	1.2232532	-3.5607863	1.6659639
H	0.8891447	-3.0114228	3.3227360

Combination of torsional angles = 35
E(BP86/def2-TZVP) = -3822.37714486595

Cl	2.5077529	-1.3458246	-0.8681500
Cl	2.5084048	1.3458128	0.8663014
Ni	0.9794544	-0.0000034	-0.0003527
P	-0.5462815	1.5606261	-0.1060963
P	-0.5461984	-1.5606375	0.1065295
C	-2.2135339	-0.7510032	-0.1517530
H	-2.4430849	-0.9164601	-1.2130634
H	-2.9962147	-1.2700334	0.4223958
C	-2.2134205	0.7509878	0.1534358
H	-2.4421739	0.9164440	1.2149182
H	-2.9965336	1.2700159	-0.4201252
C	-0.5103901	2.2034871	-1.9158964
C	-0.8906488	1.0282806	-2.8315133
H	-1.9297013	0.6994591	-2.6842252
H	-0.2172719	0.1757211	-2.6854738
H	-0.7976432	1.3545600	-3.8796754
C	0.9282384	2.6291811	-2.2700661
H	0.9520006	2.9264692	-3.3310836
H	1.6390055	1.8044785	-2.1269779
H	1.2808400	3.4776202	-1.6737453
C	-1.4896573	3.3574483	-2.1882790
H	-1.2147922	4.2816990	-1.6669535
H	-2.5269660	3.1018533	-1.9273919
H	-1.4720492	3.5757228	-3.2684975
C	-0.6459864	3.0594295	1.1052457
C	0.4101564	4.1290844	0.7706515
H	0.2022754	4.6449959	-0.1753116
H	1.4179614	3.6971919	0.7358453
H	0.3892276	4.8913390	1.5663569
C	-0.3607060	2.5292137	2.5229818
H	-0.3718747	3.3823634	3.2202806
H	0.6256465	2.0507141	2.5769909
H	-1.1304330	1.8240690	2.8655256
C	-2.0441859	3.7128666	1.1139636
H	-2.0246793	4.5373699	1.8448134
H	-2.8351278	3.0219579	1.4351219
H	-2.3309491	4.1413786	0.1476236
C	-0.6467978	-3.0594375	-1.1047429
C	0.4096056	-4.1290828	-0.7709429
H	0.3880881	-4.8913366	-1.5666337
H	0.2024390	-4.6449979	0.1751751
H	1.4174320	-3.6971800	-0.7368915
C	-0.3625828	-2.5292107	-2.5226889
H	-0.3742632	-3.3823567	-3.2199839
H	0.6237236	-2.0506999	-2.5774322
H	-1.1325731	-1.8240725	-2.8646539
C	-2.0449975	-3.7128868	-1.1124155
H	-2.8361869	-3.0219829	-1.4329744
H	-2.3310304	-4.1414079	-0.1458632
H	-2.0260329	-4.5373848	-1.8432854
C	-0.5089484	-2.2035080	1.9162987
C	-0.8885384	-1.0283118	2.8322066
H	-1.9277057	-0.6995045	2.6856987
H	-0.2152837	-0.1757412	2.6856664
H	-0.7947419	-1.3545946	3.8802971
C	-1.4879960	-3.3574840	2.1894064
H	-1.4695753	-3.5757658	3.2696099
H	-1.2135093	-4.2817271	1.6678684
H	-2.5255034	-3.1019009	1.9292990
C	0.9299495	-2.6291867	2.2693888
H	1.6405982	-1.8044730	2.1257794
H	1.2821161	-3.4776139	1.6727938
H	0.9545083	-2.9264877	3.3303846

Combination of torsional angles = 40
E(BP86/def2-TZVP) = -3822.37537972839

Cl	2.4939957	-1.2619753	-0.9987099
Cl	2.4950778	1.2620140	0.9962394
Ni	0.9732370	0.0000557	-0.0004557
P	-0.5552621	1.5538321	-0.1130522
P	-0.5552321	-1.5536386	0.1137045
C	-2.2273459	-0.7532038	-0.1410581
H	-2.4656704	-0.9345753	-1.1979254
H	-3.0029396	-1.2662765	0.4478377
C	-2.2271573	0.7534881	0.1434205
H	-2.4643878	0.9348732	1.2005309
H	-3.0033257	1.2666030	-0.4446807
C	-0.4944268	2.1782157	-1.9291517
C	-0.8988185	1.0058390	-2.8377210
H	-1.9451587	0.7008240	-2.6900408
H	-0.2439285	0.1404396	-2.6859053
H	-0.7973475	1.3238254	-3.8876484
C	0.9581703	2.5636092	-2.2737657
H	0.9985270	2.8574879	-3.3352289
H	1.6444812	1.7188785	-2.1250324
H	1.3290698	3.4039524	-1.6767579
C	-1.4413127	3.3545483	-2.2190808
H	-1.1466407	4.2762955	-1.7042618
H	-2.4868830	3.1279733	-1.9645666

H	-1.4090981	3.5619060	-3.3011209
C	-0.6508639	3.0636789	1.0823408
C	0.4398939	4.1013265	0.7588273
H	0.2671564	4.6106899	-0.1976895
H	1.4366416	3.6423352	0.7520377
H	0.4231224	4.8736200	1.5448507
C	-0.4070681	2.5418581	2.5109997
H	-0.4152890	3.4026786	3.1988505
H	0.5681955	2.0445172	2.5908699
H	-1.1985251	1.8566836	2.8447137
C	-2.0339491	3.7476840	1.0571929
H	-2.0156105	4.5697486	1.7908713
H	-2.8469039	3.0723644	1.3563830
H	-2.2874361	4.1842519	0.0854504
C	-0.6521313	-3.0634910	-1.0815735
C	0.4389041	-4.1011853	-0.7591476
H	0.4212946	-4.8734974	-1.5451345
H	0.2671162	-4.6105164	0.1975584
H	1.4356809	-3.6422424	-0.7533846
C	-0.4097685	-2.5417024	-2.5104886
H	-0.4187350	-3.4025320	-3.1983185
H	0.5654379	-2.0444112	-2.5913612
H	-1.2015317	-1.8564927	-2.8434039
C	-2.0352225	-3.7474274	-1.0549908
H	-2.8484509	-3.0720742	-1.3533612
H	-2.2877324	-4.1839600	-0.0829770
H	-2.0176784	-4.5695101	-1.7886684
C	-0.4925738	-2.1780485	1.9297296
C	-0.8959826	-1.0056694	2.8387337
H	-1.9424585	-0.7006017	2.6921275
H	-0.2412072	-0.1402977	2.6862646
H	-0.7934544	-1.3236793	3.8885510
C	-1.4392168	-3.3543457	2.2205942
H	-1.4059032	-3.5617371	3.3025945
H	-1.1451159	-4.2760910	1.7054443
H	-2.4850370	-3.1277141	1.9671583
C	0.9603563	-2.5635239	2.2728439
H	1.6465572	-1.7188236	2.1234318
H	1.3306005	-3.4038686	1.6754298
H	1.0017866	-2.8574368	3.3342563

Relaxed potential surface scan of O structure of NiCl2dtbpe

Combination of torsional angles = -5

E(BP86/def2-TZVP) = -3822.37563791622

Ni	-1.0139415	-0.0390618	-0.0001462
Cl	-2.5532638	0.0113346	-1.5946005
Cl	-2.5450283	-0.2074870	1.5939895
C	2.1313847	-0.1975924	0.7112664
C	2.1101277	0.3602929	-0.7103800
P	0.4911658	0.0486428	1.5862003
P	0.4939165	-0.0109045	-1.5859187
C	0.6224145	-1.3306082	2.9475308
C	0.5383041	-2.6850181	2.2180986
C	-0.5060139	-1.3324664	3.9972541
C	1.9735832	-1.2274227	3.6822457
C	0.5739442	1.8085414	2.3875816
C	-0.2131152	1.8731474	3.7074986
C	-0.0960874	2.7841724	1.4040555
C	2.0216482	2.2668735	2.6357972
C	0.7117561	-1.7589876	-2.3876080
C	2.1901901	-2.1038542	-2.6381463
C	0.1208447	-2.7835398	-1.4031111
C	-0.0700569	-1.8842881	-3.7063065
C	0.5190245	1.3747584	-2.9468394
C	1.8743205	1.3764331	-3.6811494
C	0.3304382	2.7182479	-2.2168066
C	-0.6057769	1.2900822	-3.9970268
H	2.9657734	0.2275553	1.2854502
H	2.2902307	-1.2847446	0.6828085
H	2.1850805	1.4564414	-0.6816161
H	2.9748762	0.0005675	-1.2843696
H	-0.4106991	-2.7855515	1.6757488
H	0.5853779	-3.4876071	2.9708985
H	1.3696859	-2.8558857	1.5210941
H	-1.4953601	-1.3388240	3.5278174
H	-0.4519701	-0.4844487	4.6855756
H	-0.3934249	-2.2487066	4.5996238
H	2.8402176	-1.2980001	3.0114931
H	2.0448584	-2.0646320	4.3952424
H	2.0578771	-0.3006056	4.2653056
H	-1.2248899	1.4620983	3.5977810
H	-0.3060474	2.9323866	3.9970427
H	0.3023072	1.3567914	4.5267556
H	0.4341801	2.8371737	0.4471674
H	-0.0865418	3.7941466	1.8462997
H	-1.1389242	2.5018576	1.2064307
H	2.5945506	2.3729865	1.7037928
H	2.5745975	1.5971593	3.3078451
H	1.9950267	3.2603540	3.1117251
H	2.2397995	-3.0962435	-3.1145061
H	2.7709735	-2.1655695	-1.7070543
H	2.6886560	-1.3931902	-3.3107581
H	0.2079885	-3.7898031	-1.8453002
H	-0.9404743	-2.5828959	-1.2039362
H	0.6550531	-2.7951820	-0.4469802
H	-0.0819426	-2.9476378	-3.9954106
H	0.4030416	-1.3302430	-4.5264551
H	-1.1102231	-1.5519347	-3.5952152
H	2.0297711	0.4592866	-4.2648667
H	2.7327971	1.5129992	-3.0101178
H	1.8811218	2.2171564	-4.3935743
H	0.3160776	3.5225382	-2.9691198
H	1.1456790	2.9521741	-1.5190405
H	-0.6239187	2.7451322	-1.6751212
H	-0.4860260	0.4492383	-4.6858469
H	-0.5641865	2.2126982	-4.5987763
H	-1.5928521	1.2196353	-3.5280440

Combination of torsional angles = 0

E(BP86/def2-TZVP) = -3822.37680712235

Ni	-0.9594058	-0.3249827	0.0000485
Cl	-2.4068941	-0.8280499	-1.6025861
Cl	-2.4140998	-0.8071168	1.6025722
C	2.1027347	0.4014545	0.7044249
C	1.9131066	0.9608175	-0.7044953
P	0.4632464	0.1691228	1.5853244
P	0.4701573	0.1483415	-1.5853100

C	0.9671368	-1.1576222	2.9091210
C	1.2823611	-2.4580537	2.1452783
C	-0.1292954	-1.5129153	3.9315951
C	2.2241484	-0.6958037	3.6724066
C	0.0777482	1.8658875	2.4346494
C	-0.6779764	1.6852519	3.7622405
C	-0.8433970	2.6487263	1.4825355
C	1.3518403	2.6917312	2.6854236
C	1.1957015	-1.4329375	-2.4350314
C	2.7092514	-1.3136455	-2.6863392
C	0.9408070	-2.6147213	-1.4830074
C	0.4854936	-1.7488187	-3.7624686
C	0.0628136	1.5082495	-2.9087937
C	1.3412921	1.9065789	-3.6721621
C	-0.4779229	2.7319912	-2.1446160
C	-1.0237620	1.1235004	-3.9311934
H	2.7915073	1.0293292	1.2856263
H	2.5563759	-0.5980647	0.6507753
H	1.6655163	2.0301078	-0.6508577
H	2.8416456	0.8810205	-1.2857746
H	0.4118545	-2.8050847	1.5736620
H	1.5371354	-3.2379160	2.8800678
H	2.1423441	-2.3679811	1.4682924
H	-1.0614197	-1.8085415	3.4385532
H	-0.3503104	-0.6976785	4.6259713
H	0.2409170	-2.3614704	4.5299809
H	3.0788409	-0.4878592	3.0147426
H	2.5297100	-1.5022521	4.3584425
H	2.0320666	0.1938329	4.2867778
H	-1.5520515	1.0322252	3.6445431
H	-1.0341170	2.6759087	4.0882675
H	-0.0348662	1.2931281	4.5600526
H	-0.3585756	2.8674689	0.5248180
H	-1.1010298	3.6122586	1.9524575
H	-1.7731628	2.0991990	1.2839386
H	1.8604603	2.9738293	1.7528509
H	2.0752494	2.1793788	3.3335852
H	1.0644629	3.6278886	3.1905807
H	3.0502613	-2.2314383	-3.1918411
H	3.2849017	-1.2284708	-1.7539501
H	2.9716073	-0.4668003	-3.3343827
H	1.3223876	-3.5361100	-1.9531756
H	-0.1313954	-2.7441053	-1.2843133
H	1.4587164	-2.4936134	-0.5252968
H	0.8050248	-2.7518066	-4.0888173
H	0.7574088	-1.0463080	-4.5601975
H	-0.6054408	-1.7619127	-3.6443969
H	1.7299621	1.0838277	-4.2868718
H	2.1462566	2.2612545	-3.0144758
H	1.0931997	2.7327290	-4.3579426
H	-0.7503267	3.5061082	-2.8791634
H	0.2596105	3.1835683	-1.4677361
H	-1.3797891	2.4777564	-1.5727972
H	-0.7032222	0.3424433	-4.6260812
H	-1.2465040	2.0224475	-4.5290308
H	-1.9432348	0.7906085	-3.4381178

Combination of torsional angles = 5
E(BP86/def2-TZVP) = -3822.37778002909

Ni	-1.0128309	0.0247064	-0.0002101
Cl	-2.5431851	-0.0689061	-1.6026705
Cl	-2.5372285	0.1925730	1.6017190
C	2.1078237	-0.3665312	0.6965377
C	2.1234313	0.2618740	-0.6965297
P	0.4916466	-0.0216046	1.5838388
P	0.4923046	-0.0028773	-1.5839866
C	0.4714513	-1.4750407	2.8666210
C	0.3296741	-2.7841822	2.0665291
C	-0.7065224	-1.4467201	3.8587337
C	1.7929149	-1.5039071	3.6593213
C	0.7464108	1.6744991	2.4838697
C	-0.0263493	1.7438925	3.8123883
C	0.1781364	2.7669531	1.5612466
C	2.2330740	1.9722786	2.7488746
C	0.6629096	-1.7096181	-2.4838879
C	2.1331054	-2.0809086	-2.7479961
C	0.0405373	-2.7724884	-1.5615747
C	-0.1117030	-1.7406712	-3.8127722
C	0.5440719	1.4496820	-2.8668427
C	1.8650404	1.4124614	-3.6600719
C	0.4681408	2.7645061	-2.0670565
C	-0.6344412	1.4799398	-3.8582721
H	2.9747532	-0.0379452	1.2854244
H	2.1785227	-1.4599501	0.6134816
H	2.2479399	1.3504698	-0.6135578
H	2.9731708	-0.1091113	-1.2852993
H	-0.5871373	-2.7863638	1.4627949
H	0.2658128	-3.6204054	2.7804029
H	1.1880789	-2.9901399	1.4134587
H	-1.6703225	-1.3982092	3.3406499
H	-0.6560862	-0.6129573	4.5643189
H	-0.6653328	-2.3782712	4.4466919
H	2.6802864	-1.5827169	3.0165980
H	1.7860754	-2.3892852	4.3154139
H	1.9079438	-0.6243252	4.3063254
H	-1.0805782	1.4698357	3.6804860
H	0.0133532	2.7841175	4.1743499
H	0.4202973	1.1126426	4.5908636
H	0.7157773	2.8237161	0.6082042
H	0.2858402	3.7434092	2.0616537
H	-0.8864156	2.5982505	1.3520846
H	2.8122212	2.0811646	1.8211541
H	2.7192938	1.2117964	3.3742879
H	2.3032607	2.9320196	3.2856014
H	2.1558602	-3.0431562	-3.2843493
H	2.7056289	-2.2181115	-1.8198977
H	2.6568415	-1.3457072	-3.3733490
H	0.0996807	-3.7530254	-2.0620991
H	-1.0143804	-2.5510006	-1.3528548
H	0.5742303	-2.8560737	-0.6083197
H	-0.1231860	-2.7815617	-4.1748396
H	0.3657829	-1.1321485	-4.5910235
H	-1.1511805	-1.4150329	-3.6811552
H	1.9359524	0.5280785	-4.3068523
H	2.7554373	1.4471405	-3.0176072
H	1.9021295	2.2969304	-4.3163762
H	0.4451241	3.6026603	-2.7811485
H	1.3363471	2.9278775	-1.4148703
H	-0.4468684	2.8123389	-1.4624457
H	-0.6267514	0.6440495	-4.5631030

H -0.5466278 2.4076947 -4.4471113
H -1.5990954 1.4805928 -3.3395209

Combination of torsional angles = 10
E(BP86/def2-TZVP) = -3822.37847871941
Ni -1.0106477 0.0405860 0.0000262
Cl -2.5431051 -0.1549901 -1.5912456
Cl -2.5225095 0.3585949 1.5912609
C 2.1001899 -0.4159651 0.6898112
C 2.1270366 0.2442417 -0.6892733
P 0.4927368 -0.0442000 1.5818794
P 0.4949732 0.0036410 -1.5816420
C 0.4073303 -1.5239034 2.8273738
C 0.2530125 -2.8119023 1.9958610
C -0.7978968 -1.4813455 3.7852223
C 1.7069606 -1.6060336 3.6513657
C 0.8063877 1.6182029 2.5263847
C 0.0227174 1.6875146 3.8488303
C 0.2959953 2.7563615 1.6255925
C 2.3010439 1.8479026 2.8148677
C 0.6729106 -1.6788946 -2.5260469
C 2.1442015 -2.0297232 -2.8127434
C 0.0702490 -2.7717080 -1.6260837
C -0.1123169 -1.6841642 -3.8493781
C 0.5299804 1.4851554 -2.8274753
C 1.8320526 1.4612604 -3.6514555
C 0.4808083 2.7817750 -1.9964460
C -0.6749534 1.5402211 -3.7851004
H 2.9753703 -0.1221172 1.2846936
H 2.1433581 -1.5085601 0.5819851
H 2.2581973 1.3297806 -0.5815527
H 2.9757600 -0.1193392 -1.2839866
H -0.6402330 -2.7737272 1.3587992
H 0.1366747 -3.6591480 2.6897926
H 1.1280988 -3.0322074 1.3703456
H -1.7450326 -1.4027748 3.2402787
H -0.7505647 -0.6572336 4.5023047
H -0.7963457 -2.4210966 4.3614178
H 2.6075295 -1.6849350 3.0268826
H 1.6653201 -2.5106700 4.2793057
H 1.8254417 -0.7492277 4.3273830
H -1.0417191 1.4692135 3.6976605
H 0.1092513 2.7139168 4.2409156
H 0.4289630 1.0135211 4.6135515
H 0.8507572 2.8166850 0.6823909
H 0.4354230 3.7140996 2.1534336
H -0.7711222 2.6357369 1.3978587
H 2.8941290 1.9619783 1.8966869
H 2.7502870 1.0507491 3.4218488
H 2.4026316 2.7877444 3.3809547
H 2.1695449 -2.9750242 -3.3783013
H 2.7250121 -2.1912700 -1.8938122
H 2.6575755 -1.2720748 -3.4194924
H 0.1312361 -3.7374665 -2.1542102
H -0.9836150 -2.5641485 -1.3992613
H 0.6173772 -2.8776006 -0.6824556
H -0.1090222 -2.7141857 -4.2415320
H 0.3480521 -1.0453588 -4.6135958
H -1.1556741 -1.3802369 -3.6992047
H 1.8809591 0.5972418 -4.3269059
H 2.7359794 1.4674137 -3.0268385
H 1.8638888 2.3659027 -4.2799775
H 0.4335368 3.6353915 -2.6907044
H 1.3709751 2.9306003 -1.3710832
H -0.4125258 2.8164746 -1.3592570
H -0.6946905 0.7149655 -4.5021532
H -0.5974526 2.4767365 -4.3613357
H -1.6251834 1.5385808 -3.2398725

Combination of torsional angles = 15
E(BP86/def2-TZVP) = -3822.37889234840
Ni -1.0062806 -0.0072972 0.0000692
Cl -2.5220117 -0.4020944 -1.5701541
Cl -2.5277870 0.3652365 1.5701418
C 2.1211663 -0.3308451 0.6824759
C 2.1162513 0.3613976 -0.6822001
P 0.5007619 -0.0352043 1.5790802
P 0.5002801 0.0425400 -1.5788528
C 0.4403460 -1.5452610 2.7845476
C 0.3500166 -2.8174920 1.9199593
C -0.7927040 -1.5592975 3.7069552
C 1.7211040 -1.6062485 3.6388728
C 0.7673651 1.6091474 2.5695282
C -0.0350188 1.6286551 3.8827163
C 0.2476712 2.7607924 1.6916020
C 2.2530544 1.8616523 2.8855069
C 0.7905977 -1.5977410 -2.5693609
C 2.2797612 -1.8287599 -2.8854335
C 0.2876582 -2.7567830 -1.6914082
C -0.0114816 -1.6287867 -3.8825149
C 0.4181203 1.5516046 -2.7842670
C 1.6977924 1.6309295 -3.6387020
C 0.3096646 2.8224373 -1.9197199
C -0.8150842 1.5479506 -3.7065599
H 2.9851315 -0.0159898 1.2828603
H 2.2064146 -1.4182055 0.5504847
H 2.1859857 1.4498640 -0.5502026
H 2.9846393 0.0588971 -1.2825476
H -0.5211048 -2.7896459 1.2522635
H 0.2340082 -3.6832401 2.5906729
H 1.2520609 -2.9984470 1.3208110
H -1.7259747 -1.4962553 3.1360794
H -0.7918499 -0.7489764 4.4412103
H -0.7807686 -2.5106605 4.2635057
H 2.6380968 -1.6336100 3.0337922
H 1.6979166 -2.5308591 4.2380448
H 1.7928254 -0.7669575 4.3426471
H -1.0935784 1.3986813 3.7101234
H 0.0306355 2.6446905 4.3047911
H 0.3712278 0.9395312 4.6338249
H 0.8173404 2.8593267 0.7603295
H 0.3582954 3.7060668 2.2478296
H -0.8127500 2.6238935 1.4433485
H 2.8550046 2.0190963 1.9796257
H 2.7126408 1.0557138 3.4726716
H 2.3258035 2.7848066 3.4826380
H 2.3657735 -2.7507077 -3.4826624
H 2.8839605 -1.9776103 -1.9795987
H 2.7276609 -1.0162335 -3.4725472
H 0.4119320 -3.7003604 -2.2476335

H	-0.7746116	-2.6352300	-1.4431055
H	0.8587394	-2.8470528	-0.7601601
H	0.0688393	-2.6437400	-4.3046511
H	0.3847263	-0.9338137	-4.6336039
H	-1.0732487	-1.4141461	-3.7098648
H	1.7814598	0.7927556	-4.3424805
H	2.6143523	1.6714271	-3.0336994
H	1.6613144	2.5551187	-4.2378599
H	0.1812894	3.6864214	-2.5904577
H	1.2090490	3.0162761	-1.3206091
H	-0.5609616	2.7822027	-1.2520122
H	-0.8027324	0.7376519	-4.4407381
H	-0.8168015	2.4993374	-4.2631987
H	-1.7473155	1.4716301	-3.1356060

Combination of torsional angles = 20

E(BP86/def2-TZVP) = -3822.37894827374

Ni	-1.0002423	-0.0350623	0.0002175
Cl	-2.4960258	-0.5895769	-1.5399300
Cl	-2.5306232	0.4122081	1.5414405
C	2.1354777	-0.2884848	0.6729193
C	2.1094595	0.4396221	-0.6739943
P	0.5099107	-0.0452446	1.5750181
P	0.5047028	0.0820986	-1.5753842
C	0.4440001	-1.5918580	2.7281757
C	0.3905384	-2.8367209	1.8217474
C	-0.8156849	-1.6416599	3.6125442
C	1.7026858	-1.6680111	3.6129131
C	0.7605945	1.5660860	2.6223625
C	-0.0659330	1.5438586	3.9207596
C	0.2599978	2.7473617	1.7732782
C	2.2404625	1.8061185	2.9745818
C	0.8685371	-1.5071842	-2.6231783
C	2.3613571	-1.6412640	-2.9770943
C	0.4542765	-2.7211500	-1.7736836
C	0.0411954	-1.5437800	-3.9207373
C	0.3286892	1.6203330	-2.7281483
C	1.5786309	1.7861992	-3.6129703
C	0.1867968	2.8578705	-1.8212606
C	-0.9313692	1.5805864	-3.6125071
H	2.9934860	0.0297026	1.2799222
H	2.2437343	-1.3699059	0.5127305
H	2.1414685	1.5259869	-0.5138287
H	2.9874171	0.1825813	-1.2814122
H	-0.4582346	-2.7937887	1.1264578
H	0.2597172	-3.7238722	2.4610102
H	1.3129410	-2.9917730	1.2469258
H	-1.7324992	-1.5633851	3.0167785
H	-0.8410038	-0.8550410	4.3718238
H	-0.8167047	-2.6105005	4.1380394
H	2.6344659	-1.6600627	3.0298363
H	1.6781558	-2.6150349	4.1759770
H	1.7452149	-0.8550782	4.3490778
H	-1.1217075	1.3238350	3.7208292
H	-0.0045872	2.5446829	4.3783868
H	0.3243754	0.8281387	4.6552689
H	0.8494926	2.8767915	0.8578936
H	0.3605723	3.6730592	2.3631952
H	-0.7953321	2.6203714	1.4998748
H	2.8578036	2.0013064	2.0866500
H	2.6912940	0.9777979	3.5366372
H	2.3008985	2.7044966	3.6096821
H	2.4847884	-2.5329075	-3.6125570
H	2.9920646	-1.7923138	-2.0899414
H	2.7515090	-0.7828526	-3.5393892
H	0.6195073	-3.6373176	-2.3639112
H	-0.6069909	-2.6694150	-1.4987540
H	1.0529149	-2.8085788	-0.8592063
H	0.1728537	-2.5378009	-4.3783500
H	0.3791585	-0.8023255	-4.6556959
H	-1.0273466	-1.3990346	-3.7198671
H	1.6786390	0.9787204	-4.3495547
H	2.5087449	1.8442167	-3.0300456
H	1.4868202	2.7293786	-4.1755403
H	-0.0069544	3.7337150	-2.4601389
H	1.0958595	3.0779508	-1.2464636
H	-0.6567311	2.7543441	-1.1259621
H	-0.9003171	0.7947910	-4.3724533
H	-1.0017484	2.5472658	-4.1372634
H	-1.8402717	1.4364156	-3.0169042

Combination of torsional angles = 25

E(BP86/def2-TZVP) = -3822.37856386406

Ni	-0.9973787	0.0157618	-0.0002041
Cl	-2.5160678	-0.5784290	-1.5019884
Cl	-2.4963855	0.6589212	1.5012017
C	2.1214149	-0.4162897	0.6649124
C	2.1340328	0.3454988	-0.6647974
P	0.5112638	-0.0983762	1.5704739
P	0.5144840	0.0805775	-1.5705890
C	0.3129335	-1.6697211	2.6694451
C	0.1973913	-2.8792758	1.7220994
C	-0.9746812	-1.6488267	3.5141275
C	1.5366128	-1.8638941	3.5840568
C	0.8689295	1.4538050	2.6739352
C	0.0099942	1.4605453	3.9515786
C	0.4909018	2.6985147	1.8524937
C	2.3540756	1.5593320	3.0686476
C	0.8212819	-1.4824678	-2.6741151
C	2.3022952	-1.6367603	-3.0682512
C	0.4022362	-2.7142233	-1.8530475
C	-0.0369553	-1.4607163	-3.9520668
C	0.3680267	1.6575238	-2.6697260
C	1.5972206	1.8108579	-3.5847173
C	0.2929587	2.8705242	-1.7227253
C	-0.9198668	1.6791611	-3.5139490
H	2.9953938	-0.1607018	1.2785436
H	2.1691475	-1.4978555	0.4788788
H	2.2171121	1.4249272	-0.4787739
H	2.9993041	0.0614401	-1.2782599
H	-0.6239058	-2.7534719	1.0040185
H	-0.0165482	-3.7733863	2.3283991
H	1.1236302	-3.0827921	1.1690961
H	-1.8634490	-1.4770353	2.8952881
H	-0.9620464	-0.8881729	4.2998617
H	-1.0704866	-2.6313466	4.0040719
H	2.4829501	-1.8990201	3.0255118
H	1.4321560	-2.8267906	4.1098721
H	1.6132345	-1.0828245	4.3511516
H	-1.0547821	1.3349021	3.7202332

H	0.1416667	2.4383406	4.4429415
H	0.3215570	0.6928946	4.6711548
H	1.1135259	2.8064274	0.9559364
H	0.6536175	3.5937954	2.4745248
H	-0.5640541	2.6692130	1.5515905
H	3.0072385	1.7397600	2.2035759
H	2.7237408	0.6762918	3.6058077
H	2.4692096	2.4243764	3.7413600
H	2.3891698	-2.5050930	-3.7409755
H	2.9487764	-1.8386243	-2.2029113
H	2.7010619	-0.7663547	-3.6052188
H	0.5355935	-3.6142181	-2.4752584
H	-0.6512770	-2.6503259	-1.5524564
H	1.0207027	-2.8427469	-0.9563451
H	0.0628181	-2.4421378	-4.4437087
H	0.2997758	-0.7034248	-4.6712683
H	-1.0971239	-1.3003814	-3.7210193
H	1.6478628	1.0274106	-4.3515311
H	2.5443158	1.8149343	-3.0263736
H	1.5244515	2.7764933	-4.1108416
H	0.1089067	3.7711037	-2.3292647
H	1.2255194	3.0432480	-1.1698359
H	-0.5320382	2.7724095	-1.0045650
H	-0.9329111	0.9181340	-4.2993047
H	-0.9830667	2.6641127	-4.0043027
H	-1.8136216	1.5373862	-2.8946886

Combination of torsional angles = 30

E(BP86/def2-TZVP) = -3822.37783707938

Ni	-0.9874784	0.0433153	-0.0009324
Cl	-2.5227009	-0.6311764	-1.4504232
Cl	-2.4560766	0.8561876	1.4466405
C	2.1189558	-0.4915714	0.6599173
C	2.1556635	0.2908477	-0.6585745
P	0.5177471	-0.1335259	1.5652762
P	0.5292867	0.0812042	-1.5655034
C	0.2207160	-1.7192273	2.6163887
C	0.0777914	-2.8991224	1.6361175
C	-1.0930767	-1.6485706	3.4175028
C	1.4030784	-1.9947889	3.5631739
C	0.9371791	1.3669507	2.7161425
C	0.0414284	1.3950475	3.9681722
C	0.6602021	2.6516406	1.9160610
C	2.4136289	1.3733651	3.1560486
C	0.8110076	-1.4511990	-2.7162351
C	2.2810912	-1.5924435	-3.1547164
C	0.4170683	-2.7052858	-1.9166975
C	-0.0822840	-1.3970535	-3.9691774
C	0.3796809	1.6874700	-2.6166692
C	1.5828127	1.8534313	-3.5628708
C	0.3453129	2.8753381	-1.6362458
C	-0.9346458	1.7379167	-3.4183720
H	2.9989628	-0.2718484	1.2787246
H	2.1338372	-1.5710561	0.4575701
H	2.2693764	1.3644666	-0.4563174
H	3.0124987	-0.0087149	-1.2764106
H	-0.7150335	-2.7180131	0.8979214
H	-0.1948281	-3.7963144	2.2136847
H	1.0098790	-3.1316815	1.1048283
H	-1.9491337	-1.4108921	2.7742516
H	-1.0659011	-0.9102237	4.2239933
H	-1.2617535	-2.6363077	3.8760494
H	2.3643192	-2.0578921	3.0328694
H	1.2383973	-2.9662678	4.0568670
H	1.4902900	-1.2397918	4.3547606
H	-1.0213624	1.3379648	3.7029229
H	0.2148983	2.3517120	4.4873892
H	0.2859280	0.5939520	4.6771681
H	1.3130864	2.7413647	1.0387744
H	0.8618680	3.5200579	2.5641713
H	-0.3861767	2.6957163	1.5885202
H	3.1015529	1.5442013	2.3163958
H	2.7170438	0.4540190	3.6730831
H	2.5570885	2.2084523	3.8604421
H	2.3483105	-2.4369474	-3.8592907
H	2.9496165	-1.8256722	-2.3144496
H	2.6677986	-0.7045734	-3.6711784
H	0.5392190	-3.5884299	-2.5647549
H	-0.6292814	-2.6537264	-1.5901882
H	1.0582473	-2.8543081	-1.0388395
H	0.0037656	-2.3652933	-4.4887548
H	0.2349789	-0.6212080	-4.6774156
H	-1.1357470	-1.2433762	-3.7049880
H	1.6006336	1.0937739	-4.3545646
H	2.5455194	1.8278846	-3.0320880
H	1.5082727	2.8360460	-4.0563455
H	0.1561058	3.7938887	-2.2135919
H	1.2947308	3.0214293	-1.1047737
H	-0.4609025	2.7674787	-0.8981771
H	-0.9754096	0.9997141	-4.2244133
H	-1.0112249	2.7367647	-3.8774775
H	-1.8092536	1.5806158	-2.7754180

Combination of torsional angles = 35

E(BP86/def2-TZVP) = -3822.37664129003

Ni	-0.9778205	0.0070400	-0.0002646
Cl	-2.4815375	-0.8528848	-1.3824442
Cl	-2.4689695	0.8892922	1.3814266
C	2.1512688	-0.4156735	0.6557065
C	2.1576067	0.3825043	-0.6549370
P	0.5356881	-0.1284869	1.5595984
P	0.5382333	0.1198404	-1.5594880
C	0.2517131	-1.7429336	2.5666457
C	0.1696248	-2.9060122	1.5599075
C	-1.0921077	-1.7114347	3.3197893
C	1.4062112	-2.0116673	3.5484993
C	0.9088287	1.3495510	2.7525262
C	-0.0282681	1.3439685	3.9743811
C	0.6474669	2.6483510	1.9699227
C	2.3704502	1.3591612	3.2400726
C	0.8895492	-1.3635518	-2.7523496
C	2.3510220	-1.3950830	-3.2394111
C	0.6084440	-2.6582651	-1.9698312
C	-0.0469332	-1.3438575	-3.9745330
C	0.2790176	1.7384095	-2.5665546
C	1.4376021	1.9896674	-3.5482253
C	0.2144416	2.9025658	-1.5597975
C	-1.0650168	1.7272492	-3.3198851
H	3.0203405	-0.1666668	1.2788459
H	2.2102005	-1.4914654	0.4424168

H	2.2327911	1.4572901	-0.4416530
H	3.0230674	0.1203349	-1.2777037
H	-0.6065258	-2.7312991	0.8025820
H	-0.0947463	-3.8214850	2.1121520
H	1.1228584	-3.1022215	1.0518056
H	-1.9286298	-1.4777929	2.6494506
H	-1.1085104	-0.9874109	4.1395532
H	-1.2603918	-2.7102202	3.7536771
H	2.3865121	-2.0381381	3.0506537
H	1.2493903	-2.9988260	4.0128131
H	1.4466431	-1.2743818	4.3601527
H	-1.0811770	1.2819942	3.6727145
H	0.1176247	2.2916103	4.5180413
H	0.2011201	0.5311545	4.6750660
H	1.3239817	2.7586976	1.1126335
H	0.8274614	3.5046656	2.6401074
H	-0.3901004	2.6940097	1.6159727
H	3.0826097	1.5611719	2.4280493
H	2.6687116	0.4296172	3.7411494
H	2.4814419	2.1761717	3.9710580
H	2.4499686	-2.2135904	-3.9704497
H	3.0597909	-1.6078555	-2.4271740
H	2.6633847	-0.4700760	-3.7402945
H	0.7758789	-3.5172144	-2.6398967
H	-0.4298411	-2.6883548	-1.6163200
H	1.2828698	-2.7786751	-1.1122487
H	0.0849435	-2.2935312	-4.5182210
H	0.1948505	-0.5345089	-4.6750684
H	-1.0989081	-1.2661360	-3.6732417
H	1.4669733	1.2519131	-4.3599188
H	2.4181124	2.0012480	-3.0502200
H	1.2958372	2.9791276	-4.0124828
H	-0.0360413	3.8219502	-2.1120178
H	1.1705146	3.0843281	-1.0516476
H	-0.5642907	2.7395741	-0.8025108
H	-1.0922988	1.0034624	-4.1395704
H	-1.2180663	2.7284291	-3.7538944
H	-1.9050801	1.5063873	-2.6496428

Combination of torsional angles = 40
E(BP86/def2-TZVP) = -3822.37490685822

Ni	-0.9683519	0.0013002	-0.0001995
Cl	-2.4605155	-0.9969370	-1.2993460
Cl	-2.4577184	1.0038785	1.2988128
C	2.1694624	-0.4050164	0.6540858
C	2.1706949	0.3984600	-0.6542155
P	0.5483882	-0.1374170	1.5531402
P	0.5489226	0.1355928	-1.5534073
C	0.2317005	-1.7667807	2.5240194
C	0.1874512	-2.9181805	1.5019553
C	-1.1435129	-1.7338234	3.2192275
C	1.3432206	-2.0524030	3.5492528
C	0.9157039	1.3118249	2.7801961
C	-0.0666687	1.3091097	3.9660866
C	0.7117930	2.6272936	2.0080977
C	2.3590141	1.2824321	3.3194034
C	0.9121300	-1.3147228	-2.7804111
C	2.3555652	-1.2895285	-3.3194973
C	0.7043389	-2.6295737	-2.0082949
C	-0.0701278	-1.3091823	-3.9663874
C	0.2370686	1.7658695	-2.5243165
C	1.3495194	2.0482692	-3.5494333
C	0.1960603	2.9173815	-1.5022452
C	-1.1381618	1.7369104	-3.2196684
H	3.0330869	-0.1473918	1.2813310
H	2.2419035	-1.4792411	0.4376399
H	2.2462630	1.4724710	-0.4377710
H	3.0336176	0.1383102	-1.2813838
H	-0.5639349	-2.7370776	0.7216447
H	-0.0926031	-3.8402110	2.0353498
H	1.1582157	-3.1060353	1.0244679
H	-1.9500532	-1.4988292	2.5132103
H	-1.1943000	-1.0100029	4.0379018
H	-1.3335296	-2.7326233	3.6438789
H	2.3434050	-2.0721689	3.0920891
H	1.1662580	-3.0470995	3.9896519
H	1.3502060	-1.3290845	4.3741601
H	-1.1087391	1.2750380	3.6241216
H	0.0782468	2.2452834	4.5295016
H	0.1184872	0.4812692	4.6622756
H	1.4156925	2.7312635	1.1718662
H	0.8952628	3.4694496	2.6950602
H	-0.3139645	2.7052904	1.6267202
H	3.1033814	1.4847541	2.5369140
H	2.6217292	0.3388390	3.8133725
H	2.4598560	2.0842982	4.0684503
H	2.4541395	-2.0916857	-4.0685335
H	3.0992757	-1.4940099	-2.5369447
H	2.6210635	-0.3467039	-3.8134472
H	0.8854239	-3.4722788	-2.6952161
H	-0.3216723	-2.7045813	-1.6270006
H	1.4078611	-2.7355589	-1.1719992
H	0.0721118	-2.2457894	-4.5297627
H	0.1175003	-0.4819039	-4.6625843
H	-1.1121248	-1.2720647	-3.6245170
H	1.3544912	1.3249350	-4.3743406
H	2.3497094	2.0651338	-3.0921650
H	1.1754896	3.0434766	-3.9898473
H	-0.0812372	3.8402328	-2.0356605
H	1.1673134	3.1023916	-1.0246411
H	-0.5559409	2.7384639	-0.7220227
H	-1.1909534	1.0132679	-4.0383742
H	-1.3252466	2.7362687	-3.6443068
H	-1.9454526	1.5042252	-2.5137445

Relaxed potential surface scan of P structure of NiBr2dtbpe

Combination of torsional angles = -40
E(BP86/def2-TZVP) = -8050.73856872186

Br	2.2115189	-1.3996366	0.9383717
Br	2.2115021	1.3996445	-0.9384300
Ni	0.5534552	0.0000030	-0.0000157
P	-0.9811543	1.5643061	0.2356298
P	-0.9811606	-1.5642978	-0.2356376
C	-2.5911650	-0.6350106	-0.4296512
H	-2.6797502	-0.3739747	-1.4922323
H	-3.4516188	-1.2761644	-0.1869232

C	-2.5911584	0.6350225	0.4296617
H	-2.6797318	0.3739863	1.4922438
H	-3.4516136	1.2761782	0.1869441
C	-1.4561313	2.9104927	-1.0753132
C	-2.0122552	2.1640784	-2.3031694
H	-2.9595521	1.6471045	-2.0972344
H	-1.2847805	1.4444758	-2.6999768
H	-2.2124735	2.9016285	-3.0962517
C	-0.2564725	3.7468436	-1.5535162
H	-0.6210333	4.4530514	-2.3181189
H	0.5279777	3.1205956	-1.9918108
H	0.2011680	4.3345632	-0.7508171
C	-2.5434562	3.8696875	-0.5551719
H	-2.1529861	4.5636924	0.1991941
H	-3.4216639	3.3571641	-0.1382509
H	-2.8957181	4.4800132	-1.4026554
C	-0.6676808	2.3900040	1.9456042
C	0.3550154	3.5303766	1.8015145
H	-0.0740321	4.4124242	1.3089204
H	1.2476393	3.2121273	1.2443612
H	0.6756423	3.8413555	2.8084676
C	-0.0604887	1.3109133	2.8627963
H	0.1785575	1.7745373	3.8338145
H	0.8618371	0.8784590	2.4510079
H	-0.7650337	0.4915124	3.0583094
C	-1.9522123	2.9157730	2.6140605
H	-1.6839472	3.3020541	3.6107130
H	-2.7003813	2.1260216	2.7689438
H	-2.4248614	3.7350426	2.0624048
C	-0.6677120	-2.3900130	-1.9456089
C	0.3549802	-3.5303895	-1.8015228
H	0.6755939	-3.8413772	-2.8084773
H	-0.0740659	-4.4124314	-1.3089174
H	1.2476122	-3.2121404	-1.2443822
C	-0.0605261	-1.3109346	-2.8628195
H	0.1785066	-1.7745700	-3.8338357
H	0.8618065	-0.8784799	-2.4510467
H	-0.7650700	-0.4915332	-3.0583330
C	-1.9522544	-2.9157817	-2.6140446
H	-2.7004216	-2.1260280	-2.7689256
H	-2.4249005	-3.7350443	-2.0623759
H	-1.6840036	-3.3020728	-3.6106971
C	-1.4561330	-2.9104662	1.0753254
C	-2.0122389	-2.1640303	2.3031767
H	-2.9595329	-1.6470503	2.0972429
H	-1.2847542	-1.4444287	2.6999678
H	-2.2124569	-2.9015677	3.0962708
C	-2.5434711	-3.8696583	0.5552070
H	-2.8957299	-4.4799703	1.4027017
H	-2.1530144	-4.5636761	-0.1991540
H	-3.4216786	-3.3571327	0.1382881
C	-0.2564764	-3.7468203	1.5535285
H	0.5279824	-3.1205731	1.9918086
H	0.2011526	-4.3345536	0.7508330
H	-0.6210363	-4.4530157	2.3181431

Combination of torsional angles = -35

E(BP86/def2-TZVP) = -8050.74075155264

Br	2.2157702	-1.4745641	0.8126452
Br	2.2157648	1.4745594	-0.8126745
Ni	0.5555817	-0.0000013	-0.0000070
P	-0.9746104	1.5679896	0.2141602
P	-0.9746132	-1.5679912	-0.2141594
C	-2.5832834	-0.6392628	-0.4230242
H	-2.6684349	-0.3888648	-1.4881181
H	-3.4456796	-1.2765020	-0.1767385
C	-2.5832786	0.6392619	0.4230420
H	-2.6684185	0.3888639	1.4881368
H	-3.4456772	1.2765016	0.1767656
C	-1.4566747	2.8865367	-1.1221937
C	-2.0339120	2.1218722	-2.3290647
H	-2.9851705	1.6208419	-2.1035554
H	-1.3199825	1.3851312	-2.7194956
H	-2.2330613	2.8457507	-3.1348976
C	-0.2600402	3.7077254	-1.6324490
H	-0.6350797	4.4122346	-2.3936514
H	0.5077235	3.0709391	-2.0841853
H	0.2236559	4.2942183	-0.8444257
C	-2.5335067	3.8592709	-0.6049802
H	-2.1354831	4.5559008	0.1429709
H	-3.4135514	3.3557108	-0.1810856
H	-2.8850650	4.4653531	-1.4557644
C	-0.6693558	2.4277331	1.9097856
C	0.3081394	3.6044969	1.7464770
H	-0.1528958	4.4610288	1.2378295
H	1.2130996	3.3092621	1.1969055
H	0.6136281	3.9447413	2.7487732
C	-0.0103473	1.3797170	2.8278305
H	0.2161889	1.8565585	3.7955260
H	0.9269824	0.9882801	2.4090647
H	-0.6757702	0.5299543	3.0307312
C	-1.9648385	2.9140568	2.5870824
H	-1.6976544	3.3397586	3.5677953
H	-2.6745077	2.0970892	2.7769377
H	-2.4826301	3.6961276	2.0214818
C	-0.6693737	-2.4277370	-1.9097872
C	0.3081234	-3.6045004	-1.7464866
H	0.6136041	-3.9447444	-2.7487853
H	-0.1529073	-4.4610325	-1.2378356
H	1.2130879	-3.3092652	-1.1969224
C	-0.0103723	-1.3797221	-2.8278384
H	0.2161569	-1.8565650	-3.7955349
H	0.9269602	-0.9882841	-2.4090800
H	-0.6757971	-0.5299601	-3.0307356
C	-1.9648616	-2.9140606	-2.5870740
H	-2.6745328	-2.0970932	-2.7769229
H	-2.4826484	-3.6961320	-2.0214700
H	-1.6976853	-3.3397615	-3.5677894
C	-1.4566643	-2.8865340	1.1222035
C	-2.0338864	-2.1218643	2.3290785
H	-2.9851464	-1.6208326	2.1035782
H	-1.3199508	-1.3851236	2.7194988
H	-2.2330282	-2.8457397	3.1349159
C	-2.5335039	-3.8592685	0.6050062
H	-2.8850536	-4.4653467	1.4557968
H	-2.1354898	-4.5559023	-0.1429464
H	-3.4135526	-3.3557088	0.1811194
C	-0.2600256	-3.7077229	1.6324492
H	0.5077430	-3.0709364	2.0841768
H	0.2236624	-4.2942181	0.8444227

H -0.6350585 -4.4122301 2.3936567

Combination of torsional angles = -30
E(BP86/def2-TZVP) = -8050.74247546104
Br 2.2225747 -1.5333927 0.6891057
Br 2.2225548 1.5333786 -0.6892421
Ni 0.5579148 -0.0000004 -0.0000333
P -0.9693730 1.5732739 0.1886688
P -0.9693803 -1.5732769 -0.1886682
C -2.5780250 -0.6468528 -0.4107429
H -2.6643448 -0.4161017 -1.4799118
H -3.4406038 -1.2791391 -0.1524904
C -2.5780101 0.6468494 0.4107972
H -2.6642940 0.4160979 1.4799688
H -3.4405975 1.2791357 0.1525743
C -1.4469022 2.8564276 -1.1829416
C -2.0222106 2.0647190 -2.3731429
H -2.9757717 1.5722685 -2.1389105
H -1.3097749 1.3163291 -2.7437358
H -2.2163803 2.7697001 -3.1967517
C -0.2485493 3.6645296 -1.7092279
H -0.6218907 4.3539306 -2.4849948
H 0.5177465 3.0172113 -2.1481809
H 0.2372638 4.2647464 -0.9330191
C -2.5258840 3.8401881 -0.6912865
H -2.1348332 4.5476060 0.0500708
H -3.4109366 3.3442202 -0.2688818
H -2.8682377 4.4332524 -1.5548725
C -0.6870111 2.4761136 1.8675403
C 0.2538507 3.6803194 1.6895657
H -0.2274124 4.5110435 1.1573767
H 1.1741353 3.4013072 1.1579241
H 0.5348923 4.0509856 2.6883217
C 0.0026114 1.4629180 2.8022440
H 0.2090454 1.9586573 3.7649477
H 0.9544636 1.1009161 2.3901872
H -0.6338225 0.5929736 3.0126443
C -1.9973510 2.9368499 2.5346538
H -1.7424480 3.4038247 3.4996748
H -2.6770127 2.1022942 2.7544375
H -2.5444176 3.6813966 1.9459033
C -0.6870786 -2.4761365 -1.8675394
C 0.2537913 -3.6803385 -1.6895817
H 0.5347963 -4.0510205 -2.6883422
H -0.2274510 -4.5110547 -1.1573613
H 1.1740953 -3.4013165 -1.1579781
C 0.0025089 -1.4629523 -2.8022811
H 0.2089091 -1.9587047 -3.7649851
H 0.9543753 -1.1009438 -2.3902630
H -0.6339339 -0.5930116 -3.0126702
C -1.9974421 -2.9368834 -2.5345996
H -2.6771086 -2.1023302 -2.7543783
H -2.5444911 -3.6814160 -1.9458150
H -1.7425725 -3.4038795 -3.4996192
C -1.4468512 -2.8564158 1.1829796
C -2.0221190 -2.0646929 2.3731911
H -2.9756932 -1.5722539 2.1389878
H -1.3096745 -1.3162913 2.7437440
H -2.2162508 -2.7696623 3.1968191
C -2.5258462 -3.8401926 0.6913852
H -2.8681653 -4.4332392 1.5549973
H -2.1348195 -4.5476253 -0.0499710
H -3.4109168 -3.3442381 0.2690023
C -0.2484696 -3.6644977 1.7092314
H 0.5178437 -3.0171630 2.1481312
H 0.2373105 -4.2647327 0.9330153
H -0.6217707 -4.3538800 2.4850343

Combination of torsional angles = -25
E(BP86/def2-TZVP) = -8050.74385551872
Br 2.2273256 -1.5798353 0.5676335
Br 2.2273628 1.5798267 -0.5674897
Ni 0.5585112 0.0000014 0.0000332
P -0.9662198 1.5789458 0.1615757
P -0.9662212 -1.5789340 -0.1615765
C -2.5758558 -0.6561852 -0.3951028
H -2.6664994 -0.4505133 -1.4687938
H -3.4372626 -1.2828214 -0.1195750
C -2.5758673 0.6562037 0.3950448
H -2.6665502 0.4505317 1.4687327
H -3.4372618 1.2828434 0.1194864
C -1.4294493 2.8188220 -1.2535653
C -1.9900603 1.9932169 -2.4274587
H -2.9468529 1.5082961 -2.1908436
H -1.2738196 1.2338894 -2.7670855
H -2.1734032 2.6739873 -3.2736114
C -0.2248397 3.6119338 -1.7878793
H -0.5882877 4.2780773 -2.5882660
H 0.5468005 2.9525781 -2.1988100
H 0.2517686 4.2339071 -1.0232352
C -2.5163886 3.8140021 -0.8039149
H -2.1402115 4.5380611 -0.0711433
H -3.4090865 3.3266635 -0.3875781
H -2.8429572 4.3870721 -1.6868736
C -0.7164926 2.5341940 1.8186120
C 0.1917384 3.7608399 1.6239356
H -0.3027337 4.5628212 1.0607575
H 1.1294186 3.4938900 1.1180144
H 0.4417307 4.1659835 2.6176330
C -0.0082071 1.5623372 2.7826311
H 0.1723560 2.0835609 3.7370201
H 0.9584605 1.2229672 2.3867595
H -0.6207098 0.6780256 3.0040897
C -2.0447661 2.9775490 2.4624795
H -1.8094984 3.4903719 3.4089739
H -2.6986678 2.1314263 2.7131100
H -2.6123508 3.6806588 1.8425809
C -0.7164418 -2.5341711 -1.8186105
C 0.1917724 -3.7608256 -1.6239105
H 0.4417955 -4.1659648 -2.6176019
H -0.3027260 -4.5628065 -1.0607545
H 1.1294373 -3.4938868 -1.1179553
C -0.0081175 -1.5623126 -2.7826000
H 0.1724709 -2.0835302 -3.7369877
H 0.9585408 -1.2229542 -2.3866957
H -0.6206055 -0.6779942 -3.0040705
C -2.0446974 -2.9775138 -2.4625228
H -2.6985870 -2.1313856 -2.7131656
H -2.6123047 -3.6806262 -1.8426470
H -1.8094034 -3.4903297 -3.4090144

C	-1.4295127	-2.8188235	1.2535292
C	-1.9901637	-1.9932307	2.4274126
H	-2.9469419	-1.5082966	2.1907658
H	-1.2739295	-1.2339151	2.7670808
H	-2.1735479	-2.6740124	3.2735470
C	-2.5164400	-3.8139883	0.8038158
H	-2.8430453	-4.3870766	1.6867490
H	-2.1402385	-4.5380325	0.0710417
H	-3.4091194	-3.3266357	0.3874555
C	-0.2249278	-3.6119523	1.7878741
H	0.5467001	-2.9526091	2.1988481
H	0.2517069	-4.2339125	1.0232356
H	-0.5884103	-4.2781103	2.5882329

Combination of torsional angles = -20
E(BP86/def2-TZVP) = -8050.74494530890

Br	2.2301936	-1.6142422	0.4524263
Br	2.2302155	1.6142383	-0.4523181
Ni	0.5582503	0.0000003	0.0000210
P	-0.9639799	1.5849884	0.1290192
P	-0.9639811	-1.5849814	-0.1290437
C	-2.5753554	-0.6674999	-0.3750495
H	-2.6722901	-0.4936203	-1.4536353
H	-3.4346922	-1.2867455	-0.0770812
C	-2.5753703	0.6675146	0.3749467
H	-2.6723581	0.4936357	1.4535278
H	-3.4346897	1.2867644	0.0769368
C	-1.4044775	2.7726132	-1.3362503
C	-1.9410168	1.9063315	-2.4916104
H	-2.9013547	1.4277768	-2.2564306
H	-1.2172176	1.1372977	-2.7906994
H	-2.1093152	2.5571239	-3.3640704
C	-0.1899057	3.5483625	-1.8732956
H	-0.5366918	4.1837457	-2.7054155
H	0.5911706	2.8760957	-2.2437718
H	0.2696447	4.1984194	-1.1217567
C	-2.5025779	3.7792145	-0.9425379
H	-2.1466084	4.5251154	-0.2218697
H	-3.4045643	3.3017509	-0.5348361
H	-2.8082470	4.3253637	-1.8496859
C	-0.7533159	2.6018881	1.7571885
C	0.1274030	3.8450999	1.5405382
H	-0.3737515	4.6152726	0.9402509
H	1.0828022	3.5855373	1.0659110
H	0.3429781	4.2889162	2.5258238
C	-0.0375773	1.6779550	2.7616322
H	0.1143813	2.2316569	3.7025824
H	0.9431602	1.3529964	2.3897061
H	-0.6321276	0.7858400	3.0001417
C	-2.1007950	3.0365038	2.3672817
H	-1.8895239	3.5980636	3.2914496
H	-2.7345450	2.1855186	2.6503495
H	-2.6802439	3.6953723	1.7104896
C	-0.7532397	-2.6018851	-1.7572009
C	0.1274662	-3.8450984	-1.5405060
H	0.3430899	-4.2889153	-2.5257807
H	-0.3737193	-4.6152701	-0.9402436
H	1.0828421	-3.5855371	-1.0658311
C	-0.0374479	-1.6779548	-2.7616088
H	0.1145566	-2.2316575	-3.7025511
H	0.9432717	-1.3529988	-2.3896333
H	-0.6319837	-0.7858381	-3.0001487
C	-2.1006889	-3.0364974	-2.3673630
H	-2.7344219	-2.1855108	-2.6504640
H	-2.6801734	-3.6953640	-1.7106006
H	-1.8893718	-3.5980582	-3.2915198
C	-1.4045551	-2.7725994	1.3362095
C	-1.9411497	-1.9063126	2.4915399
H	-2.9014749	-1.4277567	2.2563110
H	-1.2173637	-1.1372793	2.7906623
H	-2.1094927	-2.5571016	3.3639939
C	-2.5026394	-3.7791994	0.9424492
H	-2.8083540	-4.3253429	1.8495853
H	-2.1466376	-4.5251051	0.2218022
H	-3.4046046	-3.3017348	0.5347017
C	-0.1900125	-3.5483497	1.8733194
H	0.5910469	-2.8760833	2.2438321
H	0.2695742	-4.1984109	1.1218064
H	-0.5368420	-4.1837284	2.7054247

Combination of torsional angles = -15
E(BP86/def2-TZVP) = -8050.74570825355

Br	2.2372330	-1.6400899	0.3368437
Br	2.2372237	1.6400856	-0.3369112
Ni	0.5615980	-0.0000035	-0.0000162
P	-0.9597546	1.5902103	0.0978674
P	-0.9597516	-1.5902216	-0.0978667
C	-2.5734862	-0.6787105	-0.3535513
H	-2.6785954	-0.5383526	-1.4361616
H	-3.4297539	-1.2899791	-0.0310843
C	-2.5734811	0.6786939	0.3535850
H	-2.6785676	0.5383360	1.4361975
H	-3.4297573	1.2899602	0.0311354
C	-1.3701779	2.7229111	-1.4174540
C	-1.8747084	1.8145092	-2.5542865
H	-2.8383051	1.3395298	-2.3252100
H	-1.1403153	1.0393599	-2.8077461
H	-2.0248066	2.4333261	-3.4529551
C	-0.1427113	3.4815274	-1.9495974
H	-0.4664223	4.0817904	-2.8162997
H	0.6505878	2.7980052	-2.2706847
H	0.2930944	4.1624898	-1.2114584
C	-2.4812295	3.7383077	-1.0882462
H	-2.1494513	4.5083396	-0.3817231
H	-3.3933211	3.2701777	-0.6922754
H	-2.7620527	4.2536811	-2.0210450
C	-0.7942535	2.6694474	1.6935461
C	0.0678692	3.9219929	1.4552607
H	-0.4312802	4.6604853	0.8149637
H	1.0405665	3.6649885	1.0168398
H	0.2466533	4.4043615	2.4297904
C	-0.0861128	1.7939936	2.7452293
H	0.0377608	2.3833684	3.6683994
H	0.9065994	1.4723069	2.4041327
H	-0.6732592	0.9026546	3.0040403
C	-2.1615238	3.1036069	2.2595845
H	-1.9775070	3.7101165	3.1608373
H	-2.7844213	2.2544013	2.5701708
H	-2.7411571	3.7212725	1.5638603
C	-0.7942782	-2.6694598	-1.6935471

C	0.0678552	-3.9220013	-1.4552787
H	0.2466228	-4.4043687	-2.4298121
H	-0.4312781	-4.6604961	-0.8149729
H	1.0405595	-3.6649924	-1.0168770
C	-0.0861620	-1.7940045	-2.7452452
H	0.0376978	-2.3833806	-3.6684164
H	0.9065545	-1.4723114	-2.4041679
H	-0.6733182	-0.9026692	-3.0040474
C	-2.1615572	-3.1036251	-2.2595600
H	-2.7844629	-2.2544222	-2.5701373
H	-2.7411761	-3.7212908	-1.5638246
H	-1.9775544	-3.7101359	-3.1608146
C	-1.3701347	-2.7229170	1.4174693
C	-1.8746400	-1.8145104	2.5543089
H	-2.8382450	-1.3395375	2.3252547
H	-1.1402444	-1.0393559	2.8077439
H	-2.0247115	-2.4333220	3.4529856
C	-2.4811908	-3.7383201	1.0882972
H	-2.7619885	-4.2536868	2.0211072
H	-2.1494276	-4.5083565	0.3817726
H	-3.3932940	-3.2701970	0.6923457
C	-0.1426521	-3.4815240	1.9495890
H	0.6506527	-2.7979961	2.2706490
H	0.2931369	-4.1624925	1.2114465
H	-0.4663390	-4.0817790	2.8163059

Combination of torsional angles = -10
E(BP86/def2-TZVP) = -8050.74621414554

Br	2.2432284	-1.6579985	0.2184826
Br	2.2432514	1.6579498	-0.2186003
Ni	0.5645024	-0.0000079	-0.0000238
P	-0.9566667	1.5942747	0.0703915
P	-0.9566851	-1.5942749	-0.0703746
C	-2.5736016	-0.6893060	-0.3316923
H	-2.6892051	-0.5828638	-1.4170762
H	-3.4255132	-1.2924079	0.0168262
C	-2.5735800	0.6893217	0.3317838
H	-2.6891353	0.5828813	1.4171730
H	-3.4255014	1.2924320	-0.0166964
C	-1.3288467	2.6686410	-1.4951701
C	-1.7930354	1.7161565	-2.6124376
H	-2.7600850	1.2428054	-2.3947084
H	-1.0460283	0.9379390	-2.8135203
H	-1.9197654	2.3002235	-3.5376126
C	-0.0862024	3.4108653	-2.0153629
H	-0.3810560	3.9728501	-2.9172395
H	0.7202033	2.7184149	-2.2803914
H	0.3211984	4.1239891	-1.2915614
C	-2.4537398	3.6896417	-1.2394755
H	-2.1497809	4.4860790	-0.5500253
H	-3.3765114	3.2303245	-0.8580612
H	-2.7055533	4.1699202	-2.1988889
C	-0.8408786	2.7366947	1.6284292
C	0.0104260	3.9925426	1.3680628
H	-0.4788416	4.6982724	0.6847249
H	0.9999717	3.7341946	0.9710846
H	0.1502457	4.5144586	2.3285214
C	-0.1530486	1.9114109	2.7323545
H	-0.0556241	2.5396469	3.6327089
H	0.8495623	1.5840284	2.4281454
H	-0.7420099	1.0284090	3.0143985
C	-2.2279769	3.1765952	2.1405460
H	-2.0736958	3.8251699	3.0177298
H	-2.8482163	2.3343307	2.4740387
H	-2.7975099	3.7552046	1.4039956
C	-0.8409713	-2.7366855	-1.6284252
C	0.0103343	-3.9925424	-1.3681047
H	0.1501132	-4.5144491	-2.3285743
H	-0.4789120	-4.6982759	-0.6847556
H	0.9998974	-3.7342056	-0.9711622
C	-0.1531779	-1.9113991	-2.7323712
H	-0.0557978	-2.5396278	-3.6327355
H	0.8494491	-1.5840308	-2.4282003
H	-0.7421407	-1.0283877	-3.0143824
C	-2.2280937	-3.1765688	-2.1404919
H	-2.8483367	-2.3342961	-2.4739569
H	-2.7976051	-3.7551759	-1.4039233
H	-2.0738525	-3.8251405	-3.0176849
C	-1.3287942	-2.6686458	1.4952017
C	-1.7929132	-1.7161616	2.6124980
H	-2.7599696	-1.2427997	2.3948230
H	-1.0458871	-0.9379528	2.8135436
H	-1.9195995	-2.3002312	3.5376776
C	-2.4537105	-3.6896357	1.2395657
H	-2.7054768	-4.1699134	2.1989919
H	-2.1497960	-4.4860747	0.5500982
H	-3.3764985	-3.2303098	0.8582019
C	-0.0861284	-3.4108820	2.0153268
H	0.7202984	-2.7184390	2.2803111
H	0.3212261	-4.1240101	1.2915036
H	-0.3809381	-3.9728637	2.9172198

Combination of torsional angles = -5
E(BP86/def2-TZVP) = -8050.74659101436

Br	2.2424661	-1.6674163	0.1031260
Br	2.2424721	1.6674050	-0.1032333
Ni	0.5622742	-0.0000011	-0.0000216
P	-0.9587050	1.5970805	0.0407882
P	-0.9587254	-1.5970651	-0.0407729
C	-2.5796250	-0.7001510	-0.3075403
H	-2.7071689	-0.6309191	-1.3946583
H	-3.4261697	-1.2935973	0.0696004
C	-2.5796052	0.7001864	0.3076177
H	-2.7071088	0.6309563	1.3947405
H	-3.4261569	1.2936428	-0.0694913
C	-1.2858379	2.6073912	-1.5750414
C	-1.7060816	1.6081715	-2.6680761
H	-2.6765403	1.1359388	-2.4632213
H	-0.9471078	0.8288967	-2.8111986
H	-1.8058838	2.1535092	-3.6198622
C	-0.0263775	3.3319621	-2.0801021
H	-0.2877907	3.8518321	-3.0167995
H	0.7916328	2.6320551	-2.2836633
H	0.3510445	4.0784461	-1.3739355
C	-2.4222466	3.6321689	-1.3998293
H	-2.1465242	4.4564355	-0.7315929
H	-3.3561905	3.1827654	-1.0339519
H	-2.6416675	4.0733477	-2.3856139
C	-0.8930777	2.8043078	1.5543099
C	-0.0449590	4.0572899	1.2696132

H	-0.5180021	4.7289818	0.5419970
H	0.9594859	3.7935733	0.9169498
H	0.0569851	4.6198875	2.2117308
C	-0.2359027	2.0314127	2.7130793
H	-0.1634427	2.7003775	3.5859614
H	0.7747631	1.6925915	2.4513376
H	-0.8337037	1.1625461	3.0192411
C	-2.2981216	3.2556330	2.0052281
H	-2.1732424	3.9445534	2.8559124
H	-2.9226685	2.4250906	2.3590903
H	-2.8494955	3.7961640	1.2271064
C	-0.8931783	-2.8042946	-1.5542960
C	-0.0450713	-4.0572919	-1.2696315
H	0.0568234	-4.6198935	-2.2117520
H	-0.5180972	-4.7289734	-0.5419944
H	0.9593930	-3.7935936	-0.9170101
C	-0.2360382	-2.0314128	-2.7130943
H	-0.1636261	-2.7003805	-3.5859781
H	0.7746443	-1.6926084	-2.4513955
H	-0.8338371	-1.1625366	-3.0192330
C	-2.2982486	-3.2555967	-2.0051545
H	-2.9227959	-2.4250446	-2.3589931
H	-2.8495995	-3.7961159	-1.2270080
H	-2.1734168	-3.9445218	-2.8558418
C	-1.2858130	-2.6073713	1.5750681
C	-1.7060009	-1.6081460	2.6681193
H	-2.6764599	-1.1358979	2.4633007
H	-0.9470098	-0.8288831	2.8112145
H	-1.8057767	-2.1534829	3.6199085
C	-2.4222443	-3.6321308	1.3998951
H	-2.6416356	-4.0733092	2.3856864
H	-2.1465593	-4.4563997	0.7316459
H	-3.3561947	-3.1827118	1.0340535
C	-0.0263463	-3.3319637	2.0800820
H	0.7916827	-2.6320707	2.2836153
H	0.3510380	-4.0784526	1.3739005
H	-0.2877345	-3.8518311	3.0167877

Combination of torsional angles = 0

E(BP86/def2-TZVP) = -8050.74691726040

Br	2.2404974	-1.6697486	-0.0006971
Br	2.2405003	1.6697416	0.0006674
Ni	0.5601936	-0.0000019	-0.0000046
P	-0.9609784	1.5982057	0.0006558
P	-0.9609818	-1.5982066	-0.0006502
C	-2.5864055	-0.7121778	-0.2779933
H	-2.7264799	-0.6879722	-1.3656476
H	-3.4268438	-1.2923449	0.1321152
C	-2.5864018	0.7121819	0.2780134
H	-2.7264668	0.6879771	1.3656689
H	-3.4268421	1.2923511	-0.1320881
C	-1.2390735	2.5324362	-1.6671969
C	-1.6170770	1.4809807	-2.7255847
H	-2.5913913	1.0123160	-2.5306537
H	-0.8495697	0.7009943	-2.8046284
H	-1.6876085	1.9799842	-3.7050520
C	0.0384367	3.2346920	-2.1590446
H	-0.1858812	3.7043975	-3.1310962
H	0.8649543	2.5278926	-2.2939598
H	0.3864236	4.0181048	-1.4782383
C	-2.3823903	3.5602928	-1.5801841
H	-2.1325269	4.4154419	-0.9412023
H	-3.3276773	3.1242188	-1.2273257
H	-2.5677397	3.9548953	-2.5923714
C	-0.9432638	2.8761542	1.4581204
C	-0.0911580	4.1192398	1.1429021
H	-0.5424205	4.7527563	0.3686861
H	0.9258210	3.8454405	0.8378365
H	-0.0247647	4.7265455	2.0601374
C	-0.3247288	2.1620827	2.6741839
H	-0.2764160	2.8748387	3.5133694
H	0.6923459	1.8089129	2.4607589
H	-0.9357857	1.3121544	3.0061915
C	-2.3633067	3.3443317	1.8410440
H	-2.2661089	4.0750168	2.6598868
H	-2.9976518	2.5308224	2.2161381
H	-2.8905120	3.8441420	1.0201733
C	-0.9432792	-2.8761492	-1.4581217
C	-0.0911697	-4.1192368	-1.1429209
H	-0.0247819	-4.7265336	-2.0601626
H	-0.5424259	-4.7527615	-0.3687083
H	0.9258112	-3.8454392	-0.8378597
C	-0.3247518	-2.1620696	-2.6741839
H	-0.2764453	-2.8748193	-3.5133752
H	0.6923248	-1.8089025	-2.4607629
H	-0.9358100	-1.3121380	-3.0061810
C	-2.3633244	-3.3443231	-1.8410426
H	-2.9976708	-2.5308106	-2.2161277
H	-2.8905264	-3.8441397	-1.0201740
H	-2.2661306	-4.0750017	-2.6598918
C	-1.2390654	-2.5324355	1.6672075
C	-1.6170569	-1.4809770	2.7255961
H	-2.5913711	-1.0123094	2.5306717
H	-0.8495462	-0.7009934	2.8046321
H	-1.6875825	-1.9799785	3.7050649
C	-2.3823868	-3.5602885	1.5802112
H	-2.5677288	-3.9548834	2.5924029
H	-2.1325322	-4.4154428	0.9412334
H	-3.3276754	-3.1242133	1.2273584
C	0.0384460	-3.2346928	2.1590502
H	0.8649662	-2.5278951	2.2939580
H	0.3864270	-4.0181091	1.4782451
H	-0.1858675	-3.7043940	3.1311050

Combination of torsional angles = 5

E(BP86/def2-TZVP) = -8050.74705787813

Br	2.2385970	-1.6672633	-0.1093039
Br	2.2386210	1.6672107	0.1092547
Ni	0.5593491	-0.0000155	-0.0000060
P	-0.9630832	1.5971944	-0.0349447
P	-0.9630913	-1.5972166	0.0349560
C	-2.5933579	-0.7223023	-0.2498800
H	-2.7466416	-0.7404381	-1.3360497
H	-3.4268455	-1.2891178	0.1918775
C	-2.5933509	0.7222895	0.2499130
H	-2.7466198	0.7404257	1.3360847
H	-3.4268415	1.2891097	-0.1918333
C	-1.1902010	2.4573054	-1.7475291
C	-1.5291013	1.3578760	-2.7693966
H	-2.5083664	0.8947833	-2.5856638

H	-0.7576308	0.5778974	-2.7852488
H	-1.5675982	1.8111072	-3.7726507
C	0.1060312	3.1371079	-2.2225113
H	-0.0787642	3.5579558	-3.2246858
H	0.9371982	2.4257701	-2.2897722
H	0.4266844	3.9538243	-1.5679100
C	-2.3358988	3.4856511	-1.7466845
H	-2.1092952	4.3690421	-1.1381068
H	-3.2923396	3.0630011	-1.4075867
H	-2.4864291	3.8343122	-2.7812656
C	-0.9904637	2.9387605	1.3652170
C	-0.1293946	4.1687203	1.0235537
H	-0.5556227	4.7657634	0.2073097
H	0.8975598	3.8845928	0.7655338
H	-0.0950675	4.8165421	1.9144687
C	-0.4153557	2.2812254	2.6331641
H	-0.3914594	3.0330543	3.4385535
H	0.6068729	1.9164233	2.4697827
H	-1.0410792	1.4501745	2.9851194
C	-2.4225051	3.4229255	1.6787506
H	-2.3512746	4.1908202	2.4655855
H	-3.0697334	2.6275706	2.0702064
H	-2.9219782	3.8841653	0.8189148
C	-0.9904886	-2.9387665	-1.3652215
C	-0.1294126	-4.1687312	-1.0235931
H	-0.0950907	-4.8165322	-1.9145233
H	-0.5556316	-4.7657947	-0.2073604
H	0.8975430	-3.8846063	-0.7655754
C	-0.4153897	-2.2812091	-2.6331607
H	-0.3915013	-3.0330226	-3.4385647
H	0.6068410	-1.9164123	-2.4697802
H	-1.0411141	-1.4501496	-2.9850950
C	-2.4225329	-3.4229222	-1.6787580
H	-3.0697613	-2.6275580	-2.0701950
H	-2.9220033	-3.8841781	-0.8189301
H	-2.3513079	-4.1908010	-2.4656089
C	-1.1901961	-2.4573236	1.7475465
C	-1.5290788	-1.3578867	2.7694103
H	-2.5083402	-0.8947847	2.5856814
H	-0.7576003	-0.5779167	2.7852535
H	-1.5675738	-1.8111124	3.7726670
C	-2.3359039	-3.4856581	1.7467267
H	-2.4864267	-3.8343039	2.7813139
H	-2.1093156	-4.3690591	1.1381594
H	-3.2923441	-3.0630032	1.4076337
C	0.1060350	-3.1371294	2.2225275
H	0.9372065	-2.4257965	2.2897767
H	0.4266794	-3.9538541	1.5679340
H	-0.0787572	-3.5579656	3.2247075

Combination of torsional angles = 10
E(BP86/def2-TZVP) = -8050.74708625789

Br	2.2374346	-1.6577461	-0.2214121
Br	2.2374570	1.6577233	0.2211986
Ni	0.5602785	-0.0000085	-0.0000420
P	-0.9638490	1.5941578	-0.0677160
P	-0.9638444	-1.5941746	0.0677436
C	-2.5993014	-0.7309993	-0.2228248
H	-2.7663179	-0.7895922	-1.3057309
H	-3.4249883	-1.2842109	0.2497785
C	-2.5992857	0.7309823	0.2229668
H	-2.7662267	0.7895752	1.3058844
H	-3.4250055	1.2841940	-0.2495789
C	-1.1406536	2.3830230	-1.8180887
C	-1.4525230	1.2418878	-2.8018403
H	-2.4384540	0.7894069	-2.6267751
H	-0.6839950	0.4598318	-2.7605578
H	-1.4600156	1.6514631	-3.8244423
C	0.1761022	3.0346373	-2.2768213
H	0.0311773	3.4093011	-3.3034861
H	1.0048478	2.3169571	-2.2809175
H	0.4776957	3.8795332	-1.6493760
C	-2.2801773	3.4146450	-1.8971163
H	-2.0685730	4.3226012	-1.3200962
H	-3.2483224	3.0094572	-1.5697936
H	-2.3973907	3.7190036	-2.9498336
C	-1.0293974	2.9923584	1.2747969
C	-0.1528827	4.2048328	0.9103888
H	-0.5503087	4.7677967	0.0562781
H	0.8809063	3.9078636	0.6986321
H	-0.1456271	4.8896293	1.7738767
C	-0.5010967	2.3872002	2.5883158
H	-0.4988694	3.1734115	3.3604695
H	0.5238041	2.0112300	2.4745579
H	-1.1437328	1.5756888	2.9552169
C	-2.4689659	3.4940879	1.5200942
H	-2.4195272	4.2934745	2.2766650
H	-3.1328390	2.7180907	1.9222523
H	-2.9374148	3.9216346	0.6261365
C	-1.0294837	-2.9923764	-1.2747637
C	-0.1529409	-4.2048490	-0.9104168
H	-0.1457419	-4.8896441	-1.7739062
H	-0.5503076	-4.7678152	-0.0562801
H	0.8808618	-3.9078772	-0.6987298
C	-0.5012730	-2.3872170	-2.5883183
H	-0.4990974	-3.1734279	-3.3604726
H	0.5236352	-2.0112457	-2.4746297
H	-1.1439348	-1.5757059	-2.9551751
C	-2.4690682	-3.4941079	-1.5199640
H	-3.1329695	-2.7181116	-1.9220773
H	-2.9374562	-3.9216554	-0.6259749
H	-2.4196792	-4.2934943	-2.2765383
C	-1.1405266	-2.3830345	1.8181316
C	-1.4523270	-1.2418954	2.8019004
H	-2.4382695	-0.7894140	2.6269013
H	-0.6838009	-0.4598406	2.7605619
H	-1.4597497	-1.6514669	3.8245044
C	-2.2800460	-3.4146549	1.8972441
H	-2.3971862	-3.7190080	2.9499712
H	-2.0684834	-4.3226144	1.3202139
H	-3.2482137	-3.0094676	1.5699872
C	0.1762606	-3.0346471	2.2767761
H	1.0050070	-2.3169673	2.2808111
H	0.4778101	-3.8795467	1.6493147
H	0.0314068	-3.4093052	3.3034531

Combination of torsional angles = 15
E(BP86/def2-TZVP) = -8050.74701779508

Br	2.2305862	-1.6406729	-0.3359897
Br	2.2306066	1.6406597	0.3358688

Ni	0.5572276	-0.0000043	-0.0000224
P	-0.9683533	1.5897460	-0.0988165
P	-0.9683486	-1.5897551	0.0988381
C	-2.6090113	-0.7384712	-0.1967524
H	-2.7893371	-0.8358165	-1.2749257
H	-3.4266619	-1.2775037	0.3053387
C	-2.6090031	0.7384621	0.1968449
H	-2.7892823	0.8358071	1.2750260
H	-3.4266755	1.2774944	-0.3052109
C	-1.0958262	2.3114093	-1.8803012
C	-1.3907955	1.1349002	-2.8266537
H	-2.3844682	0.6965466	-2.6586534
H	-0.6300223	0.3494896	-2.7346988
H	-1.3693884	1.5039095	-3.8644338
C	0.2426329	2.9307466	-2.3218017
H	0.1371044	3.2631396	-3.3675633
H	1.0630930	2.2051763	-2.2680986
H	0.5323448	3.7984450	-1.7202631
C	-2.2221045	3.3487840	-2.0328354
H	-2.0186982	4.2771965	-1.4862605
H	-3.2026194	2.9641570	-1.7173648
H	-2.3069034	3.6118856	-3.0997092
C	-1.0654400	3.0380862	1.1870889
C	-0.1689712	4.2301842	0.8042208
H	-0.5353546	4.7618747	-0.0831627
H	0.8688478	3.9190785	0.6373130
H	-0.1839497	4.9480582	1.6403286
C	-0.5853722	2.4817070	2.5401148
H	-0.6034591	3.2979097	3.2802277
H	0.4404920	2.0968171	2.4749627
H	-1.2451920	1.6888183	2.9172774
C	-2.5086367	3.5575595	1.3661473
H	-2.4774836	4.3842282	2.0938452
H	-3.1908542	2.8012282	1.7749596
H	-2.9447093	3.9545544	0.4423291
C	-1.0654891	-3.0380895	-1.1870704
C	-0.1690019	-4.2301892	-0.8042509
H	-0.1840140	-4.9480553	-1.6403649
H	-0.5353469	-4.7618890	0.0831425
H	0.8688235	-3.9190831	-0.6373838
C	-0.5854787	-2.4817003	-2.5401123
H	-0.6035968	-3.2978974	-3.2802306
H	0.4403882	-2.0968108	-2.4750007
H	-1.2453144	-1.6888087	-2.9172409
C	-2.5086931	-3.5575618	-1.3660737
H	-3.1909275	-2.8012273	-1.7748522
H	-2.9447279	-3.9545640	-0.4422411
H	-2.4775697	-4.3842246	-2.0937795
C	-1.0957460	-2.3114178	1.8803295
C	-1.3906742	-1.1349068	2.8266918
H	-2.3843532	-0.6965518	2.6587317
H	-0.6299036	-0.3494978	2.7347037
H	-1.3692247	-1.5039140	3.8644718
C	-2.2220195	-3.3487900	2.0329162
H	-2.3067736	-3.6118862	3.0997949
H	-2.0186378	-4.2772054	1.4863376
H	-3.2025472	-2.9641630	1.7174854
C	0.2427311	-2.9307539	2.3217773
H	1.0631892	-2.2051840	2.2680382
H	0.5324183	-3.7984543	1.7202303
H	0.1372452	-3.2631431	3.3675443

Combination of torsional angles = 20
E(BP86/def2-TZVP) = -8050.74679516794

Br	2.2217678	-1.6162921	-0.4477780
Br	2.2217386	1.6163128	0.4479143
Ni	0.5526885	0.0000069	0.0000258
P	-0.9746053	1.5835881	-0.1335805
P	-0.9746109	-1.5835757	0.1335552
C	-2.6204428	-0.7453399	-0.1693538
H	-2.8133950	-0.8830440	-1.2411289
H	-3.4299974	-1.2680498	0.3623268
C	-2.6204518	0.7453504	0.1692454
H	-2.8134584	0.8830547	1.2410108
H	-3.4299800	1.2680597	-0.3624761
C	-1.0557048	2.2393837	-1.9411933
C	-1.3463584	1.0324638	-2.8495995
H	-2.3489271	0.6130526	-2.6850244
H	-0.5980821	0.2415348	-2.7133083
H	-1.2999149	1.3624931	-3.8996421
C	0.3055895	2.8198909	-2.3667668
H	0.2371683	3.1140736	-3.4268771
H	1.1112714	2.0829707	-2.2620542
H	0.5928795	3.7048627	-1.7895107
C	-2.1610832	3.2865978	-2.1611802
H	-1.9572872	4.2322091	-1.6451708
H	-3.1545899	2.9276329	-1.8559494
H	-2.2157160	3.5097995	-3.2390917
C	-1.0956799	3.0778400	1.0954936
C	-0.1729368	4.2446879	0.6975904
H	-0.5043711	4.7466291	-0.2203381
H	0.8657911	3.9157987	0.5760904
H	-0.2052070	4.9937760	1.5053593
C	-0.6664089	2.5673290	2.4833328
H	-0.7006039	3.4109245	3.1914502
H	0.3573323	2.1717916	2.4663734
H	-1.3463418	1.7951319	2.8678525
C	-2.5379274	3.6181143	1.2095436
H	-2.5207908	4.4677375	1.9108247
H	-3.2416052	2.8825946	1.6200343
H	-2.9392029	3.9892084	0.2597303
C	-1.0956240	-3.0778326	-1.0955176
C	-0.1729015	-4.2446775	-0.6975576
H	-0.2051326	-4.9937736	-1.5053206
H	-0.5043816	-4.7466090	0.2203599
H	0.8658206	-3.9157880	-0.5760097
C	-0.6662856	-2.5673315	-2.4833398
H	-0.7004463	-3.4109321	-3.1914527
H	0.3574547	-2.1717939	-2.4663338
H	-1.3461999	-1.7951372	-2.8678982
C	-2.5378655	-3.6181091	-1.2096316
H	-3.2415244	-2.8825935	-1.6201619
H	-2.9391857	-3.9891956	-0.2598339
H	-2.5206948	-4.4677382	-1.9109047
C	-1.0557983	-2.2393751	1.9411614
C	-1.3464992	-1.0324596	2.8495589
H	-2.3490612	-0.6130507	2.6849374
H	-0.5982187	-0.2415277	2.7133074
H	-1.3001054	-1.3624934	3.8996023
C	-2.1611843	-3.2865941	2.1610867

H	-2.2158693	-3.5098041	3.2389937
H	-1.9573603	-4.2322010	1.6450798
H	-3.1546770	-2.9276298	1.8558097
C	0.3054766	-2.8198827	2.3667961
H	1.1111626	-2.0829611	2.2621248
H	0.5927945	-3.7048515	1.7895486
H	0.2370061	-3.1140709	3.4269016

Combination of torsional angles = 25
E(BP86/def2-TZVP) = -8050.74631004770

Br	2.2165892	-1.5852389	-0.5591089
Br	2.2165605	1.5852458	0.5592415
Ni	0.5520950	0.0000022	0.0000258
P	-0.9778427	1.5755965	-0.1704210
P	-0.9778420	-1.5756007	0.1703972
C	-2.6288341	-0.7513620	-0.1412474
H	-2.8341920	-0.9299512	-1.2048360
H	-3.4300619	-1.2560536	0.4197241
C	-2.6288453	0.7513481	0.1411427
H	-2.8342566	0.9299361	1.2047212
H	-3.4300485	1.2560351	-0.4198681
C	-1.0172058	2.1651892	-2.0008000
C	-1.3134452	0.9314403	-2.8703235
H	-2.3256458	0.5350439	-2.7065904
H	-0.5810870	0.1337057	-2.6940077
H	-1.2453708	1.2229709	-3.9305443
C	0.3664252	2.7021558	-2.4128736
H	0.3314445	2.9599341	-3.4839526
H	1.1529091	1.9519940	-2.2626830
H	0.6585895	3.6008387	-1.8594676
C	-2.0966231	3.2239696	-2.2835812
H	-1.8862225	4.1844288	-1.7986745
H	-3.1029382	2.8942261	-1.9872141
H	-2.1239083	3.4074232	-3.3700215
C	-1.1158251	3.1131423	1.0002674
C	-0.1637605	4.2508356	0.5874876
H	-0.4594019	4.7223084	-0.3583907
H	0.8730634	3.9024563	0.5105527
H	-0.2080569	5.0305116	1.3651684
C	-0.7358953	2.6488933	2.4185354
H	-0.7815915	3.5186692	3.0935423
H	0.2832241	2.2423343	2.4476765
H	-1.4367959	1.8992658	2.8103013
C	-2.5534429	3.6749328	1.0518947
H	-2.5467689	4.5451719	1.7276619
H	-3.2791335	2.9607558	1.4619749
H	-2.9201500	4.0218025	0.0794197
C	-1.1157549	-3.1131469	-1.0002990
C	-0.1637020	-4.2508333	-0.5874732
H	-0.2079530	-5.0305082	-1.3651576
H	-0.4593874	-4.7223102	0.3583893
H	0.8731152	-3.9024458	-0.5104853
C	-0.7357563	-2.6488938	-2.4185472
H	-0.7814119	-3.5186693	-3.0935574
H	0.2833616	-2.2423273	-2.4476361
H	-1.4366424	-1.8992710	-2.8103481
C	-2.5533660	-3.6749479	-1.0520003
H	-3.2790407	-2.9607761	-1.4621173
H	-2.9201205	-4.0218210	-0.0795445
H	-2.5466509	-4.5451866	-1.7277677
C	-1.0172909	-2.1651925	2.0007749
C	-1.3135798	-0.9314440	2.8702821
H	-2.3257746	-0.5350536	2.7064988
H	-0.5812174	-0.1337056	2.6940010
H	-1.2455556	-1.2229726	3.9305067
C	-2.0967159	-3.2239784	2.2835054
H	-2.1240529	-3.4074303	3.3699447
H	-1.8862863	-4.1844373	1.7986107
H	-3.1030186	-2.8942412	1.9870889
C	0.3663230	-2.7021504	2.4129174
H	1.1528101	-1.9519846	2.2627639
H	0.6585194	-3.6008328	1.8595277
H	0.3312911	-2.9599266	3.4839953

Combination of torsional angles = 30
E(BP86/def2-TZVP) = -8050.74558738135

Br	2.2091597	-1.5428923	-0.6802027
Br	2.2092103	1.5428651	0.6800853
Ni	0.5513123	-0.0000032	-0.0000204
P	-0.9807809	1.5669523	-0.1993022
P	-0.9807824	-1.5669488	0.1993274
C	-2.6372622	-0.7558652	-0.1166776
H	-2.8553540	-0.9698661	-1.1713287
H	-3.4296047	-1.2440986	0.4708865
C	-2.6372525	0.7558782	0.1167710
H	-2.8552994	0.9698804	1.1714310
H	-3.4296163	1.2441165	-0.4707603
C	-0.9809883	2.1001530	-2.0466841
C	-1.2913668	0.8479060	-2.8840289
H	-2.3137441	0.4774186	-2.7218402
H	-0.5778738	0.0411457	-2.6755959
H	-1.2043020	1.1073285	-3.9511949
C	0.4245750	2.5907318	-2.4437736
H	0.4193104	2.8215096	-3.5214913
H	1.1873616	1.8235243	-2.2588761
H	0.7290243	3.4954707	-1.9068177
C	-2.0291802	3.1741818	-2.3830559
H	-1.8060577	4.1445087	-1.9242796
H	-3.0482430	2.8762089	-2.0966262
H	-2.0312534	3.3236794	-3.4750462
C	-1.1289852	3.1390939	0.9205681
C	-0.1435334	4.2453022	0.5009556
H	-0.4009758	4.6908200	-0.4683713
H	0.8883876	3.8754092	0.4675673
H	-0.1953751	5.0508377	1.2513073
C	-0.7991169	2.7136290	2.3634853
H	-0.8518887	3.6050820	3.0090223
H	0.2126802	2.2943796	2.4362099
H	-1.5228248	1.9870268	2.7574515
C	-2.5581017	3.7242020	0.9132855
H	-2.5591263	4.6090584	1.5699025
H	-3.3073620	3.0299484	1.3154388
H	-2.8884923	4.0546306	-0.0775402
C	-1.1290359	-3.1390908	-0.9205356
C	-0.1435684	-4.2452996	-0.5009613
H	-0.1954408	-5.0508359	-1.2513100
H	-0.4009723	-4.6908159	0.4683764
H	0.8883544	-3.8754073	-0.4676148
C	-0.7992229	-2.7136274	-2.3634659
H	-0.8520214	-3.6050806	-3.0090002

H	0.2125723	-2.2943800	-2.4362300
H	-1.5229445	-1.9870240	-2.7574043
C	-2.5581531	-3.7241966	-0.9131965
H	-3.3074281	-3.0299421	-1.3153207
H	-2.8885052	-4.0546243	0.0776422
H	-2.5592049	-4.6090533	-1.5698131
C	-0.9809148	-2.1001478	2.0467100
C	-1.2912533	-0.8478991	2.8840669
H	-2.3136359	-0.4774077	2.7219207
H	-0.5777658	-0.0411417	2.6756036
H	-1.2041449	-1.1073212	3.9512295
C	-2.0290967	-3.1741722	2.3831274
H	-2.0311248	-3.3236680	3.4751180
H	-1.8059971	-4.1445006	1.9243432
H	-3.0481703	-2.8761958	2.0967398
C	0.4246635	-2.5907315	2.4437404
H	1.1874450	-1.8235270	2.2588099
H	0.7290865	-3.4954720	1.9067722
H	0.4194437	-2.8215086	3.5214585

Combination of torsional angles = 35
E(BP86/def2-TZVP) = -8050.74467256565

Br	2.1956058	-1.4890547	-0.8059296
Br	2.1956695	1.4890203	0.8057822
Ni	0.5465479	-0.0000085	-0.0000246
P	-0.9868867	1.5576944	-0.2249703
P	-0.9868862	-1.5576991	0.2250111
C	-2.6487439	-0.7593629	-0.0945549
H	-2.8781984	-1.0050002	-1.1400113
H	-3.4327280	-1.2319043	0.5165864
C	-2.6487320	0.7593727	0.0946949
H	-2.8781218	1.0050118	1.1401651
H	-3.4327486	1.2319206	-0.5163996
C	-0.9526819	2.0445404	-2.0844939
C	-1.2850872	0.7816527	-2.8967538
H	-2.3170394	0.4382865	-2.7345251
H	-0.5914741	-0.0358286	-2.6658148
H	-1.1843733	1.0160399	-3.9685151
C	0.4730635	2.4872878	-2.4672819
H	0.4928247	2.6989202	-3.5487177
H	1.2094718	1.7003751	-2.2575655
H	0.7950641	3.3922179	-1.9406609
C	-1.9660190	3.1374041	-2.4633851
H	-1.7245202	4.1126644	-2.0249140
H	-2.9969487	2.8729360	-2.1866873
H	-1.9464865	3.2596124	-3.5586025
C	-1.1374902	3.1566399	0.8530026
C	-0.1156820	4.2293335	0.4337650
H	-0.3341970	4.6542735	-0.5541572
H	0.9081434	3.8354331	0.4408521
H	-0.1694058	5.0557226	1.1609191
C	-0.8560519	2.7614517	2.3148281
H	-0.9107853	3.6700596	2.9357924
H	0.1459062	2.3274128	2.4266273
H	-1.6035636	2.0580433	2.7066951
C	-2.5542105	3.7678687	0.7931763
H	-2.5594123	4.6612851	1.4381629
H	-3.3277885	3.0920437	1.1808257
H	-2.8480246	4.0905897	-0.2113645
C	-1.1375664	-3.1566399	-0.8529599
C	-0.1157422	-4.2293451	-0.4337910
H	-0.1695151	-5.0557275	-1.1609491
H	-0.3342027	-4.6542922	0.5541400
H	0.9080860	-3.8354529	-0.4409346
C	-0.8562098	-2.7614457	-2.3147992
H	-0.9109866	-3.6700495	-2.9357657
H	0.1457454	-2.3274144	-2.4266540
H	-1.6037386	-2.0580289	-2.7066186
C	-2.5542887	-3.7678568	-0.7930576
H	-3.3278828	-3.0920223	-1.1806582
H	-2.8480488	-4.0905830	0.2114970
H	-2.5595349	-4.6612683	-1.4380508
C	-0.9525753	-2.0445423	2.0845344
C	-1.2849200	-0.7816489	2.8968098
H	-2.3168782	-0.4382726	2.7346403
H	-0.5913121	0.0358246	2.6658274
H	-1.1841457	-1.0160337	3.9685659
C	-1.9659010	-3.1373936	2.4634921
H	-1.9463052	-3.2595949	3.5587092
H	-1.7244375	-4.1126591	2.0250136
H	-2.9968443	-2.8729171	2.1868534
C	0.4731886	-2.4873006	2.4672415
H	1.2095917	-1.7003957	2.2574784
H	0.7951506	-3.3922361	1.9406067
H	0.4930107	-2.6989276	3.5486774

Combination of torsional angles = 40
E(BP86/def2-TZVP) = -8050.74335656464

Br	2.1826843	-1.4215637	-0.9339422
Br	2.1827871	1.4215249	0.9337427
Ni	0.5418932	-0.0000038	-0.0000334
P	-0.9938032	1.5478551	-0.2484855
P	-0.9938086	-1.5478371	0.2485457
C	-2.6606138	-0.7619193	-0.0751405
H	-2.8995031	-1.0351444	-1.1117116
H	-3.4371688	-1.2201090	0.5560754
C	-2.6605940	0.7619665	0.0753443
H	-2.8993887	1.0351962	1.1119358
H	-3.4371955	1.2201698	-0.5558046
C	-0.9337260	1.9966214	-2.1170853
C	-1.2923610	0.7284610	-2.9094331
H	-2.3323268	0.4111451	-2.7445211
H	-0.6173548	-0.0998803	-2.6642320
H	-1.1840521	0.9435691	-3.9844959
C	0.5080829	2.3945649	-2.4901312
H	0.5462881	2.5904167	-3.5740246
H	1.2195277	1.5892851	-2.2626015
H	0.8487358	3.2978928	-1.9722184
C	-1.9135892	3.1083418	-2.5273315
H	-1.6508950	4.0853668	-2.1053596
H	-2.9540016	2.8762214	-2.2572644
H	-1.8787493	3.2082674	-3.6244340
C	-1.1398455	3.1675979	0.7953968
C	-0.0811549	4.2051738	0.3798307
H	-0.2633314	4.6137514	-0.6222432
H	0.9319288	3.7854729	0.4217136
H	-0.1302576	5.0483220	1.0877645
C	-0.9020014	2.7962240	2.2712914
H	-0.9534708	3.7185750	2.8719267
H	0.0883473	2.3457038	2.4165130

H	-1.6729558	2.1162460	2.6593122
C	-2.5413692	3.8068261	0.6914113
H	-2.5473851	4.7041712	1.3309982
H	-3.3382982	3.1480056	1.0611161
H	-2.8008465	4.1285670	-0.3225709
C	-1.1399662	-3.1675748	-0.7953294
C	-0.0812584	-4.2051704	-0.3798564
H	-0.1304348	-5.0483146	-1.0877899
H	-0.2633577	-4.6137493	0.6222309
H	0.9318291	-3.7854864	-0.4218227
C	-0.9022378	-2.7961993	-2.2712421
H	-0.9537710	-3.7185472	-2.8718767
H	0.0881063	-2.3456942	-2.4165436
H	-1.6732134	-2.1162077	-2.6591968
C	-2.5414922	-3.8067798	-0.6912310
H	-3.3384410	-3.1479440	-1.0608659
H	-2.8008907	-4.1285218	0.3227710
H	-2.5475765	-4.7041214	-1.3308221
C	-0.9335796	-1.9966070	2.1171400
C	-1.2921202	-0.7284400	2.9095200
H	-2.3320935	-0.4111022	2.7446974
H	-0.6171178	0.0998876	2.6642620
H	-1.1837238	-0.9435520	3.9845731
C	-1.9134309	-3.1083073	2.5274693
H	-1.8785009	-3.2082329	3.6245690
H	-1.6507918	-4.0853378	2.1054761
H	-2.9538613	-2.8761662	2.2574895
C	0.5082528	-2.3945805	2.4900630
H	1.2196950	-1.5893154	2.2624731
H	0.8488432	-3.2979151	1.9721210
H	0.5465461	-2.5904336	3.5739531

Relaxed potential surface scan of O structure of NiBr2dtbpe

Combination of torsional angles = -40

E(BP86/def2-TZVP) = -8050.74335639522

Ni	-0.5436760	-0.0000133	0.0000064
Br	-2.1845439	0.9326984	-1.4222492
Br	-2.1845032	-0.9327754	1.4222754
C	2.6588349	-0.0745882	0.7619851
C	2.6588183	0.0747209	-0.7620254
P	0.9920485	0.2497352	1.5476478
P	0.9920360	-0.2496924	-1.5476582
C	1.1381649	-0.7928987	3.1681890
C	0.9004870	-2.2690971	2.7979221
C	0.0793988	-0.3766573	4.2054191
C	2.5396569	-0.6882761	3.8073790
C	0.9318666	2.1186825	1.9949843
C	-0.5100144	2.4919573	2.3924518
C	1.2906496	2.9100759	0.7262704
C	1.9115571	2.5298195	3.1065225
C	0.9319424	-2.1186454	-1.9949822
C	1.9116147	-2.5297393	-3.1065522
C	1.2908131	-2.9100124	-0.7262767
C	-0.5099335	-2.4919974	-2.3923961
C	1.1380579	0.7929415	-3.1682067
C	2.5395374	0.6883899	-3.8074356
C	0.9003121	2.2691286	-2.7979382
C	0.0792817	0.3766431	-4.2054038
H	3.4354098	0.5569769	1.2196614
H	2.8977060	-1.1109513	1.0360091
H	2.8976295	1.1110964	-1.0360542
H	3.4354190	-0.5568034	-1.2197143
H	-0.0898201	-2.4147592	2.3474516
H	0.9519499	-2.8690226	3.7207354
H	1.6715302	-2.6575600	2.1182963
H	-0.9336717	-0.4190429	3.7857384
H	0.2614034	0.6257818	4.6131764
H	0.1286108	-1.0838871	5.0491518
H	3.3366679	-1.0582635	3.1488146
H	2.5457603	-1.3272882	4.7051330
H	2.7989499	0.3259548	4.1284801
H	-1.2213237	2.2639067	1.5872007
H	-0.5482676	3.5759723	2.5876237
H	-0.8508045	1.9745947	3.2960451
H	2.3306608	2.7449407	0.4092229
H	1.1822802	3.9853009	0.9405377
H	0.6157587	2.6642330	-0.1019727
H	2.9520127	2.2596235	2.8747483
H	1.6487509	2.1085917	4.0838379
H	1.8766472	3.6269974	3.2055951
H	1.8767553	-3.6269195	-3.2056176
H	2.9520648	-2.2594911	-2.8748145
H	1.6487546	-2.1085300	-4.0838608
H	1.1824933	-3.9852445	-0.9405337
H	0.6159385	-2.6642013	0.1019890
H	2.3308268	-2.7448200	-0.4092672
H	-0.5481366	-3.5760142	-2.5875678
H	-0.8507847	-1.9746515	-3.2959761
H	-1.2212248	-2.2639851	-1.5871184
H	2.7988727	-0.3258273	-4.1285452
H	3.3365479	1.0584166	-3.1488927
H	2.5455840	1.3274034	-4.7051889
H	0.9517215	2.8690541	-3.7207544
H	1.6713506	2.6576340	-2.1183316
H	-0.0899919	2.4147400	-2.3474446
H	0.2613215	-0.6257899	-4.6131599
H	0.1284351	1.0838699	-5.0491424
H	-0.9337784	0.4189830	-3.7856934

Combination of torsional angles = -35

E(BP86/def2-TZVP) = -8050.74467282893

Ni	-0.5461586	0.0000361	-0.0000196
Br	-2.1951805	0.8048129	-1.4897184
Br	-2.1953242	-0.8046012	1.4895959
C	2.6491082	-0.0941411	0.7594926
C	2.6491514	0.0939394	-0.7593889
P	0.9872508	0.2261618	1.5575353
P	0.9873019	-0.2262200	-1.5575051
C	1.1378054	-0.8505719	3.1573181
C	0.8563435	-2.3126974	2.7632571
C	0.1159863	-0.4304869	4.2296701
C	2.5545180	-0.7903081	3.7685231
C	0.9530725	2.0860669	2.0429261
C	-0.4726758	2.4692355	2.4853332
C	1.2855327	2.8973373	0.7794175
C	1.9663896	2.4657948	3.1355193

C	0.9529838	-2.0861188	-2.0429028
C	1.9663185	-2.4659224	-3.1354534
C	1.2853139	-2.8974263	-0.7793832
C	-0.4727766	-2.4691568	-2.4853833
C	1.1380144	0.8504869	-3.1572893
C	2.5547464	0.7900920	-3.7684362
C	0.8566570	2.3126405	-2.7632571
C	0.1162052	0.4304691	-4.2296768
H	3.4331239	0.5173054	1.2315860
H	2.8784809	-1.1394246	1.0059411
H	2.8786258	1.1392031	-1.0058265
H	3.4331354	-0.5175751	-1.2314469
H	-0.1456082	-2.4248092	2.3292847
H	0.9110475	-2.9329597	3.6723457
H	1.6038602	-2.7051245	2.0601655
H	-0.9078321	-0.4378522	3.8357573
H	0.3345168	0.5577546	4.6538579
H	0.1696788	-1.1570091	5.0566163
H	3.3280961	-1.1784946	3.0930065
H	2.5596909	-1.4346089	4.6624343
H	2.8483513	0.2144729	4.0904763
H	-1.2090670	2.2589128	1.6985663
H	-0.4924205	3.5508385	2.6961100
H	-0.7947102	1.9433374	3.3906709
H	2.3174917	2.7348223	0.4362070
H	1.1848382	3.9692820	1.0129716
H	0.5919396	2.6657798	-0.0379043
H	2.9973201	2.1888684	2.8712946
H	1.7248566	2.0280945	4.1111166
H	1.9468766	3.5611079	3.2568670
H	1.9467163	-3.5612323	-3.2568151
H	2.9972607	-2.1890879	-2.8711780
H	1.7248684	-2.0281888	-4.1110569
H	1.1845359	-3.9693606	-1.0129487
H	0.5917035	-2.6658128	0.0379083
H	2.3172713	-2.7350045	-0.4361238
H	-0.4926078	-3.5507566	-2.6961684
H	-0.7947184	-1.9432234	-3.3907339
H	-1.2091884	-2.2587731	-1.6986518
H	2.8485055	-0.2147198	-4.0903628
H	3.3283311	1.1782212	-3.0928943
H	2.5600111	1.4343791	-4.6623567
H	0.9114483	2.9328872	-3.6723510
H	1.6041779	2.7050147	-2.0601407
H	-0.1453030	2.4248402	-2.3293262
H	0.3346718	-0.5577982	-4.6538385
H	0.1699922	1.1569729	-5.0566330
H	-0.9076289	0.4379256	-3.8358065

Combination of torsional angles = -30
E(BP86/def2-TZVP) = -8050.74558742270

Ni	-0.5504358	-0.0000129	0.0000127
Br	-2.2083369	0.6804703	-1.5426936
Br	-2.2082899	-0.6805420	1.5427491
C	2.6381267	-0.1168676	0.7558326
C	2.6381111	0.1169225	-0.7558617
P	0.9816533	0.1989550	1.5669953
P	0.9816317	-0.1989407	-1.5669961
C	1.1299141	-0.9212812	3.1388655
C	0.8000903	-2.3641119	2.7130731
C	0.1444559	-0.5019606	4.2451817
C	2.5590335	-0.9140814	3.7239663
C	0.9817942	2.0462100	2.1006319
C	-0.4237758	2.4431353	2.5913339
C	1.2921028	2.8838495	0.8485632
C	2.0299953	2.3823861	3.1747117
C	0.9818088	-2.0461938	-2.1006373
C	2.0300003	-2.3823386	-3.1747363
C	1.2921583	-2.8838300	-0.8485764
C	-0.4237593	-2.4431505	-2.5913190
C	1.1298398	0.9212972	-3.1388696
C	2.5589498	0.9141285	-3.7239932
C	0.7999881	2.3641210	-2.7130751
C	0.1443746	0.5019486	-4.2451689
H	3.4304797	0.4705916	1.2441776
H	2.8562261	-1.1715638	0.9695973
H	2.8561808	1.1716241	-0.9696300
H	3.4304702	-0.4705173	-1.2442202
H	-0.2117150	-2.4367773	2.2938343
H	0.8529125	-3.0098522	3.6043762
H	1.5237972	-2.7578761	1.9863607
H	-0.8874696	-0.4685349	3.8753037
H	0.4018603	0.4672777	4.6909127
H	0.1963367	-1.2524886	5.0505514
H	3.3083019	-1.3160551	3.0296173
H	2.5600832	-1.5708926	4.6086785
H	2.8893911	0.0766842	4.0546080
H	-1.1865771	2.2583866	1.8241065
H	-0.4185390	3.5207979	2.8223689
H	-0.7281769	1.9059542	3.4959555
H	2.3144672	2.7217592	0.4779976
H	1.2050253	3.9509562	1.1082257
H	0.5785849	2.6755771	0.0417827
H	3.0490613	2.0960606	2.8766500
H	1.8069132	1.9233869	4.1449432
H	2.0320239	3.4743439	3.3244467
H	2.0320531	-3.4742955	-3.3244774
H	3.0490643	-2.0959898	-2.8766899
H	1.8068910	-1.9233392	-4.1449615
H	1.2051017	-3.9509379	-1.1082409
H	0.5786488	-2.6755771	-0.0417832
H	2.3145250	-2.7217166	-0.4780274
H	-0.4185004	-3.5208120	-2.8223588
H	-0.7281872	-1.9059726	-3.4959336
H	-1.1865530	-2.2584232	-1.8240790
H	2.8893249	-0.0766309	-4.0546367
H	3.3082201	1.3161218	-3.0296576
H	2.5599702	1.5709365	-4.6087077
H	0.8527804	3.0098605	-3.6043805
H	1.5236971	2.7579043	-1.9863752
H	-0.2118123	2.4367631	-2.2938202
H	0.4017955	-0.4672855	-4.6909000
H	0.1962250	1.2524746	-5.0505423
H	-0.8875443	0.4684993	-3.8752748

Combination of torsional angles = -25
E(BP86/def2-TZVP) = -8050.74630708090

Ni	-0.5397707	0.0002623	0.0001094
Br	-2.2041335	0.5521492	-1.5878713
Br	-2.2044039	-0.5503821	1.5882396

C	2.6409944	-0.1381868	0.7521696
C	2.6410811	0.1367570	-0.7519244
P	0.9901137	0.1780339	1.5748548
P	0.9900297	-0.1785204	-1.5746118
C	1.1277312	-0.9850867	3.1182031
C	0.7471747	-2.4054964	2.6610658
C	0.1759770	-0.5662602	4.2539411
C	2.5653853	-1.0344944	3.6801161
C	1.0300444	2.0113058	2.1553675
C	-0.3533122	2.4264609	2.6906812
C	1.3261200	2.8745701	0.9171893
C	2.1098376	2.2990482	3.2124239
C	1.0288591	-2.0118175	-2.1550840
C	2.1081278	-2.3001843	-3.2125017
C	1.3249054	-2.8752420	-0.9170142
C	-0.3549269	-2.4261734	-2.6899118
C	1.1283304	0.9844775	-3.1179778
C	2.5659646	1.0328911	-3.6800250
C	0.7488114	2.4051562	-2.6607991
C	0.1761477	0.5663314	-4.2536107
H	3.4424240	0.4250185	1.2540461
H	2.8459956	-1.2009438	0.9360180
H	2.8467213	1.1993867	-0.9357966
H	3.4421736	-0.4269405	-1.2537912
H	-0.2719774	-2.4362321	2.2547038
H	0.7926280	-3.0761664	3.5342021
H	1.4478696	-2.8013002	1.9133674
H	-0.8608522	-0.4905814	3.9053032
H	0.4721032	0.3818079	4.7206953
H	0.2200325	-1.3400851	5.0374546
H	3.2908595	-1.4484309	2.9679471
H	2.5585104	-1.7058993	4.5537231
H	2.9325068	-0.0604372	4.0220857
H	-1.1400956	2.2726151	1.9415759
H	-0.3179555	3.4988436	2.9429298
H	-0.6453055	1.8777811	3.5923087
H	2.3381624	2.7085926	0.5213236
H	1.2583975	3.9362527	1.2034264
H	0.5934903	2.6944027	0.1205663
H	3.1159847	2.0007454	2.8839161
H	1.8995373	1.8189872	4.1753376
H	2.1374803	3.3863791	3.3904660
H	2.1350770	-3.3875334	-3.3905422
H	3.1145545	-2.0024666	-2.8843180
H	1.8977947	-1.8200071	-4.1753465
H	1.2565029	-3.9368883	-1.2032253
H	0.5926469	-2.6946872	-0.1201398
H	2.3371781	-2.7098112	-0.5215062
H	-0.3202480	-3.4985331	-2.9423535
H	-0.6469915	-1.8771734	-3.5913251
H	-1.1413293	-2.2720233	-1.9404676
H	2.9323385	0.0586080	-4.0221467
H	3.2918114	1.4462131	-2.9678782
H	2.5594941	1.7044050	-4.5535513
H	0.7947185	3.0758148	-3.5339189
H	1.4497943	2.8004462	-1.9130999
H	-0.2703106	2.4366038	-2.2544158
H	0.4714806	-0.3819929	-4.7203475
H	0.2207307	1.3400823	-5.0371670
H	-0.8607056	0.4914720	-3.9048671

Combination of torsional angles = -20

E(BP86/def2-TZVP) = -8050.74679919830

Ni	-0.5481371	-0.0017844	-0.0014250
Br	-2.2162478	0.4279513	-1.6236081
Br	-2.2180535	-0.4348810	1.6180757
C	2.6244898	-0.1601325	0.7482707
C	2.6253944	0.1632848	-0.7457972
P	0.9776336	0.1494602	1.5819838
P	0.9805938	-0.1498435	-1.5822478
C	1.0987756	-1.0640015	3.0888656
C	0.6714307	-2.4574882	2.5923004
C	0.1746015	-0.6550895	4.2507703
C	2.5406878	-1.1708686	3.6314848
C	1.0562149	1.9638651	2.2192018
C	-0.3060121	2.3939446	2.7942005
C	1.3468050	2.8600784	1.0031775
C	2.1605018	2.1959054	3.2649539
C	1.0641137	-1.9640784	-2.2193079
C	2.1706255	-2.1937727	-3.2632329
C	1.3546306	-2.8596701	-1.0028050
C	-0.2962382	-2.3970783	-2.7965489
C	1.1016409	1.0638336	-3.0889580
C	2.5442226	1.1737577	-3.6291873
C	0.6705192	2.4564263	-2.5931464
C	0.1802803	0.6529178	-4.2523877
H	3.4330076	0.3777748	1.2661993
H	2.8185234	-1.2302220	0.8970557
H	2.8173827	1.2337862	-0.8942691
H	3.4359238	-0.3728855	-1.2623804
H	-0.3519927	-2.4456957	2.1957628
H	0.7056698	-3.1568421	3.4431778
H	1.3524273	-2.8492115	1.8246788
H	-0.8639835	-0.5381836	3.9197687
H	0.5045896	0.2683669	4.7434441
H	0.2071554	-1.4550180	5.0082112
H	3.2454191	-1.5881705	2.9008211
H	2.5236092	-1.8633311	4.4883103
H	2.9406125	-0.2168221	3.9930539
H	-1.1109956	2.2807331	2.0577770
H	-0.2389588	3.4571218	3.0774331
H	-0.5933981	1.8255973	3.6848885
H	2.3498902	2.6923166	0.5862720
H	1.2989123	3.9134161	1.3223087
H	0.5993126	2.7147667	0.2131182
H	3.1546458	1.8881329	2.9099433
H	1.9565212	1.6894567	4.2156802
H	2.2137299	3.2761271	3.4770636
H	2.2265451	-3.2738856	-3.4752013
H	3.1635188	-1.8838358	-2.9066084
H	1.9671159	-1.6878082	-4.2143172
H	1.3095725	-3.9131070	-1.3220226
H	0.6055061	-2.7160130	-0.2139917
H	2.3566483	-2.6897145	-0.5842328
H	-0.2264519	-3.4601209	-3.0796269
H	-0.5833609	-1.8293737	-3.6877301
H	-1.1026814	-2.2855551	-2.0614612
H	2.9467734	0.2205618	-3.9900852
H	3.2468550	1.5925585	-2.8973601
H	2.5271016	1.8661784	-4.4860451

H	0.7047216	3.1558294	-3.4439834
H	1.3493830	2.8495962	-1.8243757
H	-0.3535428	2.4424848	-2.1983333
H	0.5130910	-0.2698240	-4.7445031
H	0.2123583	1.4529073	-5.0097834
H	-0.8585995	0.5337739	-3.9231138

Combination of torsional angles = -15
E(BP86/def2-TZVP) = -8050.74701336213

Ni	-0.5565990	0.0008975	0.0002405
Br	-2.2301710	0.3151986	-1.6447022
Br	-2.2300404	-0.3117415	1.6457027
C	2.6097020	-0.1874243	0.7408665
C	2.6096788	0.1860044	-0.7412832
P	0.9693610	0.1206778	1.5882519
P	0.9687892	-0.1204515	-1.5882033
C	1.0661716	-1.1454667	3.0539005
C	0.5854142	-2.5057052	2.5160113
C	0.1700726	-0.7460607	4.2408475
C	2.5093852	-1.3181173	3.5755045
C	1.0978835	1.9117282	2.2856208
C	-0.2402734	2.3622390	2.8990979
C	1.3931881	2.8419397	1.0963848
C	2.2243888	2.0777231	3.3206766
C	1.0953027	-1.9116364	-2.2855994
C	2.2213376	-2.0787732	-3.3209832
C	1.3900208	-2.8421306	-1.0964382
C	-0.2434821	-2.3608073	-2.8986836
C	1.0664556	1.1455895	-3.0538866
C	2.5096885	1.3167795	-3.5759179
C	0.5872364	2.5063167	-2.5158601
C	0.1696046	0.7470940	-4.2405724
H	3.4277115	0.3215326	1.2728747
H	2.7894360	-1.2642602	0.8528795
H	2.7904523	1.2626620	-0.8533467
H	3.4270308	-0.3237640	-1.2735238
H	-0.4405128	-2.4453384	2.1304987
H	0.6033707	-3.2346827	3.3421772
H	1.2448953	-2.8938610	1.7281681
H	-0.8677171	-0.5829092	3.9276615
H	0.5369463	0.1482862	4.7604003
H	0.1848019	-1.5723614	4.9699912
H	3.1912523	-1.7375511	2.8246977
H	2.4780298	-2.0344466	4.4120347
H	2.9459950	-0.3891881	3.9597767
H	-1.0608532	2.2991021	2.1744260
H	-0.1341859	3.4123548	3.2172881
H	-0.5301774	1.7726482	3.7748940
H	2.3866166	2.6673553	0.6600544
H	1.3726132	3.8846045	1.4513992
H	0.6321272	2.7399986	0.3124857
H	3.2046971	1.7566176	2.9402007
H	2.0208655	1.5438422	4.2564125
H	2.3097441	3.1480197	3.5693086
H	2.3055445	-3.1491588	-3.5696257
H	3.2020811	-1.7586484	-2.9408036
H	2.0180668	-1.5447006	-4.2566644
H	1.3682784	-3.8847785	-1.4514338
H	0.6292998	-2.7394063	-0.3123118
H	2.3837575	-2.6685513	-0.6604097
H	-0.1385500	-3.4110407	-3.2168695
H	-0.5330175	-1.7709500	-3.7744231
H	-1.0637990	-2.2968098	-2.1737899
H	2.9452245	0.3874172	-3.9603599
H	3.1922167	1.7354804	-2.8253030
H	2.4788161	2.0331747	-4.4124096
H	0.6056930	3.2352710	-3.3420354
H	1.2473401	2.8938063	-1.7282108
H	-0.4386378	2.4469924	-2.1300464
H	0.5354235	-0.1476175	-4.7602407
H	0.1849487	1.5733846	-4.9697151
H	-0.8682569	0.5849848	-3.9270829

Combination of torsional angles = -10
E(BP86/def2-TZVP) = -8050.74093555076

Ni	-0.5748077	-0.0000220	0.0000023
Br	-2.2366093	0.2107257	-1.6732301
Br	-2.2366150	-0.2108315	1.6732216
C	2.5675475	-0.2574607	0.7174490
C	2.5675418	0.2575250	-0.7174345
P	0.9457835	0.0795215	1.5935804
P	0.9457917	-0.0795112	-1.5935700
C	1.0848168	-1.2332203	3.0263001
C	0.8796175	-2.6132025	2.3732771
C	0.0381077	-1.1148154	4.1513757
C	2.4836030	-1.1745263	3.6727972
C	1.0863891	1.8804569	2.2934098
C	0.3272586	2.0408950	3.6214470
C	0.4214370	2.8152813	1.2674958
C	2.5491667	2.3145048	2.4904450
C	1.0864562	-1.8804389	-2.2934047
C	2.5492477	-2.3144370	-2.4904468
C	0.4215377	-2.8152903	-1.2674934
C	0.3273271	-2.0408924	-3.6214411
C	1.0847785	1.2332313	-3.0262926
C	2.4835649	1.1745817	-3.6727933
C	0.8795323	2.6132095	-2.3732750
C	0.0380704	1.1147822	-4.1513643
H	3.4199813	0.1500334	1.2776367
H	2.6808253	-1.3509888	0.7219036
H	2.6807838	1.3510567	-0.7218887
H	3.4199906	-0.1499415	-1.2776194
H	-0.1081905	-2.6857256	1.8995451
H	0.9376086	-3.3824308	3.1594714
H	1.6521778	-2.8589014	1.6321750
H	-0.9823732	-1.0592064	3.7578363
H	0.2125611	-0.2557282	4.8055495
H	0.1228813	-2.0196814	4.7749670
H	3.3016880	-1.3591048	2.9647623
H	2.5383149	-1.9599807	4.4437070
H	2.6669568	-0.2164169	4.1775516
H	-0.6904785	1.6330408	3.5642510
H	0.2478568	3.1179419	3.8403095
H	0.8565612	1.5766135	4.4623203
H	0.9274175	2.7944651	0.2964762
H	0.4707174	3.8492607	1.6473068
H	-0.6341573	2.5553149	1.1097981
H	3.1097625	2.3476532	1.5456850
H	3.0950493	1.6725557	3.1947114
H	2.5563091	3.3354679	2.9049463

H	2.5564229	-3.3353977	-2.9049535
H	3.1098472	-2.3475717	-1.5456885
H	3.0951071	-1.6724661	-3.1947114
H	0.4708508	-3.8492661	-1.6473097
H	-0.6340646	-2.5553592	-1.1097910
H	0.9275207	-2.7944625	-0.2964753
H	0.2479619	-3.1179401	-3.8403129
H	0.8566108	-1.5765848	-4.4623122
H	-0.6904239	-1.6330738	-3.5642383
H	2.6669493	0.2164767	-4.1775449
H	3.3016456	1.3591902	-2.9647613
H	2.5382481	1.9600353	-4.4437060
H	0.9374946	3.3824363	-3.1594727
H	1.6520853	2.8589391	-1.6321756
H	-0.1082773	2.6857001	-1.8995412
H	0.2125495	0.2556934	-4.8055297
H	0.1228134	2.0196447	-4.7749650
H	-0.9824078	1.0591446	-3.7578215

Combination of torsional angles = -5
E(BP86/def2-TZVP) = -8050.74206330153

Ni	-0.5749449	-0.0000253	-0.0000054
Br	-2.2346074	0.0955712	-1.6862916
Br	-2.2346178	-0.0956869	1.6862686
C	2.5624371	-0.2785175	0.7095335
C	2.5624303	0.2785867	-0.7095292
P	0.9428464	0.0489197	1.5945040
P	0.9428559	-0.0489113	-1.5945070
C	1.0604509	-1.3141213	2.9802949
C	0.8709964	-2.6716929	2.2770969
C	-0.0076279	-1.2413851	4.0884257
C	2.4484957	-1.2713631	3.6506733
C	1.1133931	1.8227814	2.3569287
C	0.3921276	1.9416219	3.7100909
C	0.4317200	2.8002270	1.3830083
C	2.5848480	2.2368191	2.5330466
C	1.1134730	-1.8227663	-2.3569324
C	2.5849441	-2.2367482	-2.5330456
C	0.4318334	-2.8002392	-1.3830161
C	0.3922166	-1.9416324	-3.7100973
C	1.0604119	1.3141349	-2.9802973
C	2.4484587	1.2714288	-3.6506747
C	0.8709061	2.6716990	-2.2770987
C	-0.0076643	1.2413599	-4.0884279
H	3.4186994	0.1063525	1.2795492
H	2.6676223	-1.3723263	0.6814206
H	2.6675750	1.3723994	-0.6814163
H	3.4187093	-0.1062519	-1.2795408
H	-0.1070362	-2.7297806	1.7815137
H	0.9134669	-3.4667580	3.0381610
H	1.6577524	-2.8931528	1.5434673
H	-1.0218297	-1.2047140	3.6770144
H	0.1289008	-0.3882406	4.7588417
H	0.0904812	-2.1540757	4.6986495
H	3.2781179	-1.4219311	2.9479064
H	2.4984235	-2.0857147	4.3913026
H	2.6169613	-0.3320060	4.1944216
H	-0.6376131	1.5649973	3.6584490
H	0.3489856	3.0092241	3.9799141
H	0.9282293	1.4244580	4.5154764
H	0.9112928	2.8078235	0.3982411
H	0.5031644	3.8195794	1.7971711
H	-0.6302473	2.5557251	1.2464444
H	3.1226562	2.3003763	1.5767248
H	3.1417183	1.5649968	3.2000352
H	2.6109582	3.2417198	2.9842832
H	2.6110938	-3.2416473	-2.9842831
H	3.1227508	-2.3002858	-1.5767217
H	3.1417915	-1.5649042	-3.2000313
H	0.5033177	-3.8195881	-1.7971805
H	-0.6301436	-2.5557776	-1.2464555
H	0.9114031	-2.8078194	-0.3982473
H	0.3491163	-3.0092358	-3.9799226
H	0.9283015	-1.4244467	-4.5154801
H	-0.6375386	-1.5650471	-3.6584583
H	2.6169589	0.3320793	-4.1944254
H	3.2780748	1.4220247	-2.9479067
H	2.4983579	2.0857842	-4.3913017
H	0.9133491	3.4667664	-3.0381619
H	1.6576523	2.8931871	-1.5434671
H	-0.1071301	2.7297508	-1.7815181
H	0.1288953	0.3882204	-4.7588442
H	0.0904108	2.1540543	-4.6986517
H	-1.0218648	1.2046513	-3.6770161

Combination of torsional angles = 0
E(BP86/def2-TZVP) = -8050.74316887107

Ni	-0.5752835	-0.0004778	-0.0000209
Br	-2.2317897	-0.0157907	-1.6920877
Br	-2.2319541	0.0133907	1.6918948
C	2.5583948	-0.3016690	0.6999796
C	2.5581659	0.3037092	-0.6997044
P	0.9411160	0.0139917	1.5942278
P	0.9412897	-0.0135416	-1.5941171
C	1.0305447	-1.3981113	2.9295448
C	0.8615335	-2.7318118	2.1768560
C	-0.0665754	-1.3665448	4.0101735
C	2.4028905	-1.3753717	3.6321423
C	1.1438825	1.7558645	2.4224497
C	0.4312898	1.8373537	3.7831021
C	0.4776829	2.7817651	1.4886157
C	2.6231608	2.1376713	2.6080577
C	1.1458269	-1.7552295	-2.4222857
C	2.6254925	-2.1356005	-2.6077515
C	0.4805355	-2.7817570	-1.4884947
C	0.4334380	-1.8374344	-3.7830014
C	1.0294742	1.3986343	-2.9294385
C	2.4019617	1.3773276	-3.6318027
C	0.8589346	2.7321485	-2.1767645
C	-0.0674164	1.3659165	-4.0102674
H	3.4184396	0.0574687	1.2808161
H	2.6550864	-1.3945031	0.6346016
H	2.6537691	1.3966394	-0.6343152
H	3.4186232	-0.0545766	-1.2804562
H	-0.0992062	-2.7716642	1.6467968
H	0.8755742	-3.5505981	2.9133931
H	1.6717783	-2.9335152	1.4635684
H	-1.0701098	-1.3484710	3.5721915
H	0.0271159	-0.5182811	4.6937844
H	0.0384873	-2.2846156	4.6112137

H	3.2481878	-1.4857547	2.9403991
H	2.4453392	-2.2228376	4.3351387
H	2.5511489	-0.4607881	4.2218352
H	-0.6098251	1.4962112	3.7179742
H	0.4232827	2.8929293	4.0997672
H	0.9529291	1.2685021	4.5629901
H	0.9570487	2.8192643	0.5042536
H	0.5675268	3.7828779	1.9417154
H	-0.5882551	2.5602061	1.3454731
H	3.1582132	2.2307609	1.6526406
H	3.1715687	1.4312722	3.2456423
H	2.6670994	3.1234078	3.0984122
H	2.6704380	-3.1213047	-3.0980798
H	3.1605503	-2.2281435	-1.6522848
H	3.1732681	-1.4286813	-3.2453040
H	0.5713879	-3.7827913	-1.9415669
H	-0.5856296	-2.5612260	-1.3454525
H	0.9598487	-2.8187745	-0.5040897
H	0.4264528	-2.8930277	-4.0996315
H	0.9546185	-1.2681198	-4.5628575
H	-0.6080030	-1.4972665	-3.7179883
H	2.5512898	0.4628781	-4.2214348
H	3.2470268	1.4886387	-2.9399255
H	2.4436239	2.2248093	-4.3348275
H	0.8722703	3.5509627	-2.9132834
H	1.6688314	2.9346731	-1.4633141
H	-0.1019481	2.7709927	-1.6468878
H	0.0273627	0.5178109	-4.6939256
H	0.0367249	2.2841480	-4.6112216
H	-1.0710109	1.3466881	-3.5724718

Combination of torsional angles = 5

E(BP86/def2-TZVP) = -8050.74413949050

Ni	-0.5764062	0.0000378	0.0000045
Br	-2.2290475	-0.1247884	-1.6921150
Br	-2.2290325	0.1249732	1.6921319
C	2.5541090	-0.3282676	0.6886330
C	2.5541304	0.3281311	-0.6886289
P	0.9402100	-0.0217376	1.5924270
P	0.9402096	0.0217103	-1.5924205
C	0.9930817	-1.4815084	2.8735534
C	0.8398503	-2.7880470	2.0712135
C	-0.1355455	-1.4816341	3.9210544
C	2.3471865	-1.4899906	3.6106273
C	1.1803904	1.6827916	2.4881045
C	0.4652673	1.7299657	3.8493332
C	0.5454912	2.7609946	1.5923621
C	2.6678109	2.0214983	2.6939094
C	1.1802656	-1.6828287	-2.4881090
C	2.6676615	-2.0216387	-2.6939244
C	0.5452898	-2.7609936	-1.5923747
C	0.4651340	-1.7299316	-3.8493360
C	0.9931834	1.4814718	-2.8735513
C	2.3472926	1.4898558	-3.6106181
C	0.8400338	2.7880257	-2.0712197
C	-0.1354346	1.4816584	-3.9210621
H	3.4188376	0.0011702	1.2798718
H	2.6393334	-1.4188195	0.5835375
H	2.6394283	1.4186771	-0.5835336
H	3.4188363	-0.0013650	-1.2798687
H	-0.0992777	-2.8007576	1.5024572
H	0.8160519	-3.6299998	2.7808419
H	1.6755849	-2.9761654	1.3843053
H	-1.1255453	-1.4677217	3.4528930
H	-0.0765321	-0.6428272	4.6199464
H	-0.0374113	-2.4083309	4.5099721
H	3.2087240	-1.5643839	2.9338950
H	2.3762375	-2.3706379	4.2723354
H	2.4784946	-0.6047684	4.2469734
H	-0.5870243	1.4303200	3.7650284
H	0.4945604	2.7702439	4.2121303
H	0.9620354	1.1087791	4.6053056
H	1.0355973	2.8282826	0.6147105
H	0.6541573	3.7402142	2.0871130
H	-0.5236644	2.5694000	1.4322053
H	3.2083593	2.1432462	1.7448493
H	3.1977893	1.2767494	3.3026775
H	2.7318260	2.9844268	3.2255764
H	2.7316060	-2.9845662	-3.2256019
H	3.2082061	-2.1434352	-1.7448683
H	3.1976899	-1.2769208	-3.3026873
H	0.6538828	-3.7402164	-2.0871352
H	-0.5238513	-2.5693223	-1.4322130
H	1.0353938	-2.8283268	-0.6147252
H	0.4943524	-2.7702061	-4.2121497
H	0.9619427	-1.1087671	-4.6053004
H	-0.5871362	-1.4302127	-3.7650226
H	2.4785456	0.6046167	-4.2469524
H	3.2088317	1.5642010	-2.9338823
H	2.3764047	2.3704929	-4.2723371
H	0.8162961	3.6299760	-2.7808530
H	1.6757767	2.9760926	-1.3843070
H	-0.0990966	2.8008018	-1.5024691
H	-0.0764680	0.6428385	-4.6199438
H	-0.0372355	2.4083416	-4.5099900
H	-1.1254395	1.4678150	-3.4529095

Combination of torsional angles = 10

E(BP86/def2-TZVP) = -8050.74491790243

Ni	-0.5751421	0.0000017	0.0000063
Br	-2.2231467	-0.2376685	-1.6845678
Br	-2.2231039	0.2376708	1.6846225
C	2.5525458	-0.3528807	0.6768324
C	2.5525320	0.3528802	-0.6768854
P	0.9419200	-0.0556349	1.5895850
P	0.9418866	0.0556373	-1.5896047
C	0.9511413	-1.5620066	2.8120737
C	0.8070881	-2.8368977	1.9585556
C	-0.2091084	-1.5848068	3.8237053
C	2.2851193	-1.6139242	3.5827521
C	1.2191145	1.6058022	2.5545127
C	0.4905099	1.6196802	3.9096580
C	0.6278943	2.7377671	1.6962547
C	2.7131536	1.8936281	2.7901516
C	1.2190591	-1.6058008	-2.5545367
C	2.7130928	-1.8936288	-2.7902078
C	0.6278564	-2.7377641	-1.6962642
C	0.4904246	-1.6196804	-3.9096660
C	0.9510891	1.5620081	-2.8120949
C	2.2850503	1.6139171	-3.5828029

C	0.8070633	2.8369015	-1.9585756
C	-0.2091828	1.5848151	-3.8237009
H	3.4215993	-0.0528743	1.2771970
H	2.6265466	-1.4396949	0.5329755
H	2.6265376	1.4396942	-0.5330297
H	3.4215724	0.0528727	-1.2772682
H	-0.1078842	-2.8132095	1.3518710
H	0.7398221	-3.7020359	2.6367555
H	1.6668094	-3.0164937	1.2997249
H	-1.1840763	-1.5550141	3.3251907
H	-0.1718727	-0.7631669	4.5441806
H	-0.1329294	-2.5264131	4.3918514
H	3.1627186	-1.6582317	2.9238259
H	2.2947853	-2.5268736	4.1997782
H	2.4039554	-0.7622819	4.2653832
H	-0.5706877	1.3628731	3.8010652
H	0.5537591	2.6414262	4.3180133
H	0.9554472	0.9484229	4.6427943
H	1.1378346	2.8341736	0.7310394
H	0.7538135	3.6914834	2.2346306
H	-0.4428864	2.5817207	1.5111152
H	3.2668918	2.0447327	1.8530261
H	3.2168146	1.1081655	3.3691957
H	2.7963433	2.8292393	3.3660635
H	2.7962688	-2.8292405	-3.3661210
H	3.2668509	-2.0447337	-1.8530941
H	3.2167424	-1.1081673	-3.3692631
H	0.7537635	-3.6914813	-2.2346411
H	-0.4429202	-2.5817166	-1.5111021
H	1.1378172	-2.8341693	-0.7310595
H	0.5536647	-2.6414270	-4.3180214
H	0.9553457	-0.9484240	-4.6428134
H	-0.5707706	-1.3628732	-3.8010500
H	2.4038651	0.7622748	-4.2654377
H	3.1626646	1.6582174	-2.9238961
H	2.2947090	2.5268673	-4.1998280
H	0.7397866	3.7020389	-2.6367754
H	1.6668008	3.0164937	-1.2997650
H	-0.1078953	2.8132197	-1.3518699
H	-0.1719706	0.7631725	-4.5441742
H	-0.1330082	2.5264189	-4.3918517
H	-1.1841399	1.5550325	-3.3251645

Combination of torsional angles = 15

E(BP86/def2-TZVP) = -8050.74552726438

Ni	-0.5721829	-0.0000006	0.0000004
Br	-2.2148562	-0.3489476	-1.6692745
Br	-2.2148397	0.3489412	1.6692928
C	2.5531541	-0.3776352	0.6640264
C	2.5531476	0.3776249	-0.6640592
P	0.9454343	-0.0920176	1.5852722
P	0.9454170	0.0920120	-1.5852881
C	0.9057193	-1.6437452	2.7436258
C	0.7653394	-2.8819724	1.8370184
C	-0.2852518	-1.6818456	3.7181260
C	2.2178107	-1.7490487	3.5451131
C	1.2572002	1.5206021	2.6209952
C	0.5092050	1.5011224	3.9657950
C	0.7153728	2.7053846	1.8025345
C	2.7555037	1.7533463	2.8900135
C	1.2571543	-1.5206150	-2.6210082
C	2.7554513	-1.7533792	-2.8900471
C	0.7153233	-2.7053865	-1.8025338
C	0.5091386	-1.5011329	-3.9657965
C	0.9057010	1.6437346	-2.7436496
C	2.2177856	1.7490242	-3.5451497
C	0.7653399	2.8819683	-1.8370489
C	-0.2852771	1.6818398	-3.7181408
H	3.4258219	-0.1070158	1.2729229
H	2.6168660	-1.4590540	0.4809281
H	2.6168641	1.4590435	-0.4809611
H	3.4258082	0.1070043	-1.2729649
H	-0.1249426	-2.8148804	1.1975376
H	0.6538992	-3.7700518	2.4787164
H	1.6453604	-3.0558096	1.2041340
H	-1.2439150	-1.6179366	3.1913303
H	-0.2585244	-0.8852676	4.4667553
H	-0.2429728	-2.6434317	4.2554138
H	3.1109689	-1.7709649	2.9058090
H	2.2026313	-2.6913639	4.1162107
H	2.3285976	-0.9332901	4.2712998
H	-0.5583925	1.2872158	3.8312943
H	0.6023168	2.5012265	4.4195785
H	0.9392702	0.7825547	4.6749936
H	1.2480103	2.8290998	0.8525828
H	0.8580878	3.6305356	2.3846322
H	-0.3554970	2.5888270	1.5914340
H	3.3264674	1.9344911	1.9687293
H	3.2291355	0.9272077	3.4367029
H	2.8558013	2.6574216	3.5117394
H	2.8557282	-2.6574571	-3.5117727
H	3.3264258	-1.9345302	-1.9687709
H	3.2290862	-0.9272480	-3.4367448
H	0.8580192	-3.6305424	-2.3846282
H	-0.3555424	-2.5888145	-1.5914199
H	1.2479717	-2.8291030	-0.8525882
H	0.6022330	-2.5012397	-4.4195776
H	0.9391999	-0.7825722	-4.6750044
H	-0.5584547	-1.2872147	-3.8312801
H	2.3285605	0.9332601	-4.2713318
H	3.1109499	1.7709390	-2.9058539
H	2.2026071	2.6913356	-4.1162536
H	0.6538995	3.7700443	-2.4787517
H	1.6453688	3.0558034	-1.2041751
H	-0.1249357	2.8148869	-1.1975581
H	-0.2585633	0.8852560	-4.4667647
H	-0.2429923	2.6434215	-4.2554360
H	-1.2439367	1.6179443	-3.1913375

Combination of torsional angles = 20

E(BP86/def2-TZVP) = -8050.74584017360

Ni	-0.5695032	0.0000184	0.0000083
Br	-2.2067497	-0.4576379	-1.6469077
Br	-2.2066759	0.4577190	1.6469856
C	2.5547387	-0.4026139	0.6499939
C	2.5547382	0.4025667	-0.6500270
P	0.9494128	-0.1321674	1.5791651
P	0.9493909	0.1321620	-1.5791751
C	0.8577211	-1.7261086	2.6694656
C	0.7203736	-2.9243012	1.7101040

C	-0.3641652	-1.7731362	3.6043586
C	2.1447109	-1.8899457	3.5005285
C	1.2927516	1.4267453	2.6855394
C	0.5180772	1.3766854	4.0147026
C	0.8075766	2.6622218	1.9074928
C	2.7921772	1.5996175	2.9924851
C	1.2926981	-1.4267687	-2.6855350
C	2.7921207	-1.5996646	-2.9924807
C	0.8075110	-2.6622294	-1.9074702
C	0.5180235	-1.3767180	-4.0146985
C	0.8577436	1.7261041	-2.6694811
C	2.1447338	1.8898933	-3.5005529
C	0.7204489	2.9243049	-1.7101229
C	-0.3641476	1.7731800	-3.6043655
H	3.4301422	-0.1610047	1.2669762
H	2.6097349	-1.4768706	0.4269530
H	2.6097656	1.4768222	-0.4269873
H	3.4301261	0.1609352	-1.2670232
H	-0.1443607	-2.8109692	1.0424980
H	0.5659664	-3.8335757	2.3119395
H	1.6182831	-3.0938776	1.1018043
H	-1.3040512	-1.6648637	3.0509541
H	-0.3433100	-1.0061947	4.3835979
H	-0.3629214	-2.7553572	4.1045335
H	3.0541379	-1.8945070	2.8837132
H	2.1012416	-2.8584448	4.0244797
H	2.2475673	-1.1118033	4.2678153
H	-0.5533633	1.2067300	3.8516793
H	0.6371660	2.3526880	4.5127810
H	0.9090366	0.6139831	4.7000306
H	1.3681278	2.8104062	0.9769336
H	0.9648728	3.5562249	2.5327752
H	-0.2609027	2.5890845	1.6673789
H	3.3855117	1.8094786	2.0917103
H	3.2312571	0.7338773	3.5054462
H	2.9066436	2.4685748	3.6601542
H	2.9065752	-2.4686333	-3.6601369
H	3.3854539	-1.8095194	-2.0917033
H	3.2312108	-0.7339375	-3.5054553
H	0.9647953	-3.5562428	-2.5327410
H	-0.2609667	-2.5890769	-1.6673544
H	1.3680633	-2.8104077	-0.9769104
H	0.6370994	-2.3527297	-4.5127621
H	0.9089930	-0.6140316	-4.7000384
H	-0.5534145	-1.2067462	-3.8516771
H	2.2475564	1.1117468	-4.2678400
H	3.0541650	1.8944210	-2.8837434
H	2.1012969	2.8583940	-4.0245040
H	0.5660712	3.8335830	-2.3119606
H	1.6183697	3.0938498	-1.1018310
H	-0.1442846	2.8110079	-1.0425099
H	-0.3433306	1.0062365	-4.3836032
H	-0.3628660	2.7554000	-4.1045424
H	-1.3040340	1.6649485	-3.0509542

Combination of torsional angles = 25
E(BP86/def2-TZVP) = -8050.74588213065

Ni	-0.5656185	-0.0000087	-0.0000007
Br	-2.1966727	-0.5713047	-1.6168638
Br	-2.1966676	0.5712775	1.6168707
C	2.5592041	-0.4241046	0.6369811
C	2.5592018	0.4240985	-0.6369847
P	0.9551678	-0.1696901	1.5718604
P	0.9551655	0.1696816	-1.5718633
C	0.8100686	-1.8008464	2.5935862
C	0.6758731	-2.9577584	1.5844764
C	-0.4420608	-1.8503420	3.4875284
C	2.0689183	-2.0253404	3.4523638
C	1.3256040	1.3328790	2.7451845
C	0.5182737	1.2570268	4.0538148
C	0.9020447	2.6143255	2.0064911
C	2.8224001	1.4428055	3.0927996
C	1.3256085	-1.3328768	-2.7451992
C	2.8224059	-1.4427934	-3.0928122
C	0.9020538	-2.6143317	-2.0065182
C	0.5182812	-1.2570168	-4.0538309
C	0.8100670	1.8008468	-2.5935747
C	2.0689181	2.0253482	-3.4523480
C	0.6758716	2.9577488	-1.5844529
C	-0.4420609	1.8503527	-3.4875184
H	3.4360868	-0.2067068	1.2607156
H	2.6084806	-1.4907551	0.3793431
H	2.6084764	1.4907491	-0.3793466
H	3.4360844	0.2067030	-1.2607203
H	-0.1645694	-2.7988954	0.8951796
H	0.4829352	-3.8855716	2.1455076
H	1.5884830	-3.1237415	0.9975332
H	-1.3605712	-1.6915780	2.9102388
H	-0.4246571	-1.1159752	4.2977311
H	-0.4861014	-2.8514448	3.9464083
H	2.9950263	-2.0175576	2.8604225
H	1.9950700	-3.0160393	3.9293867
H	2.1630761	-1.2850479	4.2571657
H	-0.5540606	1.1303603	3.8602853
H	0.6581641	2.2079051	4.5933578
H	0.8676003	0.4550003	4.7163719
H	1.4916857	2.7804797	1.0967471
H	1.0739539	3.4765792	2.6711856
H	-0.1619794	2.5879527	1.7388677
H	3.4421359	1.6786484	2.2166391
H	3.2238097	0.5400519	3.5713487
H	2.9472509	2.2741696	3.8050033
H	2.9472622	-2.2741515	-3.8050218
H	3.4421411	-1.6786398	-2.2166522
H	3.2238120	-0.5400342	-3.5713537
H	1.0739675	-3.4765786	-2.6712206
H	-0.1619707	-2.5879660	-1.7388960
H	1.4916944	-2.7804919	-1.0967753
H	0.6581772	-2.2078898	-4.5933817
H	0.8676060	-0.4549830	-4.7163802
H	-0.5540541	-1.1303569	-3.8603030
H	2.1630774	1.2850626	-4.2571562
H	2.9950251	2.0175601	-2.8604050
H	1.9950708	3.0160512	-3.9293623
H	0.4829353	3.8855680	-2.1454746
H	1.5884811	3.1237246	-0.9975066
H	-0.1645718	2.7988795	-0.8951587
H	-0.4246573	1.1159936	-4.2977280
H	-0.4860990	2.8514599	-3.9463890
H	-1.3605725	1.6915852	-2.9102318

Combination of torsional angles = 30
E(BP86/def2-TZVP) = -8050.74560635336

Ni	-0.5596578	-0.0000065	0.0000043
Br	-2.1834476	-0.6875318	-1.5771901
Br	-2.1834316	0.6875036	1.5772215
C	2.5670087	-0.4420939	0.6253902
C	2.5669991	0.4421153	-0.6254075
P	0.9624527	-0.2065471	1.5634736
P	0.9624381	0.2065509	-1.5634776
C	0.7629589	-1.8723722	2.5125168
C	0.6366709	-2.9855334	1.4544048
C	-0.5204927	-1.9219756	3.3613141
C	1.9886310	-2.1588624	3.3995596
C	1.3528671	1.2350946	2.8034974
C	0.5062522	1.1358803	4.0856898
C	0.9954564	2.5587652	2.1051812
C	2.8422765	1.2793140	3.1958384
C	1.3528654	-1.2350805	-2.8035083
C	2.8422733	-1.2792726	-3.1958575
C	0.9954793	-2.5587605	-2.1051969
C	0.5062429	-1.1358692	-4.0856962
C	0.7629207	1.8723723	-2.5125209
C	1.9885843	2.1588707	-3.3995727
C	0.6366279	2.9855350	-1.4544106
C	-0.5205358	1.9219576	-3.3613117
H	3.4437418	-0.2431353	1.2553674
H	2.6147072	-1.5012471	0.3385794
H	2.6146886	1.5012691	-0.3385974
H	3.4437293	0.2431657	-1.2553919
H	-0.1792673	-2.7823082	0.7472482
H	0.4090866	-3.9304866	1.9722323
H	1.5631978	-3.1461930	0.8881909
H	-1.4138028	-1.7117401	2.7607849
H	-0.5101026	-1.2221616	4.2018011
H	-0.6105313	-2.9392007	3.7756022
H	2.9329234	-2.1415430	2.8368138
H	1.8827619	-3.1686757	3.8280823
H	2.0702030	-1.4575245	4.2397367
H	-0.5637419	1.0527835	3.8584071
H	0.6614241	2.0598370	4.6662473
H	0.8107279	0.2975186	4.7250432
H	1.6166010	2.7390744	1.2189368
H	1.1795486	3.3875731	2.8080135
H	-0.0611573	2.5815065	1.8096116
H	3.4929156	1.5390183	2.3494105
H	3.2031312	0.3420612	3.6386458
H	2.9721921	2.0702307	3.9518687
H	2.9721985	-2.0701838	-3.9518919
H	3.4929215	-1.5389690	-2.3494340
H	3.2031093	-0.3420114	-3.6386629
H	1.1795809	-3.3875617	-2.8080346
H	-0.0611324	-2.5815202	-1.8096218
H	1.6166317	-2.7390646	-1.2189569
H	0.6614270	-2.0598186	-4.6662621
H	0.8107022	-0.2974969	-4.7250440
H	-0.5637514	-1.0527914	-3.8584078
H	2.0701583	1.4575293	-4.2397470
H	2.9328804	2.1415634	-2.8368325
H	1.8827025	3.1686809	-3.8280996
H	0.4090305	3.9304845	-1.9722391
H	1.5631567	3.1462058	-0.8882030
H	-0.1793037	2.7823031	-0.7472483
H	-0.5101428	1.2221383	-4.2017946
H	-0.6105871	2.9391793	-3.7756054
H	-1.4138406	1.7117163	-2.7607765

Combination of torsional angles = 35
E(BP86/def2-TZVP) = -8050.74483535377

Ni	-0.5527853	-0.0000282	-0.0000048
Br	-2.1684850	-0.8068423	-1.5261683
Br	-2.1685700	0.8066843	1.5261224
C	2.5771933	-0.4563823	0.6157951
C	2.5771708	0.4565584	-0.6157389
P	0.9702816	-0.2418951	1.5539957
P	0.9702963	0.2419445	-1.5539739
C	0.7192838	-1.9351684	2.4357375
C	0.6126410	-3.0112859	1.3380246
C	-0.5980286	-1.9806274	3.2320722
C	1.9052292	-2.2746168	3.3567231
C	1.3721615	1.1415305	2.8532391
C	0.4795403	1.0289540	4.1028537
C	1.0844770	2.4997761	2.1895967
C	2.8486735	1.1207694	3.2943815
C	1.3723155	-1.1414528	-2.8532050
C	2.8488408	-1.1205837	-3.2942972
C	1.0847064	-2.4997200	-2.1895743
C	0.4797299	-1.0289377	-4.1028504
C	0.7191940	1.9351980	-2.4357238
C	1.9051510	2.2747413	-3.3566596
C	0.6124193	3.0113029	-1.3380108
C	-0.5980880	1.9805546	-3.2321142
H	3.4519627	-0.2693512	1.2520902
H	2.6278240	-1.5087272	0.3057387
H	2.6277111	1.5089075	-0.3056820
H	3.4519690	0.2695961	-1.2520147
H	-0.1779520	-2.7741526	0.6127450
H	0.3567537	-3.9691044	1.8176927
H	1.5547833	-3.1657793	0.7962284
H	-1.4617899	-1.7302192	2.6038689
H	-0.6049796	-1.3071531	4.0939837
H	-0.7294262	-3.0074850	3.6096584
H	2.8701275	-2.2510638	2.8298863
H	1.7684690	-3.2983552	3.7412745
H	1.9655218	-1.6073870	4.2258318
H	-0.5843722	0.9892078	3.8379007
H	0.6442882	1.9276973	4.7192309
H	0.7350709	0.1604502	4.7231841
H	1.7381901	2.6856982	1.3277394
H	1.2788927	3.2976313	2.9247025
H	0.0382201	2.5721152	1.8667034
H	3.5343184	1.3959257	2.4811973
H	3.1667451	0.1550079	3.7070800
H	2.9774651	1.8745957	4.0876116
H	2.9777148	-1.8744008	-4.0875228
H	3.5344785	-1.3956888	-2.4810895
H	3.1668549	-0.1547986	-3.7069855
H	1.2792060	-3.2975601	-2.9246743
H	0.0384434	-2.5721353	-1.8667180
H	1.7384023	-2.6855955	-1.3276940

H	0.6445619	-1.9276693	-4.7192223
H	0.7352221	-0.1604157	-4.7231712
H	-0.5841946	-0.9892657	-3.8379348
H	1.9655345	1.6075138	-4.2257639
H	2.8700289	2.2512682	-2.8297822
H	1.7683236	3.2984674	-3.7412197
H	0.3564788	3.9691036	-1.8176862
H	1.5545252	3.1658667	-0.7961717
H	-0.1781871	2.7741048	-0.6127667
H	-0.6049429	1.3070930	-4.0940365
H	-0.7295579	3.0074063	-3.6096911
H	-1.4618551	1.7300630	-2.6039520

Combination of torsional angles = 40
E(BP86/def2-TZVP) = -8050.74357760205

Ni	-0.5468722	0.0000042	-0.0000034
Br	-2.1556127	-0.9308814	-1.4610203
Br	-2.1556114	0.9308905	1.4610145
C	2.5893063	-0.4665104	0.6087744
C	2.5893043	0.4665134	-0.6087929
P	0.9783618	-0.2729251	1.5435415
P	0.9783561	0.2729302	-1.5435541
C	0.6838286	-1.9855610	2.3696288
C	0.6097634	-3.0364050	1.2454003
C	-0.6679584	-2.0241232	3.1074972
C	1.8255279	-2.3627139	3.3304736
C	1.3832073	1.0611698	2.8901202
C	0.4429275	0.9457955	4.1040833
C	1.1618486	2.4441745	2.2522224
C	2.8426342	0.9828456	3.3799665
C	1.3831915	-1.0611676	-2.8901329
C	2.8426167	-0.9828513	-3.3799856
C	1.1618295	-2.4441702	-2.2522319
C	0.4429070	-0.9457931	-4.1040924
C	0.6838224	1.9855671	-2.3696395
C	1.8255194	2.3627205	-3.3304869
C	0.6097616	3.0364099	-1.2454097
C	-0.6679668	2.0241333	-3.1075036
H	3.4602136	-0.2844121	1.2518091
H	2.6469694	-1.5135102	0.2827402
H	2.6469697	1.5135130	-0.2827584
H	3.4602091	0.2844145	-1.2518306
H	-0.1551884	-2.7796558	0.4997600
H	0.3333322	-4.0027411	1.6958011
H	1.5694599	-3.1841502	0.7329720
H	-1.4995236	-1.7504699	2.4459892
H	-0.7026501	-1.3640510	3.9792230
H	-0.8325073	-3.0545589	3.4613505
H	2.8118289	-2.3362801	2.8446805
H	1.6618757	-3.3950084	3.6801328
H	1.8563859	-1.7203653	4.2194476
H	-0.6116011	0.9462588	3.8005767
H	0.6118241	1.8234187	4.7490879
H	0.6490827	0.0546433	4.7105478
H	1.8457137	2.6276847	1.4130933
H	1.3637991	3.2168804	3.0117556
H	0.1277283	2.5611293	1.9044125
H	3.5632460	1.2630403	2.5994186
H	3.1198058	-0.0034366	3.7722583
H	2.9652926	1.7083349	4.2001741
H	2.9652681	-1.7083427	-4.2001923
H	3.5632305	-1.2630483	-2.5994404
H	3.1197914	0.0034287	-3.7722804
H	1.3637747	-3.2168784	-3.0117641
H	0.1277098	-2.5611204	-1.9044185
H	1.8456961	-2.6276815	-1.4131044
H	0.6117973	-1.8234190	-4.7490949
H	0.6490634	-0.0546439	-4.7105605
H	-0.6116203	-0.9462510	-3.8005814
H	1.8563730	1.7203746	-4.2194628
H	2.8118220	2.3362834	-2.8446973
H	1.6618681	3.3950163	-3.6801426
H	0.3333313	4.0027471	-1.6958087
H	1.5694595	3.1841527	-0.7329833
H	-0.1551890	2.7796612	-0.4997680
H	-0.7026621	1.3640642	-3.9792316
H	-0.8325155	3.0545704	-3.4613530
H	-1.4995304	1.7504790	-2.4459941

Combination of torsional angles = 45
E(BP86/def2-TZVP) = -8050.74183921463

Ni	-0.5400404	-0.0000726	-0.0000137
Br	-2.1403817	-1.0633828	-1.3773808
Br	-2.1406157	1.0629619	1.3772926
C	2.6038475	-0.4700808	0.6063427
C	2.6037914	0.4704748	-0.6062435
P	0.9869757	-0.2948932	1.5336222
P	0.9869870	0.2950101	-1.5335879
C	0.6556069	-2.0205010	2.3168769
C	0.6293820	-3.0589639	1.1796030
C	-0.7321667	-2.0516566	2.9864715
C	1.7459485	-2.4192588	3.3270007
C	1.3852593	1.0007488	2.9161771
C	0.3941656	0.8934539	4.0898068
C	1.2290135	2.3997601	2.2936261
C	2.8227749	0.8723103	3.4581621
C	1.3855508	-1.0005591	-2.9161305
C	2.8230688	-0.8718737	-3.4580502
C	1.2295150	-2.3995999	-2.2935933
C	0.3944923	-0.8934263	-4.0898046
C	0.6553582	2.0205644	-2.3168504
C	1.7456824	2.4195137	-3.3269175
C	0.6288992	3.0590158	-1.1795711
C	-0.7323873	2.0514865	-2.9865139
H	3.4689637	-0.2836952	1.2560888
H	2.6726171	-1.5146045	0.2750108
H	2.6723691	1.5150106	-0.2749096
H	3.4689657	0.2842371	-1.2559547
H	-0.1059351	-2.7958057	0.4072965
H	0.3360839	-4.0298244	1.6092422
H	1.6099501	-3.2008880	0.7059893
H	-1.5277979	-1.7780375	2.2817773
H	-0.8082894	-1.3875794	3.8527425
H	-0.9199648	-3.0800116	3.3346500
H	2.7550184	-2.3915231	2.8903458
H	1.5591525	-3.4562754	3.6501425
H	1.7366526	-1.7924567	4.2272470
H	-0.6470197	0.9319509	3.7445867
H	0.5622965	1.7543141	4.7571890
H	0.5482800	-0.0139375	4.6875862

H	1.9430853	2.5731681	1.4774118
H	1.4342428	3.1537998	3.0708334
H	0.2095127	2.5563708	1.9193190
H	3.5792814	1.1453642	2.7096977
H	3.0587940	-0.1271467	3.8428079
H	2.9348673	1.5807891	4.2946395
H	2.9353195	-1.5803290	-4.2945263
H	3.5795878	-1.1448029	-2.7095528
H	3.0589354	0.1276256	-3.8426800
H	1.4349074	-3.1536010	-3.0707949
H	0.2100241	-2.5563857	-1.9193326
H	1.9435798	-2.5728904	-1.4773478
H	0.5627972	-1.7542561	-4.7571820
H	0.5484823	0.0139929	-4.6875740
H	-0.6467021	-0.9320985	-3.7446317
H	1.7365393	1.7927134	-4.2271668
H	2.7547350	2.3919491	-2.8902121
H	1.5587248	3.4564995	-3.6500647
H	0.3354603	4.0298297	-1.6092198
H	1.6094185	3.2011018	-0.7059052
H	-0.1064135	2.7957290	-0.4073042
H	-0.8083499	1.3874088	-3.8527984
H	-0.9203479	3.0798136	-3.3346868
H	-1.5280060	1.7777182	-2.2818635

Combination of torsional angles = 50
E(BP86/def2-TZVP) = -8050.73953791391

Ni	-0.5324837	0.0000129	-0.0000047
Br	-2.1232273	-1.2016780	-1.2732205
Br	-2.1232160	1.2017388	1.2731924
C	2.6202586	-0.4693187	0.6073310
C	2.6202722	0.4692689	-0.6073258
P	0.9965707	-0.3080699	1.5241426
P	0.9965848	0.3080577	-1.5241451
C	0.6369940	-2.0384359	2.2850234
C	0.6708487	-3.0811422	1.1525561
C	-0.7853527	-2.0616935	2.8797101
C	1.6712313	-2.4379154	3.3520936
C	1.3804113	0.9669364	2.9272300
C	0.3392583	0.8793877	4.0583538
C	1.2836866	2.3722694	2.3065545
C	2.7930176	0.8013406	3.5223550
C	1.3803945	-0.9669688	-2.9272235
C	2.7930069	-0.8014205	-3.5223477
C	1.2836280	-2.3722933	-2.3065357
C	0.3392448	-0.8794036	-4.0583490
C	0.6370505	2.0384308	-2.2850319
C	1.6712991	2.4378865	-3.3520999
C	0.6709262	3.0811387	-1.1525671
C	-0.7852946	2.0617213	-2.8797211
H	3.4783663	-0.2725197	1.2635309
H	2.7017144	-1.5137163	0.2789624
H	2.7017503	1.5136645	-0.2789567
H	3.4783784	0.2724504	-1.2635217
H	-0.0314763	-2.8273457	0.3477345
H	0.3645094	-4.0517638	1.5736187
H	1.6737901	-3.2188017	0.7262551
H	-1.5419125	-1.8116889	2.1245894
H	-0.9117088	-1.3761453	3.7233876
H	-0.9882821	-3.0821982	3.2422367
H	2.7021530	-2.4109654	2.9698348
H	1.4658781	-3.4754160	3.6621545
H	1.6142386	-1.8134489	4.2519371
H	-0.6853210	0.9507057	3.6703328
H	0.5025087	1.7304725	4.7393083
H	0.4414734	-0.0362842	4.6545263
H	2.0268038	2.5289979	1.5128959
H	1.4869845	3.1168099	3.0933592
H	0.2802646	2.5595727	1.9041012
H	3.5833886	1.0529551	2.8018497
H	2.9893399	-0.2023087	3.9169134
H	2.8928821	1.5091913	4.3609676
H	2.8928517	-1.5092822	-4.3609535
H	3.5833692	-1.0530521	-2.8018389
H	2.9893602	0.2022189	-3.9169153
H	1.4869063	-3.1168470	-3.0933330
H	0.2801997	-2.5595640	-1.9040827
H	2.0267388	-2.5290359	-1.5128738
H	0.5024719	-1.7305006	-4.7392938
H	0.4414857	0.0362586	-4.6545318
H	-0.6853369	-0.9506888	-3.6703279
H	1.6142939	1.8134214	-4.2519434
H	2.7022194	2.4109132	-2.9698391
H	1.4659700	3.4753917	-3.6621615
H	0.3646094	4.0517662	-1.5736325
H	1.6738698	3.2187767	-0.7262644
H	-0.0314061	2.8273598	-0.3477463
H	-0.9116659	1.3761744	-3.7233972
H	-0.9881989	3.0822302	-3.2422503
H	-1.5418618	1.8117367	-2.1246012