

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

Schultz, Pleßow, Rominger and Weigel	
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Calculated Minimum Structures and	properties of Nickel(bispho sphine)dihali des	
NidtbpeCl2 P structure		
Cl 2.5471927	-1.5766442	H -1.5682012 4.4357287
-0.1504689		-0.9642039
Cl 2.5471256	1.5766919	H -2.7981065 3.1836237
0.1511000		-1.2767507
Ni 0.9971296	0.0000092	H -1.9728432 3.9803843
0.0001288		-2.6248030
P -0.5131563	1.5872791	C -0.4945598 2.8681423
0.0200176		1.4695084
P -0.5131356	-1.5872769	C 0.4114947 4.0768969
-0.0201218		1.1701799
C -2.1510741	-0.7156613	H 0.0064501 4.7204915
-0.2725648		0.3789581
H -2.3099846	-0.7011318	H 1.4244447 3.7599418
-1.3583231		0.8962115
H -2.9802207	-1.2986855	H 0.4737704 4.6889762
0.1565902		2.0845643
C -2.1511457	0.7156476	C 0.0669127 2.1423379
0.2720749		2.7061939
H -2.3103098	0.7011167	H 0.1301152 2.8631860
1.3577959		3.5374022
H -2.9801976	1.2986634	H 1.0714785 1.7434484
-0.1572743		2.5154559
C -0.7220480	2.5174797	H -0.5890152 1.3259293
-1.6541618		3.0364628
C -1.1099919	1.4719283	C -1.9083767 3.3846738
-2.7142449		1.8094452
H -2.0991856	1.0291310	H -1.8131914 4.1064284
-2.5325992		2.6365030
H -0.3619217	0.6722853	H -2.5830487 2.5912325
-2.7763492		2.1567564
H -1.1517662	1.9679109	H -2.3901489 3.9075475
-3.6969125		0.9751739
C 0.5995491	3.1625071	C -0.4941935 -2.8681310
-2.1086840		-1.4696159
H 0.4355488	3.6114765	C 0.4117959 -4.0768843
-3.1021938		-1.1700855
H 1.4065766	2.4246480	H 0.4742828 -4.6889592
-2.1841209		-2.0844586
H 0.9430608	3.9531183	H 0.0065722 -4.7204840
-1.4339010		-0.3789597
C -1.8292146	3.5859130	H 1.4246819 -3.7599275
-1.6057790		-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 Oscillator
strength

/ Hartree /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	H	1.5851467	-2.6437703
	3.6388359			4.2242915	
C	0.9310047	1.5574377	H	1.7751852	-0.8892399
	2.5876902			4.3553248	
C	0.1147636	1.6158443	H	-0.9543133	1.4583595
	3.8913552			3.7032229	
C	0.4996474	2.7495445	H	0.2422777	2.6206273
	1.7160288			4.3260367	
C	2.4257619	1.7099429	H	0.4650043	0.8932644
	2.9251196			4.6392554	
C	0.8074265	-1.6168399	H	1.0886659	2.8211901
	-2.5879642			0.7941207	
C	2.2859205	-1.8842909	H	0.6633259	3.6796028
	-2.9254824			2.2846055	
C	0.2853733	-2.7720481	H	-0.5636980	2.6840826
	-1.7162206			1.4521112	
C	-0.0111198	-1.6121815	H	3.0478529	1.8431385
	-3.8914849			2.0290475	
C	0.5281621	1.5425472	H	2.8262946	0.8679232
	-2.7648794			3.5047197	
C	1.7948513	1.5872473	H	2.5488351	2.6175385
	-3.6405181			3.5376507	
C	0.4790666	2.8072259	H	2.3385908	-2.7988068
	-1.8860147			-3.5378313	
C	-0.7224164	1.5872318	H	2.8959250	-2.0648752
	-3.6623200			-2.0293957	
H	3.0527539	-0.1633327	H	2.7501557	-1.0757549
	1.2814755			-3.5052396	
H	2.2047221	-1.5203865	H	0.3769887	-3.7120126
	0.5408019			-2.2846902	
H	2.3148376	1.3540136	H	-0.7698558	-2.6248892
	-0.5416753			-1.4525169	
H	3.0562459	-0.0640071	H	0.8668617	-2.8886904
	-1.2825971			-0.7941646	
H	-0.5920552	-2.7423752	H	0.0386929	-2.6237674
	1.1994156			-4.3262649	
H	0.0793666	-3.6909293	H	0.3934052	-0.9185833
	2.5448951			-4.6394048	
H	1.1634731	-3.0563949	H	-1.0648685	-1.3730578
	1.3036094			-3.7030144	
H	-1.7572402	-1.3920982	H	1.8360265	0.7569731
	3.0757344			-4.3572189	
H	-0.8044165	-0.7168935	H	2.7219589	1.5850139
	4.4059289			-3.0501395	
H	-0.8988203	-2.4743363	H	1.7829677	2.5209400
	4.2091613			-4.2258056	
H	2.5929423	-1.7838209	H	0.3635764	3.6816492
	3.0476228			-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

Excitation Energy Oscillator
 strength
 / Hartree /mixed
 representation

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

 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

 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

Nidtbpel2 P structure

I 1.9954625 -1.7308072
 -0.4713829

I	1.9954290	1.7306939	C	-0.6801774	4.3388067
	0.4685300			0.3013698	
Ni	0.1624346	-0.0003227	H	-0.9983202	4.7301576
	-0.0005139			-0.6734204	
P	-1.3855578	1.5761882	H	0.3723185	4.0362855
	-0.2663823			0.2427626	
P	-1.3848260	-1.5772880	H	-0.7566097	5.1677695
	0.2669140			1.0236254	
C	-3.0262452	-0.7572949	C	-1.1891756	2.8441239
	-0.0994285			2.2431681	
H	-3.2256015	-0.9920493	H	-1.2811913	3.7536299
	-1.1529072			2.8584352	
H	-3.8333846	-1.2281890	H	-0.1521298	2.4900210
	0.4817685			2.3074697	
C	-3.0263621	0.7557195	H	-1.8543726	2.0879076
	0.1016367			2.6819120	
H	-3.2247088	0.9904170	C	-3.0391934	3.7041627
	1.1553184			0.8109081	
H	-3.8342320	1.2263780	H	-3.0595486	4.6281110
	-0.4787361			1.4107988	
C	-1.4498185	2.0384356	H	-3.7367573	3.0029345
	-2.1358426			1.2861522	
C	-1.6920879	0.7350874	H	-3.4231607	3.9551245
	-2.9169005			-0.1841187	
H	-2.6929141	0.3183387	C	-1.5812820	-3.1937002
	-2.7363444			-0.7947571	
H	-0.9369987	-0.0238950	C	-0.6792194	-4.3396979
	-2.6740051			-0.3015788	
H	-1.6188692	0.9508952	H	-0.7561434	-5.1686763
	-3.9947841			-1.0237643	
C	-0.0943765	2.6065951	H	-0.9962563	-4.7311510
	-2.5949282			0.6735304	
H	-0.1519013	2.8032393	H	0.3732460	-4.0368682
	-3.6779940			-0.2440373	
H	0.7231871	1.8968863	C	-1.1906199	-2.8451448
	-2.4171865			-2.2428452	
H	0.1686211	3.5454618	H	-1.2829866	-3.7546726
	-2.0961325			-2.8580272	
C	-2.5734994	3.0279666	H	-0.1537457	-2.4907307
	-2.4884841			-2.3081944	
H	-2.4014511	4.0291291	H	-1.8564865	-2.0891235
	-2.0759841			-2.6809074	
H	-3.5646057	2.6800693	C	-3.0389355	-3.7057346
	-2.1635763			-0.8087226	
H	-2.6114526	3.1307761	H	-3.7371839	-3.0046996
	-3.5852065			-1.2832458	
C	-1.5814058	3.1925502	H	-3.4218198	-3.9568273
	0.7954720			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

Excitation Energy Oscillator
strength
/ Hartree /mixed
representation

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

Nidtbpel2 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	H	10.1142428	-0.7727075
	9.6158083			10.7298563	
C	11.2667441	-0.0636468	H	12.5781866	1.8610330
	3.1276051			8.3010017	
C	12.6034691	-0.7673927	H	12.2480848	2.1111794
	2.8226737			10.0230795	
C	10.1825265	-1.1428902	H	10.9653529	2.4183096
	3.2939716			8.8227037	
C	10.8872084	0.8082426	H	13.4150250	-0.4086462
	1.9167388			8.9066906	
C	12.1736256	2.6781362	H	12.3694582	-1.6190888
	4.4636505			9.6952474	
C	13.5536275	2.5109078	H	12.9526587	-0.2126806
	3.8008852			10.6002943	
C	12.3532334	3.3490563	H	12.5096578	-1.2652159
	5.8397748			1.8442160	
C	11.3062052	3.6279047	H	12.8445614	-1.5500571
	3.6190315			3.5550259	
H	12.6756063	-1.5115067	H	13.4535404	-0.0762424
	7.2981462			2.7567055	
H	11.5337724	-1.7941239	H	10.1076137	-1.7136061
	5.9844015			2.3540483	
H	13.1003297	0.8154518	H	9.2014349	-0.6997664
	6.4426081			3.5079044	
H	13.4232558	-0.3522639	H	10.4290036	-1.8566936
	5.1612345			4.0899044	
H	8.4510451	-1.4966588	H	10.7194009	0.1396683
	5.9306450			1.0566909	
H	8.1771006	-3.0944011	H	11.6878766	1.5037869
	6.6642441			1.6346393	
H	9.7375369	-2.7341589	H	9.9613992	1.3704220
	5.9173776			2.0926587	
H	7.5319625	-0.6744294	H	13.4806707	2.1368555
	8.2059392			2.7716280	
H	8.3249895	-1.1393118	H	14.2196048	1.8455898
	9.7188973			4.3682299	
H	7.5014829	-2.3713557	H	14.0415400	3.4979829
	8.7466782			3.7539043	
H	11.0753704	-3.2237431	H	12.7134132	4.3774984
	8.0714875			5.6799994	
H	9.5110176	-3.8232838	H	13.0971571	2.8435005
	8.6483354			6.4687600	
H	10.4238676	-2.6745545	H	11.4043481	3.4049566
	9.6379596			6.3916973	
H	9.4431856	0.8078722	H	11.1491203	3.2773509
	10.2201322			2.5948529	
H	10.8514458	0.7307892	H	11.8255623	4.5983841
	11.3032814			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 Oscillator
strength
/ Hartree /mixed
representation

0.1467994741905383
0.6358269330584271E-02
0.1411615611975419
0.1577407259468574E-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 Oscillator
 strength
 / Hartree /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	C	0.1757103	-2.3647425
	-0.0548418			-1.5432970	
C	-0.0466508	2.3690019	C	-0.7216494	-2.2076244
	1.5413224			-2.6099294	
C	1.0378719	3.2479674	C	-0.4520199	-2.7967953
	1.7111057			-3.8483365	
C	1.2616943	3.8621270	C	0.7103101	-3.5486124
	2.9441110			-4.0312913	
C	0.4068477	3.6042456	C	1.6060815	-3.7160306
	4.0204977			-2.9704178	
C	-0.6747961	2.7363663	C	1.3419825	-3.1271760
	3.8574523			-1.7330350	
C	-0.9040170	2.1212072	H	-1.6412743	-1.6418298
	2.6235224			-2.4534941	
H	1.7045403	3.4694180	H	-1.1595667	-2.6713044
	0.8755623			-4.6690110	
H	2.1036708	4.5456465	H	0.9178603	-4.0099631
	3.0633986			-4.9979726	
H	0.5827825	4.0854671	H	2.5118132	-4.3091654
	4.9837577			-3.1052552	
H	-1.3509583	2.5393862	H	2.0426078	-3.2777678
	4.6904418			-0.9095993	
H	-1.7628940	1.4632077	C	-0.1327911	-2.8303469
	2.4830164			1.3391413	
C	-0.4591342	2.8003765	C	0.0723792	-2.4717230
	-1.3328664			2.6817190	
C	-0.8437314	4.1092167	C	0.0505655	-3.4428572
	-1.0057790			3.6833953	
C	-0.9865167	5.0710348	C	-0.1848921	-4.7809949
	-2.0074881			3.3571125	
C	-0.7579579	4.7358228	C	-0.4068889	-5.1416229
	-3.3439676			2.0261479	
C	-0.3921701	3.4294625	C	-0.3867552	-4.1728656
	-3.6788725			1.0211485	
C	-0.2474836	2.4654529	H	0.2295262	-1.4274631
	-2.6805196			2.9572654	
H	-1.0435020	4.3738433	H	0.2102593	-3.1507573
	0.0320496			4.7222098	
H	-1.2882795	6.0847871	H	-0.2056017	-5.5394315
	-1.7406374			4.1408999	
H	-0.8747808	5.4882547	H	-0.6076369	-6.1819115
	-4.1251073			1.7664416	
H	-0.2262051	3.1559061	H	-0.5808045	-4.4594804
	-4.7217418			-0.0119282	
H	0.0109436	1.4432147	C	1.3596738	0.7353499
	-2.9621372			-0.3952506	
P	-0.1495930	-1.5233025	C	1.4380047	-0.5865163
	0.0575263			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 Oscillator
 strength
 / Hartree /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

Nidppel2

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

 Excitation Energy Oscillator
 strength
 / Hartree /mixed
 representation

 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 Oscillator
strength
/ Hartree /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

Nidpppl2

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	C	-1.0844346	-2.2062569
	-1.9301352			-2.1815938	
H	-1.6713913	1.7337589	C	-0.1067251	-3.3937566
	-2.5385055			-2.1707740	
H	-2.6322271	3.2021365	H	0.1954914	-3.6073022
	-2.7882418			-3.2083875	
C	-0.7233693	3.9481756	H	-0.5665459	-4.3065619
	-1.1527949			-1.7705903	
H	-1.1241792	4.7378247	H	0.8024303	-3.1731457
	-1.8102488			-1.5933749	
H	0.0679906	3.4135213	C	-0.4391469	-1.0569047
	-1.6889102			-2.9788840	
H	-0.2632267	4.4380785	H	-0.2272050	-1.4146187
	-0.2883162			-3.9997598	
C	-3.0057905	3.8794284	H	0.5044512	-0.7152914
	-0.1525488			-2.5316429	
H	-2.6363754	4.5033339	H	-1.1066625	-0.1893304
	0.6705697			-3.0689060	
H	-3.8654051	3.2978491	C	-2.3863980	-2.6113989
	0.2079610			-2.8989196	
H	-3.3807546	4.5631412	H	-3.1023392	-1.7816844
	-0.9315010			-2.9754423	
C	-1.0839735	2.2063151	H	-2.8932742	-3.4621869
	2.1816209			-2.4317634	
C	-0.1062158	3.3937735	H	-2.1291476	-2.9074119
	2.1706307			-3.9288569	
H	-0.5660636	4.3065952	C	-1.8875455	-3.0183268
	1.7705150			0.7707195	
H	0.8028353	3.1731193	C	-2.4178709	-2.3911687
	1.5930836			2.0744347	
H	0.1961809	3.6073146	H	-3.3531290	-1.8332315
	3.2081926			1.9305541	
C	-0.4386014	1.0569376	H	-1.6710231	-1.7336733
	2.9788067			2.5386322	
H	-0.2264712	1.4146464	H	-2.6318870	-3.2020035
	3.9996452			2.7885406	
H	0.5049063	0.7152811	C	-3.0059406	-3.8792867
	2.5314078			0.1529157	
H	-1.1061400	0.1893933	H	-3.3808029	-4.5629774
	3.0689446			0.9319363	
C	-2.3857996	2.6115166	H	-2.6366986	-4.5032147
	2.8991624			-0.6702633	
H	-2.1283648	2.9075195	H	-3.8655895	-3.2976677
	3.9290565			-0.2074483	
H	-3.1017655	1.7818346	C	-0.7233495	-3.9481404
	2.9758051			1.1527667	
H	-2.8927152	3.4623270	H	0.0681298	-3.4135222
	2.4320891			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	P	-1.3585501	1.5733062
	-2.4871997			0.2973294	
H	-1.0268141	-0.2790484	P	-1.3585052	-1.5733438
	-3.0427792			-0.2973711	
C	-2.4007348	-2.6545704	C	-2.9537785	-0.6124918
	-2.8310357			-0.4587911	
H	-3.0780098	-1.7984238	H	-3.0265712	-0.2991834
	-2.9526398			-1.5074134	
H	-2.9502580	-3.4612460	H	-3.8255059	-1.2531082
	-2.3340513			-0.2591816	
H	-2.1458550	-3.0063447	C	-2.9538408	0.6124480
	-3.8438293			0.4585415	
C	-1.8914245	-2.9868443	H	-3.0267693	0.2991390
	0.8659427			1.5071544	
C	-2.4402102	-2.3192731	H	-3.8255445	1.2530610
	2.1417912			0.2588182	
H	-3.3785534	-1.7748738	C	-1.8820839	2.9476792
	1.9696046			-0.9722827	
H	-1.7043679	-1.6394286	C	-2.4264800	2.2325952
	2.5914963			-2.2240370	
H	-2.6546696	-3.1069675	H	-3.3675953	1.6985885
	2.8811970			-2.0356172	
C	-3.0013851	-3.8691476	H	-1.6911953	1.5330799
	0.2628365			-2.6434686	
H	-3.3757088	-4.5371891	H	-2.6344610	2.9916811
	1.0555336			-2.9945536	
H	-2.6260253	-4.5088459	C	-0.7198157	3.8442785
	-0.5453170			-1.4305483	
H	-3.8626916	-3.2999998	H	-1.1281385	4.5941814
	-0.1130665			-2.1288061	
C	-0.7307629	-3.9006253	H	0.0583143	3.2723946
	1.2939131			-1.9468445	
H	0.0467256	-3.3486509	H	-0.2387638	4.3807723
	1.8324176			-0.6061756	
H	-0.2490091	-4.4077609	C	-2.9956485	3.8507926
	0.4514931			-0.4075628	
H	-1.1411948	-4.6756867	H	-2.6288528	4.5131868
	1.9628026			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	
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				

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	H	-2.2655741	3.2664235
	0.2119937			3.6108847	
C	-1.8641696	2.9015684	H	-3.1015166	1.9109811
	-1.0815859			2.8470989	
C	-2.3922163	2.1357030	H	-3.0835331	3.5061890
	-2.3099403			2.0594544	
H	-3.3365759	1.6109846	C	-1.1411244	-2.4428527
	-2.1121651			-1.9698841	
H	-1.6525828	1.4185622	C	-0.2839198	-3.7158792
	-2.6898276			-1.8641620	
H	-2.5887312	2.8623539	H	-0.0553504	-4.0638553
	-3.1140091			-2.8843537	
C	-0.6957247	3.7787162	H	-0.8086533	-4.5326237
	-1.5607583			-1.3518251	
H	-1.0937340	4.4972321	H	0.6679257	-3.5259476
	-2.2969311			-1.3498481	
H	0.0899983	3.1858846	C	-0.3999810	-1.4356335
	-2.0408676			-2.8704372	
H	-0.2266316	4.3500171	H	-0.2480207	-1.8933681
	-0.7530741			-3.8616767	
C	-2.9866132	3.8248912	H	0.5830190	-1.1658360
	-0.5694474			-2.4615341	
H	-2.6357179	4.5138979	H	-0.9751954	-0.5119559
	0.2083650			-3.0206763	
H	-3.8610827	3.2813136	C	-2.4846422	-2.7952174
	-0.1862302			-2.6389649	
H	-3.3344661	4.4412835	H	-3.1018860	-1.9111703
	-1.4142808			-2.8467585	
C	-1.1409155	2.4427505	H	-3.0837117	-3.5063729
	1.9699181			-2.0591077	
C	-0.2837821	3.7158142	H	-2.2660076	-3.2665822
	1.8640650			-3.6106685	
H	-0.8086319	4.5325383	C	-1.8638717	-2.9016833
	1.3518144			1.0817404	
H	0.6679899	3.5259255	C	-2.3917522	-2.1358292
	1.3495993			2.3101735	
H	-0.0550658	4.0637961	H	-3.3361634	-1.6111481
	2.8842217			2.1125449	
C	-0.3995864	1.4355579	H	-1.6520854	-1.4186573
	2.8703484			2.6899379	
H	-0.2474892	1.8932934	H	-2.5881112	-2.8624818
	3.8615664			3.1142787	
H	0.5833607	1.1658054	C	-2.9863595	-3.8250563
	2.4612884			0.5697889	
H	-0.9747370	0.5118543	H	-3.3340518	-4.4414564
	3.0206731			1.4146828	
C	-2.4843424	2.7950551	H	-2.6355600	-4.5140546
	2.6392130			-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	I	2.0308842	-1.7603363
	-1.2666767			0.2972517	
C	-0.4396858	-1.5802378	I	2.0310665	1.7601695
	-2.8441122			-0.2971283	
H	-0.3200343	-2.0804005	Ni	0.1810262	0.0000058
	-3.8190988			0.0000190	
H	0.5576479	-1.3202171	P	-1.3601949	1.6010705
	-2.4653507			0.1548544	
H	-0.9963598	-0.6496350	P	-1.3603406	-1.6009137
	-3.0195503			-0.1548766	
C	-2.5481730	-2.8839260	C	-2.9614366	-0.6613874
	-2.5183007			-0.3820514	
H	-3.1450138	-1.9970789	H	-3.0547831	-0.4734336
	-2.7685402			-1.4580348	
H	-3.1570638	-3.5448102	H	-3.8258071	-1.2786882
	-1.8908358			-0.0954200	
H	-2.3563209	-3.4155268	C	-2.9613876	0.6616960
	-3.4641598			0.3819747	
C	-1.8407049	-2.8478997	H	-3.0547878	0.4737504
	1.1956682			1.4579550	
C	-2.3419627	-2.0279381	H	-3.8256905	1.2790784
	2.3997818			0.0953143	
H	-3.2900771	-1.5113494	C	-1.8109570	2.7845594
	2.1987319			-1.3159799	
H	-1.5941042	-1.2955693	C	-2.2763857	1.9058498
	2.7310760			-2.4922824	
H	-2.5217365	-2.7178397	H	-3.2284535	1.3960880
	3.2393580			-2.2924674	
C	-2.9753404	-3.7903917	H	-1.5175136	1.1611642
	0.7496456			-2.7656437	
H	-3.3004189	-4.3731836	H	-2.4343956	2.5533123
	1.6267698			-3.3692157	
H	-2.6463743	-4.5091590	C	-0.6177777	3.6161657
	-0.0104247			-1.8146889	
H	-3.8599107	-3.2607180	H	-0.9729500	4.2540823
	0.3701011			-2.6413342	
C	-0.6615366	-3.7032077	H	0.1937788	2.9823766
	1.6875730			-2.1884020	
H	0.1360366	-3.0893301	H	-0.1949084	4.2681326
	2.1195998			-1.0434780	
H	-0.2125942	-4.3130856	C	-2.9596614	3.7438970
	0.8968418			-0.9493474	
H	-1.0414124	-4.3846324	H	-2.6571019	4.4971576
	2.4672557			-0.2122286	
			H	-3.8552026	3.2288370
				-0.5753103	
			H	-3.2574323	4.2853607
				-1.8619220	
Combination of torsional					
angles = -15					
E(BP86/def2-TZVP) =					
-3497.56664805441					

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	H	0.4374240	1.6203270
	-0.0289060			2.4809611	
C	-2.9663949	0.6782960	H	-1.1344502	0.9790839
	0.3506218			3.0273847	
H	-3.0705420	0.5400279	C	-2.6961192	3.1010345
	1.4331258			2.2084823	
H	-3.8262507	1.2844094	H	-2.5655611	3.7471384
	0.0285869			3.0912901	
C	-1.7710256	2.7106065	H	-3.2820052	2.2325324
	-1.4382453			2.5358665	
C	-2.1915596	1.7691898	H	-3.2893976	3.6638244
	-2.5820173			1.4784989	
H	-3.1471134	1.2637882	C	-1.2922149	-2.7220016
	-2.3877165			-1.6912586	
H	-1.4194128	1.0168965	C	-0.4923913	-4.0177948
	-2.7887487			-1.4675051	
H	-2.3230975	2.3686375	H	-0.3768087	-4.5199573
	-3.4966874			-2.4416236	
C	-0.5622077	3.5189650	H	-1.0085418	-4.7201325
	-1.9378351			-0.8005550	
H	-0.8873166	4.1074201	H	0.5096618	-3.8154540
	-2.8120810			-1.0687122	
H	0.2645215	2.8689239	C	-0.5820115	-1.8957163
	-2.2448513			-2.7798217	
H	-0.1705385	4.2153903	H	-0.5221943	-2.5000944
	-1.1894112			-3.6995709	
C	-2.9350346	3.6814443	H	0.4376785	-1.6202844
	-1.1623970			-2.4807816	
H	-2.6628069	4.4728137	H	-1.1341203	-0.9790090
	-0.4540204			-3.0273847	
H	-3.8414476	3.1803920	C	-2.6959152	-3.1009556
	-0.7953788			-2.2087284	
H	-3.2019194	4.1741005	H	-3.2817471	-2.2324380
	-2.1114245			-2.5361682	
C	-1.2923589	2.7220493	H	-3.2892950	-3.6637536
	1.6912002			-1.4788353	
C	-0.4925000	4.0178316	H	-2.5652533	-3.7470408
	1.4675111			-3.0915346	
H	-1.0085657	4.7201549	C	-1.7712463	-2.7105766
	0.8004788			1.4381534	
H	0.5096002	3.8154747	C	-2.1918873	-1.7691536
	1.0688453			2.5818794	
H	-0.3770333	4.5200188	H	-3.1474090	-1.2637320
	2.4416304			2.3874734	
C	-0.5822993	1.8957783	H	-1.4197477	-1.0168775
	2.7798691			2.7886974	
H	-0.5225877	2.5001760	H	-2.3235392	-2.3686002
	3.6996123			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	H	-0.6295270	4.8916089
	0.0458609			1.8726552	
C	-2.9830281	-0.7204674	C	-0.8557776	2.3521125
	-0.2500481			2.6194525	
H	-3.1268159	-0.7369186	H	-0.8765209	3.1090553
	-1.3371574			3.4201185	
H	-3.8236805	-1.2829296	H	0.1845670	2.0338756
	0.1829952			2.4733842	
C	-2.9829125	0.7208017	H	-1.4446655	1.4935254
	0.2502775			2.9692298	
H	-3.1265739	0.7372711	C	-2.8957614	3.4100314
	1.3374034			1.6434092	
H	-3.8235465	1.2833656	H	-2.8518619	4.2005514
	-0.1826701			2.4095111	
C	-1.6193896	2.4468957	H	-3.5122298	2.6023020
	-1.7714217			2.0577534	
C	-1.9047205	1.3233245	H	-3.4133389	3.8299597
	-2.7838282			0.7731901	
H	-2.8725612	0.8332965	C	-1.4462022	-2.9729907
	-2.6111515			-1.3401429	
H	-1.1097588	0.5664448	C	-0.6363951	-4.2341084
	-2.7742870			-0.9881894	
H	-1.9385601	1.7609091	H	-0.6303260	-4.8915627
	-3.7942228			-1.8726916	
C	-0.3557156	3.1798554	H	-1.0863277	-4.8043593
	-2.2535873			-0.1654547	
H	-0.5670908	3.6005226	H	0.4034828	-3.9955137
	-3.2506400			-0.7344757	
H	0.5008129	2.5012352	C	-0.8563548	-2.3520414
	-2.3393997			-2.6194665	
H	-0.0579338	4.0036369	H	-0.8772778	-3.1089832
	-1.5969467			-3.4201288	
C	-2.8066987	3.4268816	H	0.1840440	-2.0339288
	-1.7866987			-2.4735143	
H	-2.6179543	4.3266692	H	-1.4451787	-1.4933844
	-1.1891444			-2.9691802	
H	-3.7466713	2.9709371	C	-2.8963565	-3.4097158
	-1.4454266			-1.6431950	
H	-2.9677058	3.7560341	H	-3.5127745	-2.6019156
	-2.8260981			-2.0574754	
C	-1.4456928	2.9731351	H	-3.4138883	-3.8295787
	1.3401956			-0.7729172	
C	-0.6357739	4.2341563	H	-2.8526352	-4.2002447
	0.9881531			-2.4092980	
H	-1.0857298	4.8044622	C	-1.6194793	-2.4467274
	0.1654691			1.7714949	
H	0.4040472	3.9954374	C	-1.9045520	-1.3231214
	0.7343229			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	C	-0.6735910	4.3309046
	0.3960511			0.4730378	
Ni	0.1775545	-0.0000128	H	-1.0227363	4.7660588
	-0.0000122			-0.4721297	
P	-1.3692098	1.5888150	H	0.3797064	4.0435515
	-0.2087712			0.3706830	
P	-1.3691169	-1.5889240	H	-0.7386820	5.1223202
	0.2087959			1.2373157	
C	-3.0054105	-0.7503816	C	-1.1134098	2.7368578
	-0.1382595			2.3515498	
H	-3.1924062	-0.9315281	H	-1.1945753	3.6141135
	-1.2043131			3.0134504	
H	-3.8205010	-1.2477106	H	-0.0725110	2.3887134
	0.4087189			2.3692329	
C	-3.0054472	0.7501838	H	-1.7601665	1.9540222
	0.1383345			2.7704755	
H	-3.1924197	0.9313197	C	-3.0104373	3.6476881
	1.2043940			1.0135010	
H	-3.8205816	1.2474685	H	-3.0215002	4.5447075
	-0.4086185			1.6531133	
C	-1.4715048	2.1412653	H	-3.6884011	2.9201513
	-2.0533498			1.4772879	
C	-1.7097363	0.8738391	H	-3.4246303	3.9376326
	-2.8927546			0.0413043	
H	-2.7021918	0.4352814	C	-1.5492102	-3.1517832
	-2.7186174			-0.9342937	
H	-0.9413948	0.1142965	C	-0.6733649	-4.3309728
	-2.6976490			-0.4730519	
H	-1.6552577	1.1420520	H	-0.7384329	-5.1223846
	-3.9599061			-1.2373358	
C	-0.1370062	2.7536781	H	-1.0224581	-4.7661563
	-2.5156616			0.4721210	
H	-0.2255907	3.0018945	H	0.3799191	-4.0435609
	-3.5860394			-0.3707248	
H	0.6959281	2.0506116	C	-1.1133272	-2.7369367
	-2.3929558			-2.3515366	
H	0.1238869	3.6713843	H	-1.1944624	-3.6141918
	-1.9781376			-3.0134417	
C	-2.6168779	3.1294498	H	-0.0724482	-2.3887341
	-2.3336743			-2.3692461	
H	-2.4500524	4.1114843	H	-1.7601391	-1.9541337
	-1.8754900			-2.7704381	
H	-3.5962314	2.7516741	C	-3.0102665	-3.6478813
	-2.0067285			-1.0134433	
H	-2.6791785	3.2858336	H	-3.6882827	-2.9203780
	-3.4229106			-1.4772060	
C	-1.5493559	3.1516695	H	-3.4244175	-3.9378565
	0.9343159			-0.0412382	

H	-3.0212973	-4.5448960	C	-3.0109275	0.7563373
	-1.6530627			0.1027935	
C	-1.4713264	-2.1413771	H	-3.2117181	0.9882827
	2.0533795			1.1566535	
C	-1.7096030	-0.8739617	H	-3.8171246	1.2290035
	2.8927872			-0.4782893	
H	-2.7020877	-0.4354590	C	-1.4262219	2.0457794
	2.7186775			-2.1266761	
H	-0.9413087	-0.1143777	C	-1.6700243	0.7457992
	2.6976566			-2.9128276	
H	-1.6550782	-1.1421680	H	-2.6724527	0.3312080
	3.9599380			-2.7360833	
C	-2.6166375	-3.1296220	H	-0.9176158	-0.0160801
	2.3337443			-2.6707424	
H	-2.6788967	-3.2860022	H	-1.5936010	0.9651428
	3.4229836			-3.9897775	
H	-2.4497728	-4.1116503	C	-0.0669038	2.6108873
	1.8755616			-2.5782378	
H	-3.5960213	-2.7519013	H	-0.1189616	2.8113137
	2.0068259			-3.6608749	
C	-0.1367802	-2.7537126	H	0.7474526	1.8977229
	2.5156566			-2.3993388	
H	0.6961106	-2.0505992	H	0.1970686	3.5472208
	2.3929250			-2.0751528	
H	0.1241504	-3.6714059	C	-2.5453854	3.0399996
	1.9781296			-2.4803149	
H	-0.2253210	-3.0019294	H	-2.3718265	4.0393126
	3.5860381			-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	
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				

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	H	-0.7240542	-5.1859359
	-4.0130485			-0.8694354	
C	-0.0045348	2.4675411	H	-0.9103116	-4.6853639
	-2.6321244			0.8173123	
H	-0.0236659	2.6251280	H	0.4092356	-4.0020793
	-3.7228205			-0.1786084	
H	0.7868903	1.7421731	C	-1.2501434	-2.9201992
	-2.4040671			-2.1608152	
H	0.2696134	3.4170621	H	-1.3501995	-3.8544947
	-2.1597507			-2.7363593	
C	-2.4758831	2.9565206	H	-0.2221888	-2.5535650
	-2.6122647			-2.2789248	
H	-2.2886985	3.9686969	H	-1.9443862	-2.1923253
	-2.2348779			-2.6027296	
H	-3.4833051	2.6457576	C	-3.0290866	-3.7539164
	-2.2998986			-0.6290237	
H	-2.4834212	3.0164761	H	-3.7560948	-3.0766753
	-3.7128168			-1.0951234	
C	-1.5806022	3.2190467	H	-3.3693835	-3.9826097
	0.6867482			0.3867601	
C	-0.6379636	4.3273390	H	-3.0579244	-4.6944877
	0.1838702			-1.2022604	
H	-0.9100157	4.6854451	C	-1.3882890	-1.9533592
	-0.8172750			2.1924917	
H	0.4095437	4.0020490	C	-1.6473382	-0.6278386
	0.1785525			2.9293566	
H	-0.7236145	5.1859801	H	-2.6599481	-0.2400729
	0.8694672			2.7488058	
C	-1.2497907	2.9202723	H	-0.9128661	0.1377753
	2.1608513			2.6479945	
H	-1.3497421	3.8545698	H	-1.5538783	-0.8027245
	2.7364105			4.0131028	
H	-0.2218556	2.5535616	C	-2.4759365	-2.9563538
	2.2788927			2.6123563	
H	-1.9440591	2.1924451	H	-2.4834088	-3.0163234
	2.6028027			3.7129081	
C	-3.0287695	3.7541334	H	-2.2888499	-3.9685390
	0.6291848			2.2349436	
H	-3.0575013	4.6946994	H	-3.4833558	-2.6455133
	1.2024355			2.3000584	
H	-3.7557965	3.0769392	C	-0.0045523	-2.4675576
	1.0953235			2.6320638	
H	-3.3691165	3.9828645	H	0.7869131	-1.7422475
	-0.3865733			2.4039618	
C	-1.5808842	-3.2189361	H	0.2694927	-3.4170951
	-0.6866882			2.1596622	
C	-0.6382961	-4.3272918	H	-0.0236239	-2.6251543
	-0.1838555			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	H	-3.2130146	4.0365768
	-2.9761217			-0.9419224	
H	-2.6798245	0.0088464	C	-1.5724846	-3.2627398
	-2.7746436			-0.3411949	
H	-0.9589051	-0.4615637	C	-0.5150278	-4.2446325
	-2.6097309			0.1935168	
H	-1.5273545	0.3737721	H	-0.5871986	-5.1797033
	-4.0701695			-0.3851753	
C	0.1269019	2.0566305	H	-0.6774835	-4.5027429
	-2.7899453			1.2477449	
H	0.1703242	2.1014279	H	0.5030883	-3.8526951
	-3.8902500			0.0711089	
H	0.8500391	1.3019016	C	-1.3763819	-3.1120416
	-2.4518479			-1.8616889	
H	0.4477108	3.0297401	H	-1.4656446	-4.1092794
	-2.4012167			-2.3218473	
C	-2.3028510	2.7130161	H	-0.3835640	-2.7119454
	-2.9451644			-2.1052278	
H	-2.0550961	3.7453284	H	-2.1452487	-2.4754461
	-2.6717726			-2.3210530	
H	-3.3418331	2.5090279	C	-2.9769608	-3.8628393
	-2.6485004			-0.1128002	
H	-2.2622296	2.6499081	H	-3.7768941	-3.2521756
	-4.0448577			-0.5519094	
C	-1.5724529	3.2628691	H	-3.2131320	-4.0364295
	0.3411902			0.9418192	
C	-0.5149523	4.2447439	H	-3.0078936	-4.8405760
	-0.1934675			-0.6202353	
H	-0.6773458	4.5028513	C	-1.3103695	-1.6884360
	-1.2477060			2.3715923	
H	0.5031514	3.8527925	C	-1.6427936	-0.3136524
	-0.0710011			2.9761118	
H	-0.5871418	5.1798186	H	-2.6799779	-0.0086930
	0.3852160			2.7745753	
C	-1.3764382	3.1121724	H	-0.9590422	0.4616899
	1.8616958			2.6097555	
H	-1.4657119	4.1094129	H	-1.5275850	-0.3736311
	2.3218461			4.0701662	
H	-0.3836400	2.7120621	C	-2.3030545	-2.7128666
	2.1052921			2.9451315	
H	-2.1453405	2.4755899	H	-2.2624918	-2.6497515
	2.3210186			4.0448265	
C	-2.9769070	3.8629880	H	-2.0553003	-3.7451844
	0.1127119			2.6717606	
H	-3.0078549	4.8407275	H	-3.3420175	-2.5088647
	0.6201406			2.6484098	
H	-3.7768746	3.2523380	C	0.1267168	-2.0565178
	0.5517774			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 Ni₂dtbpe**

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	H	0.6295048	-0.7723003
	2.8801699			4.7857406	
C	1.1661213	-2.8560087	H	0.5334119	-2.5249214
	2.0823165			4.5790245	
C	0.4250277	-1.5608459	H	3.6303292	-1.7317618
	4.0558150			2.7228317	
C	2.8431880	-1.5975254	H	2.9048983	-2.4544274
	3.4752077			4.1651466	
C	1.4557533	1.6213462	H	3.0692053	-0.6966965
	2.4956906			4.0618773	
C	0.7852825	1.6412142	H	-0.2449641	1.2634726
	3.8796921			3.8433602	
C	0.7445561	2.6692329	H	0.7485877	2.6870396
	1.6209800			4.2252231	
C	2.9331951	2.0216228	H	1.3536347	1.0722049
	2.6534559			4.6257524	
C	1.4539624	-1.6216815	H	1.1799853	2.7404218
	-2.4959625			0.6182889	
C	2.9310073	-2.0233124	H	0.8437826	3.6572671
	-2.6539887			2.1002276	
C	0.7419675	-2.6689008	H	-0.3250297	2.4440277
	-1.6210994			1.5134447	
C	0.7832108	-1.6409603	H	3.4418820	2.1538081
	-3.8798361			1.6884003	
C	1.4215963	1.5627138	H	3.5086145	1.3038020
	-2.8804573			3.2535096	
C	2.8443863	1.5960460	H	2.9755617	2.9914014
	-3.4755084			3.1748542	
C	1.1683900	2.8559205	H	2.9723931	-2.9931339
	-2.0825954			-3.1753862	
C	0.4262065	1.5613654	H	3.4397462	-2.1559534
	-4.0561074			-1.6890227	
H	3.7248595	-0.0342520	H	3.5069752	-1.3060226
	1.2758196			-3.2541523	
H	2.9517654	-1.4364280	H	0.8401785	-3.6570300
	0.5371260			-2.1003597	
H	2.9530330	1.4346958	H	-0.3273883	-2.4427018
	-0.5375665			-1.5133494	
H	3.7247638	0.0318097	H	1.1775350	-2.7404902
	-1.2763410			-0.6184974	
H	0.1617240	-2.8602784	H	0.7454206	-2.6867672
	1.6379885			-4.2253064	
H	1.2358400	-3.7119807	H	1.3519856	-1.0725497
	2.7720279			-4.6260289	
H	1.9073086	-3.0257300	H	-0.2466557	-1.2621991
	1.2897867			-3.8433368	
H	-0.6133406	-1.4672886	H	3.0696597	0.6950115
	3.7200295			-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	H	1.0899374	-3.9121125
	-0.6378142			2.3484953	
P	1.2744718	-0.1915490	H	1.9708516	-3.1223149
	1.5913462			1.0379226	
P	1.2738646	0.1912738	H	-0.7788852	-1.8603273
	-1.5916973			3.3117358	
C	1.3285207	-1.7943755	H	0.2827555	-1.1308917
	2.6920356			4.5274249	
C	1.1390969	-2.9935601	H	0.3387111	-2.8794355
	1.7427842			4.2543780	
C	0.2216666	-1.9031829	H	3.5431680	-1.9133639
	3.7557481			2.6993392	
C	2.6950284	-1.9116649	H	2.7218675	-2.8678471
	3.3964144			3.9434244	
C	1.5918645	1.3920717	H	2.8512791	-1.1140541
	2.6764881			4.1347018	
C	0.9221911	1.2990004	H	-0.1439881	1.0509152
	4.0586112			3.9791828	
C	0.9715318	2.5886668	H	1.0051427	2.2855174
	1.9342013			4.5431207	
C	3.0943651	1.6633524	H	1.4170679	0.5724451
	2.8765410			4.7156229	
C	1.5900929	-1.3924823	H	1.4350274	2.7542728
	-2.6769806			0.9549683	
C	3.0923868	-1.6644199	H	1.1303869	3.4986960
	-2.8776895			2.5357427	
C	0.9695631	-2.5888081	H	-0.1082501	2.4549729
	-1.9344253			1.7875537	
C	0.9198538	-1.2991161	H	3.6139637	1.8857032
	-4.0588095			1.9341986	
C	1.3281332	1.7940792	H	3.6177200	0.8375428
	-2.6924088			3.3766016	
C	2.6943776	1.9107625	H	3.1994406	2.5529991
	-3.3973985			3.5179581	
C	1.1396671	2.9933482	H	3.1967931	-2.5541111
	-1.7430728			-3.5191543	
C	0.2208510	1.9033841	H	3.6122979	-1.8870008
	-3.7556250			-1.9355738	
H	3.7480265	-0.1884396	H	3.6158855	-0.8388382
	1.2562590			-3.3779754	
H	2.9306289	-1.4862921	H	1.1277674	-3.4989067
	0.3861870			-2.5360333	
H	2.9311057	1.4852955	H	-0.1100981	-2.4546492
	-0.3872542			-1.7873137	
H	3.7475648	0.1870899	H	1.4334077	-2.7546117
	-1.2576796			-0.9553906	
H	0.2016588	-2.9142213	H	1.0021598	-2.2856683
	1.1758540			-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	H	3.7654118	1.6486398
	-4.1409063			2.1433252	
C	1.2509551	1.9259235	H	3.6608447	0.4730886
	-2.5499665			3.4804029	
C	2.5711870	2.1532230	H	3.3465060	2.1916915
	-3.3116152			3.7720791	
C	1.0695693	3.0445929	H	3.3440715	-2.1927178
	-1.5052322			-3.7734953	
C	0.0751610	2.0528929	H	3.7638922	-1.6498283
	-3.5340912			-2.1449227	
H	3.7788612	-0.2864196	H	3.6591526	-0.4742296
	1.2364813			-3.4819451	
H	2.9328142	-1.5102069	H	1.3733437	-3.3603911
	0.2895632			-2.8082957	
H	2.9332495	1.5092892	H	0.1062428	-2.4687264
	-0.2907631			-1.9241709	
H	3.7784320	0.2851887	H	1.7056708	-2.7315203
	-1.2380472			-1.1849838	
H	0.1840687	-2.8725798	H	1.1202957	-2.0075650
	0.8769831			-4.7071489	
H	0.9250084	-3.9977920	H	1.3923877	-0.2589640
	2.0377592			-4.7475501	
H	1.9443878	-3.1726148	H	-0.1032954	-0.9179684
	0.8549816			-4.0150011	
H	-0.8915437	-1.9387191	H	2.7081584	1.4358824
	3.0318269			-4.1312278	
H	0.1153809	-1.3307919	H	3.4547543	2.1120814
	4.3545861			-2.6602399	
H	0.1194989	-3.0617054	H	2.5451379	3.1586056
	3.9760451			-3.7620900	
H	3.4551429	-2.1131929	H	0.9255957	3.9976194
	2.6587839			-2.0380654	
H	2.5456353	-3.1593635	H	1.9452091	3.1720660
	3.7610595			-0.8557528	
H	2.7094652	-1.4366963	H	0.1847693	2.8726777
	4.1301006			-0.8769557	
H	-0.1012059	0.9181679	H	0.1139232	1.3309123
	4.0151286			-4.3545193	
H	1.1230787	2.0073378	H	0.1188689	3.0618288
	4.7067206			-3.9759984	
H	1.3945709	0.2586405	H	-0.8921656	1.9392339
	4.7470155			-3.0313068	
H	1.7071394	2.7310549			
	1.1842879				
H	1.3757678	3.3600594			
	2.8077438				
H	0.1079510	2.4688383			
	1.9241978				

Combination of torsional
angles = 25
E(BP86/def2-TZVP) =
-3497.56886922960
Ni -0.2147728 0.0000898
0.0000674

I	-2.0110205	-0.4838000	H	2.9448762	1.5178433
	-1.7613260			-0.2475268	
I	-2.0100350	0.4845789	H	3.7984311	0.3264404
	1.7623066			-1.2283610	
C	2.9133161	-0.4779892	H	0.1747190	-2.8419836
	0.5959054			0.7336619	
C	2.9132094	0.4770837	H	0.8479228	-4.0291405
	-0.5972216			1.8746799	
P	1.3236491	-0.2821502	H	1.9257990	-3.1894577
	1.5679973			0.7549325	
P	1.3230177	0.2818155	H	-0.9421418	-1.9487372
	-1.5685686			2.8896404	
C	1.2140327	-1.9875773	H	0.0415356	-1.4239865
	2.4728988			4.2644940	
C	1.0342344	-3.0618616	H	0.0018072	-3.1390655
	1.3821863			3.8202822	
C	0.0052594	-2.1135146	H	3.4082896	-2.2237156
	3.4163566			2.6328185	
C	2.5069535	-2.2768710	H	2.4495873	-3.3011849
	3.2590139			3.6614782	
C	1.7433545	1.1329250	H	2.6356683	-1.6005858
	2.8382083			4.1139624	
C	0.9931915	0.9585737	H	-0.0880850	0.8497030
	4.1711295			4.0192274	
C	1.2983059	2.4678014	H	1.1611416	1.8648091
	2.2157060			4.7755880	
C	3.2528230	1.2175460	H	1.3668683	0.1069265
	3.1352138			4.7537188	
C	1.7416396	-1.1333863	H	1.8524092	2.7006979
	-2.8389957			1.2983197	
C	3.2509339	-1.2184997	H	1.5003657	3.2769701
	-3.1367428			2.9363024	
C	1.2964636	-2.4681237	H	0.2246682	2.4684158
	-2.2162853			1.9874007	
C	0.9908776	-0.9587810	H	3.8400066	1.5167397
	-4.1715466			2.2561019	
C	1.2135566	1.9872899	H	3.6693987	0.2827554
	-2.4733969			3.5324206	
C	2.5061698	2.2761263	H	3.4058149	1.9951355
	-3.2601847			3.9006610	
C	1.0347181	3.0616348	H	3.4032935	-1.9961268
	-1.3825866			-3.9022778	
C	0.0043291	2.1136652	H	3.8384476	-1.5179025
	-3.4162142			-2.2579230	
H	3.7988874	-0.3276655	H	3.6676244	-0.2838408
	1.2266303			-3.5341379	
H	2.9444431	-1.5187605	H	1.4978901	-3.2773496
	0.2461962			-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	H	2.1425908	2.5917848
	-2.9331773			1.5185557	
C	3.3130740	-0.8847385	H	1.7384324	3.0798356
	-3.3176459			3.1721645	
C	1.5153064	-2.3411497	H	0.4617548	2.4428665
	-2.3858499			2.1025501	
C	0.9810258	-0.7272347	H	3.9711927	1.2214533
	-4.2064525			2.5016861	
C	1.1513960	2.1081421	H	3.6472392	-0.1096577
	-2.3103983			3.6429347	
C	2.3732630	2.5126222	H	3.4729425	1.5757741
	-3.1552353			4.1585465	
C	1.0023792	3.0965349	H	3.4700051	-1.5767709
	-1.1370075			-4.1605709	
C	-0.1296980	2.2258962	H	3.9693619	-1.2226241
	-3.1553466			-2.5040072	
H	3.8464811	-0.3884716	H	3.6451384	0.1086002
	1.2119762			-3.6450458	
H	2.9946716	-1.5301065	H	1.7356241	-3.0803053
	0.1725657			-3.1731485	
H	2.9950898	1.5291913	H	0.4597880	-2.4429455
	-0.1742555			-2.1027631	
H	3.8459092	0.3872689	H	2.1409294	-2.5923876
	-1.2141616			-1.5197818	
H	0.1918313	-2.7997334	H	1.1740126	-1.5754027
	0.4555109			-4.8833402	
H	0.7525973	-4.0874116	H	1.2592972	0.1871063
	1.5481929			-4.7459197	
H	1.9254031	-3.2144172	H	-0.0942078	-0.7085449
	0.5549681			-3.9879446	
H	-1.0231312	-1.9624015	H	2.4656987	1.9151729
	2.5778474			-4.0711512	
H	-0.1138648	-1.6013929	H	3.3169067	2.4432242
	4.0536737			-2.5955373	
H	-0.2251099	-3.2746677	H	2.2535393	3.5639238
	3.4794264			-3.4635854	
H	3.3176313	-2.4442550	H	0.7530708	4.0872543
	2.5935452			-1.5485608	
H	2.2544362	-3.5645838	H	1.9262458	3.2138942
	3.4622820			-0.5560955	
H	2.4675467	-1.9159004	H	0.1926024	2.7997680
	4.0696980			-0.4555036	
H	-0.0916426	0.7086329	H	-0.1158265	1.6014761
	3.9880722			-4.0534458	
H	1.1773744	1.5751222	H	-0.2261042	3.2748175
	4.8826942			-3.4792001	
H	1.2620515	-0.1874141	H	-1.0240098	1.9628724
	4.7452424			-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	H	-0.1619915	0.4958170
4.1808359			3.8494568		
C	1.7624439	2.0818713	H	1.0696770	1.1389505
2.5918877			4.9562660		
C	3.3067630	0.3774311	H	1.0014256	-0.6036591
3.5510657			4.6525819		
C	1.8713088	-0.6106116	H	2.4847386	2.3373840
-3.0310288			1.8049425		
C	3.3034550	-0.3787606	H	1.9874253	2.7229086
-3.5538718			3.4597620		
C	1.7591498	-2.0824438	H	0.7502600	2.3211306
-2.5933253			2.2417133		
C	0.8744613	-0.3796423	H	4.0719315	0.7247183
-4.1815018			2.8434048		
C	1.1094036	2.3005364	H	3.5180513	-0.6672585
-2.0530947			3.8068883		
C	2.1781892	2.8190438	H	3.4332888	0.9723946
-3.0313235			4.4699033		
C	1.1150974	3.1987244	H	3.4288869	-0.9738036
-0.8016878			-4.4728082		
C	-0.2917160	2.4106377	H	4.0690780	-0.7264025
-2.6854530			-2.8468766		
H	3.9163941	-0.4516758	H	3.5150206	0.6658220
1.2008043			-3.8099008		
H	3.1083315	-1.5383619	H	1.9830494	-2.7235949
0.0707396			-3.4613954		
H	3.1089796	1.5371668	H	0.7471585	-2.3212059
-0.0733662			-2.2422556		
H	3.9155548	0.4501100	H	2.4820143	-2.3383069
-1.2041388			-1.8070179		
H	0.3996477	-2.8470468	H	1.0647619	-1.1391963
0.0444437			-4.9570983		
H	0.8086322	-4.2121923	H	0.9976164	0.6034469
1.1060472			-4.6533594		
H	2.1081032	-3.2883566	H	-0.1656197	-0.4954666
0.3418628			-3.8492044		
H	-1.0742997	-2.0912459	H	2.1459901	2.3110544
1.9865500			-4.0028834		
H	-0.3968721	-1.8220273	H	3.1964859	2.7357043
3.6028279			-2.6244204		
H	-0.4710568	-3.4667136	H	1.9883620	3.8887652
2.9413441			-3.2169183		
H	3.1974747	-2.7369940	H	0.8097112	4.2120955
2.6216217			-1.1067219		
H	1.9893222	-3.8894789	H	2.1094393	3.2876585
3.2151815			-0.3437025		
H	2.1484279	-2.3118624	H	0.4010456	2.8471654
4.0010393			-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	Cl	2.5280370	-1.3313116
	-0.9572340			0.8752752	
C	0.3867583	-1.5145791	Cl	2.5334334	1.3313944
	-2.7497244			-0.8591878	
H	0.6543519	-2.0585615	Ni	0.9901567	0.0000203
	-3.6702484			0.0032144	
H	1.2873394	-1.0110738	P	-0.5344139	1.5680093
	-2.3715738			0.0970148	
H	-0.3457910	-0.7455087	P	-0.5337629	-1.5680040
	-3.0289820			-0.1001551	
C	-1.4591830	-3.1457466	C	-2.1512839	-0.6722602
	-2.3641349			-0.3767605	
H	-2.2317720	-2.3951738	H	-2.2433755	-0.5094951
	-2.5822270			-1.4585066	
H	-1.9066034	-3.9313050	H	-3.0077157	-1.2935422
	-1.7463870			-0.0745842	
H	-1.1773276	-3.6039437	C	-2.1535928	0.6722297
	-3.3259752			0.3635571	
C	-0.9854218	-2.8011731	H	-2.2523683	0.5094609
	1.3085174			1.4447112	
C	-1.5745001	-1.9653465	H	-3.0081521	1.2934959
	2.4610278			0.0560867	
H	-2.5308092	-1.4907615	C	-0.9734767	2.7838763
	2.2010981			-1.3421459	
H	-0.8690502	-1.1971280	C	-1.5711219	1.9405970
	2.8016860			-2.4849299	
H	-1.7676850	-2.6364997	H	-2.5334958	1.4811390
	3.3126297			-2.2207016	
C	-2.0386632	-3.8371435	H	-0.8754861	1.1590856
	0.8738805			-2.8160591	
H	-2.3743498	-4.3830593	H	-1.7547060	2.6034522
	1.7706568			-3.3451036	
H	-1.6241976	-4.5805886	C	0.2572001	3.5144896
	0.1820987			-1.9074940	
H	-2.9311348	-3.3896308	H	-0.0797805	4.1435867
	0.4138046			-2.7482873	
C	0.2429695	-3.5447862	H	1.0173337	2.8121324
	1.8624070			-2.2653618	
H	1.0161990	-2.8501733	H	0.7378907	4.1692099
	2.2082431			-1.1730316	
H	0.7043307	-4.2099994	C	-2.0208720	3.8295316
	1.1247606			-0.9160286	
H	-0.0912213	-4.1669591	H	-1.6060009	4.5711977
	2.7093359			-0.2225947	
			H	-2.9191400	3.3885064
				-0.4610209	
			H	-2.3474186	4.3757782
				-1.8159419	
Combination of torsional					
angles = -35					
E(BP86/def2-TZVP) =					
-3822.37354396726					

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	H	1.3287084	1.1798999
	-0.0952964			2.3466043	
C	-2.1495502	0.6752127	H	-0.2873706	0.7928338
	0.3347105			2.9867306	
H	-2.2608861	0.5214798	C	-1.5511643	3.1318737
	1.4157510			2.3008484	
H	-3.0011221	1.2932642	H	-1.3000529	3.6477496
	0.0126685			3.2416865	
C	-0.9461816	2.7621987	H	-2.2688086	2.3391082
	-1.3836541			2.5534194	
C	-1.5316886	1.9045055	H	-2.0541949	3.8587210
	-2.5219408			1.6537445	
H	-2.4996367	1.4532784	C	-0.1981354	-2.5786396
	-2.2641985			-1.7010156	
H	-0.8355719	1.1148344	C	0.7854723	-3.7289416
	-2.8322505			-1.4231210	
H	-1.7004176	2.5553080	H	1.0960295	-4.1606162
	-3.3942728			-2.3880480	
C	0.2921606	3.4830895	H	0.3278380	-4.5366284
	-1.9442500			-0.8373094	
H	-0.0353412	4.1068946	H	1.6845354	-3.3737328
	-2.7927510			-0.9007668	
H	1.0516697	2.7748994	C	0.4664667	-1.6134767
	-2.2914485			-2.7026239	
H	0.7712714	4.1399327	H	0.7104507	-2.1751401
	-1.2108079			-3.6191826	
C	-1.9985712	3.8139429	H	1.3946158	-1.1790131
	-0.9851150			-2.3065633	
H	-1.5964559	4.5598939	H	-0.2027841	-0.7923357
	-0.2888886			-2.9921734	
H	-2.9060694	3.3771579	C	-1.4848842	-3.1317102
	-0.5446096			-2.3426722	
H	-2.3071310	4.3538656	H	-2.1951549	-2.3390285
	-1.8951018			-2.6154934	
C	-0.2466278	2.5789768	H	-2.0059672	-3.8586256
	1.6959720			-1.7100976	
C	0.7441937	3.7294454	H	-1.2071048	-3.6475566
	1.4457852			-3.2760064	
H	0.3032748	4.5367967	C	-0.9846239	-2.7627158
	0.8468347			1.3575534	
H	1.6578522	3.3742497	C	-1.6011591	-1.9050741
	0.9493873			2.4793958	
H	1.0270314	4.1615529	H	-2.5612717	-1.4531734
	2.4190077			2.1949157	
C	0.3895812	1.6141299	H	-0.9134713	-1.1159466
	2.7161630			2.8092725	
H	0.6073610	2.1759745	H	-1.7945420	-2.5560746
	3.6391901			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	H	0.7901121	4.4311172
	-0.0479795			2.2687121	
C	-2.1348232	-0.6929047	C	0.3586874	1.8520219
	-0.3296816			2.6868011	
H	-2.2480238	-0.5942776	H	0.5110374	2.4757863
	-1.4164967			3.5827134	
H	-2.9853666	-1.2962100	H	1.3355917	1.4753852
	0.0222288			2.3563646	
C	-2.1354175	0.6927544	H	-0.2639845	0.9987182
	0.3262783			2.9869977	
H	-2.2503911	0.5941173	C	-1.6709786	3.2107043
	1.4129060			2.1435199	
H	-2.9854310	1.2959929	H	-1.4719289	3.8317860
	-0.0270266			3.0316335	
C	-0.8883551	2.6650844	H	-2.3286813	2.3931345
	-1.5075879			2.4678598	
C	-1.4250273	1.7307971	H	-2.2205580	3.8323454
	-2.6080996			1.4273245	
H	-2.3992845	1.2899096	C	-0.3151160	-2.7098021
	-2.3564038			-1.6006160	
H	-0.7133156	0.9280530	C	0.5951306	-3.9173605
	-2.8380924			-1.3128870	
H	-1.5647844	2.3212328	H	0.7942720	-4.4309906
	-3.5272735			-2.2672995	
C	0.3692366	3.3545450	H	0.1246366	-4.6488032
	-2.0643322			-0.6434905	
H	0.0761454	3.9154117	H	1.5547575	-3.6017183
	-2.9675005			-0.8843031	
H	1.1450866	2.6292905	C	0.3633186	-1.8519287
	-2.3321020			-2.6860675	
H	0.8160099	4.0617801	H	0.5172347	-2.4756717
	-1.3581072			-3.5817273	
C	-1.9646929	3.7290239	H	1.3396285	-1.4751942
	-1.2205319			-2.3539917	
H	-1.6084094	4.5141469	H	-0.2589374	-0.9986891
	-0.5431693			-2.9873049	
H	-2.8913617	3.3052774	C	-1.6671274	-3.2108003
	-0.8080637			-2.1461972	
H	-2.2283670	4.2172463	H	-2.3243599	-2.3932845
	-2.1727796			-2.4716229	
C	-0.3180112	2.7098198	H	-2.2178474	-3.8325031
	1.6002072			-1.4309330	
C	0.5926041	3.9174560	H	-1.4665348	-3.8318492
	1.3139769			-3.0339866	
H	0.1231589	4.6488465	C	-0.8906609	-2.6651554
	0.6437876			1.5062210	
H	1.5529717	3.6018934	C	-1.4292656	-1.7309279
	0.8869958			2.6058393	

H	-2.4031385	-1.2901279	C	-0.8505572	2.6257454
	2.3525108			-1.5548838	
H	-0.7180162	-0.9281192	C	-1.3521779	1.6600334
	2.8370343			-2.6442087	
H	-1.5705113	-2.3213866	H	-2.3292552	1.2180471
	3.5247705			-2.4055664	
C	-1.9664185	-3.7291892	H	-0.6286106	0.8575689
	1.2173413			-2.8338428	
H	-2.2316499	-4.2174483	H	-1.4727540	2.2252880
	2.1691375			-3.5817852	
H	-1.6089232	-4.5142707	C	0.4204339	3.3047998
	0.5405691			-2.0940261	
H	-2.8924310	-3.3055235	H	0.1531032	3.8360959
	0.8033190			-3.0226335	
C	0.3660541	-3.3545136	H	1.2072689	2.5757225
	2.0650675			-2.3162713	
H	1.1413839	-2.6291948	H	0.8424222	4.0355257
	2.3341647			-1.3965803	
H	0.8140855	-4.0616861	C	-1.9391638	3.6909641
	1.3595768			-1.3255357	
H	0.0714926	-3.9154334	H	-1.6075452	4.4942140
	2.9677241			-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	

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				

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	C	0.4462592	4.0689528
	-0.0009618			1.1362076	
Ni	0.9993463	0.0000048	H	0.0185511	4.7184854
	0.0001260			0.3619705	
P	-0.5101403	1.5876664	H	1.4500210	3.7525697
	-0.0013307			0.8291326	
P	-0.5101282	-1.5876693	H	0.5376247	4.6745363
	0.0012227			2.0524462	
C	-2.1438527	-0.7152449	C	0.1484048	2.1246657
	-0.2740853			2.6680772	
H	-2.2909910	-0.6984937	H	0.2319790	2.8378696
	-1.3613302			3.5041219	
H	-2.9791969	-1.2962257	H	1.1487010	1.7314409
	0.1456759			2.4457441	
C	-2.1439225	0.7152300	H	-0.4936304	1.3015761
	0.2735943			3.0088549	
H	-2.2913137	0.6984776	C	-1.8546709	3.3718234
	1.3608050			1.8402961	
H	-2.9791735	1.2962043	H	-1.7360945	4.0873394
	-0.1463615			2.6697487	
C	-0.7645948	2.5274183	H	-2.5180015	2.5747593
	-1.6655967			2.2010705	
C	-1.1868941	1.4899182	H	-2.3613020	3.9003249
	-2.7208794			1.0244713	
H	-2.1716233	1.0485660	C	-0.4512285	-2.8590590
	-2.5138850			-1.4546930	
H	-0.4433151	0.6888192	C	0.4465537	-4.0689460
	-2.8119467			-1.1361058	
H	-1.2559861	1.9932883	H	0.5381374	-4.6745223
	-3.6981910			-2.0523274	
C	0.5400790	3.1777473	H	0.0186686	-4.7184868
	-2.1588820			-0.3619737	
H	0.3406307	3.6378051	H	1.4502415	-3.7525586
	-3.1408626			-0.8287939	
H	1.3439023	2.4412984	C	0.1490456	-2.1246519
	-2.2704831			-2.6680326	
H	0.9071489	3.9608191	H	0.2328231	-2.8378513
	-1.4877290			-3.5040607	
C	-1.8699836	3.5954388	H	1.1492862	-1.7314194
	-1.5754003			-2.4454622	
H	-1.5887311	4.4408719	H	-0.4929163	-1.3015662
	-0.9366367			-3.0089580	
H	-2.8284783	3.1915436	C	-1.8542156	-3.3718259
	-1.2192326			-1.8407291	
H	-2.0448377	3.9967553	H	-2.5174665	-2.5747632
	-2.5868403			-2.2016534	
C	-0.4515899	2.8590624	H	-2.3610350	-3.9003366
	1.4545931			-1.0250274	

H	-1.7354400	-4.0873350	C	-2.1496051	0.7223564
	-2.6701590			0.2548487	
C	-0.7649738	-2.5274248	H	-2.3091976	0.7354669
	1.6654272			1.3405405	
C	-1.1875335	-1.4899276	H	-2.9783541	1.2944696
	2.7206086			-0.1894583	
H	-2.1722171	-1.0485840	C	-0.7182589	2.4740142
	2.5133790			-1.7160692	
H	-0.4439833	-0.6888218	C	-1.1040636	1.4011104
	2.8118522			-2.7492226	
H	-1.2568536	-1.9932975	H	-2.0935540	0.9630814
	3.6979041			-2.5578838	
C	-1.8703341	-3.5954524	H	-0.3557969	0.6002051
	1.5749669			-2.7887922	
H	-2.0454274	-3.9967694	H	-1.1440006	1.8711579
	2.5863652			-3.7446329	
H	-1.5889233	-4.4408840	C	0.6039637	3.1074469
	0.9362711			-2.1849155	
H	-2.8287462	-3.1915636	H	0.4415875	3.5303009
	1.2185698			-3.1900801	
C	0.5395857	-3.1777449	H	1.4113335	2.3681359
	2.1590270			-2.2397078	
H	1.3433762	-2.4412900	H	0.9460448	3.9155339
	2.2708252			-1.5304180	
H	0.9068249	-3.9608118	C	-1.8258168	3.5429268
	1.4879609			-1.6970610	
H	0.3399030	-3.6378072	H	-1.5661664	4.4090724
	3.1409580			-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	
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				

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	H	0.4186215	-4.7920247
	-3.7778564			-1.8925380	
C	0.6654916	3.0369671	H	0.0091418	-4.7313707
	-2.2022009			-0.1730304	
H	0.5395122	3.4276055	H	1.4053424	-3.7975261
	-3.2253684			-0.7897367	
H	1.4701474	2.2923176	C	-0.0217282	-2.2841361
	-2.2067325			-2.6386323	
H	0.9903065	3.8643816	H	0.0181483	-3.0504240
	-1.5631649			-3.4295999	
C	-1.7772673	3.4980556	H	0.9862873	-1.8712432
	-1.8008015			-2.5043072	
H	-1.5317237	4.3810100	H	-0.6941968	-1.4910237
	-1.1990765			-2.9918463	
H	-2.7573240	3.1169528	C	-1.9578507	-3.4815102
	-1.4794630			-1.6077261	
H	-1.8885587	3.8363785	H	-2.6480279	-2.7107809
	-2.8437809			-1.9749951	
C	-0.5312479	2.9424352	H	-2.4086332	-3.9597694
	1.3466555			-0.7305194	
C	0.3883899	4.1310141	H	-1.8864161	-4.2471847
	1.0099171			-2.3968236	
H	0.0098053	4.7313177	C	-0.6693082	-2.4248192
	0.1728878			1.7589569	
H	1.4079950	3.7974550	C	-1.0260548	-1.3230206
	0.7850389			2.7715638	
H	0.4249197	4.7920085	H	-2.0218930	-0.8923186
	1.8910409			2.5964569	
C	-0.0130044	2.2841310	H	-0.2790908	-0.5199379
	2.6386249			2.7641675	
H	0.0294390	3.0504184	H	-1.0352711	-1.7633833
	3.4294592			3.7812533	
H	0.9945788	1.8712722	C	-1.7714418	-3.4979385
	2.5009918			1.8066445	
H	-0.6842832	1.4909918	H	-1.8793091	-3.8362426
	2.9940365			2.8499891	
C	-1.9524974	3.4815236	H	-1.5279901	-4.3809252
	1.6141016			1.2041136	
H	-1.8784399	4.2472187	H	-2.7525187	-3.1167351
	2.4029374			1.4885522	
H	-2.6414609	2.7108110	C	0.6726849	-3.0371349
	1.9836749			2.1999185	
H	-2.4061755	3.9597647	H	1.4774503	-2.2925931
	0.7383805			2.2017436	
C	-0.5357150	-2.9424486	H	0.9952545	-3.8646182
	-1.3449674			1.5598364	
C	0.3849974	-4.1310540	H	0.5500629	-3.4277200
	-1.0112803			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	H	-2.3935278	4.0625559
	-2.8160971			0.3327615	
H	-1.9251187	0.7327819	C	-0.6190301	-3.0322988
	-2.6637318			-1.1795268	
H	-0.1926516	0.2839926	C	0.3721851	-4.1589092
	-2.7033752			-0.8328056	
H	-0.8412307	1.4696461	H	0.3587172	-4.8899198
	-3.8558693			-1.6575004	
C	0.8423800	2.7863636	H	0.0919839	-4.6990615
	-2.2552448			0.0804313	
H	0.8189698	3.1023274	H	1.3938302	-3.7747381
	-3.3109390			-0.7291267	
H	1.6024879	2.0029483	C	-0.2425502	-2.4670887
	-2.1432990			-2.5617000	
H	1.1631461	3.6432577	H	-0.2454763	-3.2950467
	-1.6536321			-3.2888317	
C	-1.6028611	3.3868456	H	0.7598561	-2.0201732
	-2.0811694			-2.5492167	
H	-1.3586728	4.3061976	H	-0.9695395	-1.7241454
	-1.5362285			-2.9168191	
H	-2.6188106	3.0724645	C	-2.0380168	-3.6320917
	-1.8011044			-1.2768899	
H	-1.6271017	3.6409478	H	-2.7848659	-2.9094447
	-3.1533656			-1.6311244	
C	-0.6196726	3.0322751	H	-2.3933086	-4.0626024
	1.1791948			-0.3340074	
C	0.3717036	4.1589045	H	-2.0071224	-4.4474559
	0.8329963			-2.0174383	
H	0.0919670	4.6990599	C	-0.5608899	-2.2756500
	-0.0803804			1.8722825	
H	1.3934075	3.7747520	C	-0.9054761	-1.1110036
	0.7298445			2.8156128	
H	0.3577958	4.8899083	H	-1.9264826	-0.7328010
	1.6576896			2.6627189	
C	-0.2439030	2.4670578	H	-0.1940404	-0.2839947
	2.5615583			2.7032574	
H	-0.2472192	3.2950086	H	-0.8432040	-1.4696522
	3.2886960			3.8554179	
H	0.7585150	2.0201576	C	-1.6038953	-3.3868653
	2.5495914			2.0803352	
H	-0.9710658	1.7241010	H	-1.6286847	-3.6409630
	2.9162926			3.1525201	
C	-2.0387189	3.6320447	H	-1.3594161	-4.3062175
	1.2758249			1.5355236	
H	-2.0082220	4.4474038	H	-2.6197046	-3.0724968
	2.0163947			1.7997460	
H	-2.7857407	2.9093839	C	0.8412495	-2.7863549
	1.6296662			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	Ni	0.9794544	-0.0000034
	-3.2528277			-0.0003527	
H	0.6936161	-2.0414568	P	-0.5462815	1.5606261
	-2.5633353			-0.1060963	
H	-1.0495642	-1.7778962	P	-0.5461984	-1.5606375
	-2.8917646			0.1065295	
C	-2.0438352	-3.6734176	C	-2.2135339	-0.7510032
	-1.1917775			-0.1517530	
H	-2.8120745	-2.9664384	H	-2.4430849	-0.9164601
	-1.5319852			-1.2130634	
H	-2.3658616	-4.1002864	H	-2.9962147	-1.2700334
	-0.2356143			0.4223958	
H	-2.0195934	-4.4953411	C	-2.2134205	0.7509878
	-1.9253347			0.1534358	
C	-0.5332184	-2.2374516	H	-2.4421739	0.9164440
	1.8954644			1.2149182	
C	-0.8930939	-1.0651117	H	-2.9965336	1.2700159
	2.8231875			-0.4201252	
H	-1.9233063	-0.7109239	C	-0.5103901	2.2034871
	2.6735510			-1.9158964	
H	-0.2000247	-0.2257480	C	-0.8906488	1.0282806
	2.6913190			-2.8315133	
H	-0.8141507	-1.4057453	H	-1.9297013	0.6994591
	3.8679223			-2.6842252	
C	-1.5458937	-3.3690706	H	-0.2172719	0.1757211
	2.1388429			-2.6854738	
H	-1.5485345	-3.6037017	H	-0.7976432	1.3545600
	3.2157541			-3.8796754	
H	-1.2881099	-4.2923984	C	0.9282384	2.6291811
	1.6071537			-2.2700661	
H	-2.5727905	-3.0831684	H	0.9520006	2.9264692
	1.8683165			-3.3310836	
C	0.8878853	-2.7065136	H	1.6390055	1.8044785
	2.2635897			-2.1269779	
H	1.6243490	-1.9030382	H	1.2808400	3.4776202
	2.1335068			-1.6737453	
H	1.2232532	-3.5607863	C	-1.4896573	3.3574483
	1.6659639			-2.1882790	
H	0.8891447	-3.0114228	H	-1.2147922	4.2816990
	3.3227360			-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	
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				

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	C	-2.0339491	3.7476840
	1.2005309			1.0571929	
H	-3.0033257	1.2666030	H	-2.0156105	4.5697486
	-0.4446807			1.7908713	
C	-0.4944268	2.1782157	H	-2.8469039	3.0723644
	-1.9291517			1.3563830	
C	-0.8988185	1.0058390	H	-2.2874361	4.1842519
	-2.8377210			0.0854504	
H	-1.9451587	0.7008240	C	-0.6521313	-3.0634910
	-2.6900408			-1.0815735	
H	-0.2439285	0.1404396	C	0.4389041	-4.1011853
	-2.6859053			-0.7591476	
H	-0.7973475	1.3238254	H	0.4212946	-4.8734974
	-3.8876484			-1.5451345	
C	0.9581703	2.5636092	H	0.2671162	-4.6105164
	-2.2737657			0.1975584	
H	0.9985270	2.8574879	H	1.4356809	-3.6422424
	-3.3352289			-0.7533846	
H	1.6444812	1.7188785	C	-0.4097685	-2.5417024
	-2.1250324			-2.5104886	
H	1.3290698	3.4039524	H	-0.4187350	-3.4025320
	-1.6767579			-3.1983185	
C	-1.4413127	3.3545483	H	0.5654379	-2.0444112
	-2.2190808			-2.5913612	
H	-1.1466407	4.2762955	H	-1.2015317	-1.8564927
	-1.7042618			-2.8434039	
H	-2.4868830	3.1279733	C	-2.0352225	-3.7474274
	-1.9645666			-1.0549908	
H	-1.4090981	3.5619060	H	-2.8484509	-3.0720742
	-3.3011209			-1.3533612	
C	-0.6508639	3.0636789	H	-2.2877324	-4.1839600
	1.0823408			-0.0829770	
C	0.4398939	4.1013265	H	-2.0176784	-4.5695101
	0.7588273			-1.7886684	
H	0.2671564	4.6106899	C	-0.4925738	-2.1780485
	-0.1976895			1.9297296	
H	1.4366416	3.6423352	C	-0.8959826	-1.0056694
	0.7520377			2.8387337	
H	0.4231224	4.8736200	H	-1.9424585	-0.7006017
	1.5448507			2.6921275	
C	-0.4070681	2.5418581	H	-0.2412072	-0.1402977
	2.5109997			2.6862646	
H	-0.4152890	3.4026786	H	-0.7934544	-1.3236793
	3.1988505			3.8885510	
H	0.5681955	2.0445172	C	-1.4392168	-3.3543457
	2.5908699			2.2205942	
H	-1.1985251	1.8566836	H	-1.4059032	-3.5617371
	2.8447137			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	H	0.2658128	-3.6204054
	-0.6965297			2.7804029	
P	0.4916466	-0.0216046	H	1.1880789	-2.9901399
	1.5838388			1.4134587	
P	0.4923046	-0.0028773	H	-1.6703225	-1.3982092
	-1.5839866			3.3406499	
C	0.4714513	-1.4750407	H	-0.6560862	-0.6129573
	2.8666210			4.5643189	
C	0.3296741	-2.7841822	H	-0.6653328	-2.3782712
	2.0665291			4.4466919	
C	-0.7065224	-1.4467201	H	2.6802864	-1.5827169
	3.8587337			3.0165980	
C	1.7929149	-1.5039071	H	1.7860754	-2.3892852
	3.6593213			4.3154139	
C	0.7464108	1.6744991	H	1.9079438	-0.6243252
	2.4838697			4.3063254	
C	-0.0263493	1.7438925	H	-1.0805782	1.4698357
	3.8123883			3.6804860	
C	0.1781364	2.7669531	H	0.0133532	2.7841175
	1.5612466			4.1743499	
C	2.2330740	1.9722786	H	0.4202973	1.1126426
	2.7488746			4.5908636	
C	0.6629096	-1.7096181	H	0.7157773	2.8237161
	-2.4838879			0.6082042	
C	2.1331054	-2.0809086	H	0.2858402	3.7434092
	-2.7479961			2.0616537	
C	0.0405373	-2.7724884	H	-0.8864156	2.5982505
	-1.5615747			1.3520846	
C	-0.1117030	-1.7406712	H	2.8122212	2.0811646
	-3.8127722			1.8211541	
C	0.5440719	1.4496820	H	2.7192938	1.2117964
	-2.8668427			3.3742879	
C	1.8650404	1.4124614	H	2.3032607	2.9320196
	-3.6600719			3.2856014	
C	0.4681408	2.7645061	H	2.1558602	-3.0431562
	-2.0670565			-3.2843493	
C	-0.6344412	1.4799398	H	2.7056289	-2.2181115
	-3.8582721			-1.8198977	
H	2.9747532	-0.0379452	H	2.6568415	-1.3457072
	1.2854244			-3.3733490	
H	2.1785227	-1.4599501	H	0.0996807	-3.7530254
	0.6134816			-2.0620991	
H	2.2479399	1.3504698	H	-1.0143804	-2.5510006
	-0.6135578			-1.3528548	
H	2.9731708	-0.1091113	H	0.5742303	-2.8560737
	-1.2852993			-0.6083197	
H	-0.5871373	-2.7863638	H	-0.1231860	-2.7815617
	1.4627949			-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	H	2.8550046	2.0190963
	-3.8825149			1.9796257	
C	0.4181203	1.5516046	H	2.7126408	1.0557138
	-2.7842670			3.4726716	
C	1.6977924	1.6309295	H	2.3258035	2.7848066
	-3.6387020			3.4826380	
C	0.3096646	2.8224373	H	2.3657735	-2.7507077
	-1.9197199			-3.4826624	
C	-0.8150842	1.5479506	H	2.8839605	-1.9776103
	-3.7065599			-1.9795987	
H	2.9851315	-0.0159898	H	2.7276609	-1.0162335
	1.2828603			-3.4725472	
H	2.2064146	-1.4182055	H	0.4119320	-3.7003604
	0.5504847			-2.2476335	
H	2.1859857	1.4498640	H	-0.7746116	-2.6352300
	-0.5502026			-1.4431055	
H	2.9846393	0.0588971	H	0.8587394	-2.8470528
	-1.2825476			-0.7601601	
H	-0.5211048	-2.7896459	H	0.0688393	-2.6437400
	1.2522635			-4.3046511	
H	0.2340082	-3.6832401	H	0.3847263	-0.9338137
	2.5906729			-4.6336039	
H	1.2520609	-2.9984470	H	-1.0732487	-1.4141461
	1.3208110			-3.7098648	
H	-1.7259747	-1.4962553	H	1.7814598	0.7927556
	3.1360794			-4.3424805	
H	-0.7918499	-0.7489764	H	2.6143523	1.6714271
	4.4412103			-3.0336994	
H	-0.7807686	-2.5106605	H	1.6613144	2.5551187
	4.2635057			-4.2378599	
H	2.6380968	-1.6336100	H	0.1812894	3.6864214
	3.0337922			-2.5904577	
H	1.6979166	-2.5308591	H	1.2090490	3.0162761
	4.2380448			-1.3206091	
H	1.7928254	-0.7669575	H	-0.5609616	2.7822027
	4.3426471			-1.2520122	
H	-1.0935784	1.3986813	H	-0.8027324	0.7376519
	3.7101234			-4.4407381	
H	0.0306355	2.6446905	H	-0.8168015	2.4993374
	4.3047911			-4.2631987	
H	0.3712278	0.9395312	H	-1.7473155	1.4716301
	4.6338249			-3.1356060	
H	0.8173404	2.8593267			
	0.7603295				
H	0.3582954	3.7060668			
	2.2478296				
H	-0.8127500	2.6238935			
	1.4433485				

Combination of torsional
angles = 20
E(BP86/def2-TZVP) =
-3822.37894827374
Ni -1.0002423 -0.0350623
0.0002175

Cl	-2.4960258	-0.5895769	H	2.1414685	1.5259869
	-1.5399300			-0.5138287	
Cl	-2.5306232	0.4122081	H	2.9874171	0.1825813
	1.5414405			-1.2814122	
C	2.1354777	-0.2884848	H	-0.4582346	-2.7937887
	0.6729193			1.1264578	
C	2.1094595	0.4396221	H	0.2597172	-3.7238722
	-0.6739943			2.4610102	
P	0.5099107	-0.0452446	H	1.3129410	-2.9917730
	1.5750181			1.2469258	
P	0.5047028	0.0820986	H	-1.7324992	-1.5633851
	-1.5753842			3.0167785	
C	0.4440001	-1.5918580	H	-0.8410038	-0.8550410
	2.7281757			4.3718238	
C	0.3905384	-2.8367209	H	-0.8167047	-2.6105005
	1.8217474			4.1380394	
C	-0.8156849	-1.6416599	H	2.6344659	-1.6600627
	3.6125442			3.0298363	
C	1.7026858	-1.6680111	H	1.6781558	-2.6150349
	3.6129131			4.1759770	
C	0.7605945	1.5660860	H	1.7452149	-0.8550782
	2.6223625			4.3490778	
C	-0.0659330	1.5438586	H	-1.1217075	1.3238350
	3.9207596			3.7208292	
C	0.2599978	2.7473617	H	-0.0045872	2.5446829
	1.7732782			4.3783868	
C	2.2404625	1.8061185	H	0.3243754	0.8281387
	2.9745818			4.6552689	
C	0.8685371	-1.5071842	H	0.8494926	2.8767915
	-2.6231783			0.8578936	
C	2.3613571	-1.6412640	H	0.3605723	3.6730592
	-2.9770943			2.3631952	
C	0.4542765	-2.7211500	H	-0.7953321	2.6203714
	-1.7736836			1.4998748	
C	0.0411954	-1.5437800	H	2.8578036	2.0013064
	-3.9207373			2.0866500	
C	0.3286892	1.6203330	H	2.6912940	0.9777979
	-2.7281483			3.5366372	
C	1.5786309	1.7861992	H	2.3008985	2.7044966
	-3.6129703			3.6096821	
C	0.1867968	2.8578705	H	2.4847884	-2.5329075
	-1.8212606			-3.6125570	
C	-0.9313692	1.5805864	H	2.9920646	-1.7923138
	-3.6125071			-2.0899414	
H	2.9934860	0.0297026	H	2.7515090	-0.7828526
	1.2799222			-3.5393892	
H	2.2437343	-1.3699059	H	0.6195073	-3.6373176
	0.5127305			-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	H	1.3130864	2.7413647
	-2.7162351			1.0387744	
C	2.2810912	-1.5924435	H	0.8618680	3.5200579
	-3.1547164			2.5641713	
C	0.4170683	-2.7052858	H	-0.3861767	2.6957163
	-1.9166975			1.5885202	
C	-0.0822840	-1.3970535	H	3.1015529	1.5442013
	-3.9691774			2.3163958	
C	0.3796809	1.6874700	H	2.7170438	0.4540190
	-2.6166692			3.6730831	
C	1.5828127	1.8534313	H	2.5570885	2.2084523
	-3.5628708			3.8604421	
C	0.3453129	2.8753381	H	2.3483105	-2.4369474
	-1.6362458			-3.8592907	
C	-0.9346458	1.7379167	H	2.9496165	-1.8256722
	-3.4183720			-2.3144496	
H	2.9989628	-0.2718484	H	2.6677986	-0.7045734
	1.2787246			-3.6711784	
H	2.1338372	-1.5710561	H	0.5392190	-3.5884299
	0.4575701			-2.5647549	
H	2.2693764	1.3644666	H	-0.6292814	-2.6537264
	-0.4563174			-1.5901882	
H	3.0124987	-0.0087149	H	1.0582473	-2.8543081
	-1.2764106			-1.0388395	
H	-0.7150335	-2.7180131	H	0.0037656	-2.3652933
	0.8979214			-4.4887548	
H	-0.1948281	-3.7963144	H	0.2349789	-0.6212080
	2.2136847			-4.6774156	
H	1.0098790	-3.1316815	H	-1.1357470	-1.2433762
	1.1048283			-3.7049880	
H	-1.9491337	-1.4108921	H	1.6006336	1.0937739
	2.7742516			-4.3545646	
H	-1.0659011	-0.9102237	H	2.5455194	1.8278846
	4.2239933			-3.0320880	
H	-1.2617535	-2.6363077	H	1.5082727	2.8360460
	3.8760494			-4.0563455	
H	2.3643192	-2.0578921	H	0.1561058	3.7938887
	3.0328694			-2.2135919	
H	1.2383973	-2.9662678	H	1.2947308	3.0214293
	4.0568670			-1.1047737	
H	1.4902900	-1.2397918	H	-0.4609025	2.7674787
	4.3547606			-0.8981771	
H	-1.0213624	1.3379648	H	-0.9754096	0.9997141
	3.7029229			-4.2244133	
H	0.2148983	2.3517120	H	-1.0112249	2.7367647
	4.4873892			-3.8774775	
H	0.2859280	0.5939520	H	-1.8092536	1.5806158
	4.6771681			-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	P	0.5483882	-0.1374170
	-2.4271740			1.5531402	
H	2.6633847	-0.4700760	P	0.5489226	0.1355928
	-3.7402945			-1.5534073	
H	0.7758789	-3.5172144	C	0.2317005	-1.7667807
	-2.6398967			2.5240194	
H	-0.4298411	-2.6883548	C	0.1874512	-2.9181805
	-1.6163200			1.5019553	
H	1.2828698	-2.7786751	C	-1.1435129	-1.7338234
	-1.1122487			3.2192275	
H	0.0849435	-2.2935312	C	1.3432206	-2.0524030
	-4.5182210			3.5492528	
H	0.1948505	-0.5345089	C	0.9157039	1.3118249
	-4.6750684			2.7801961	
H	-1.0989081	-1.2661360	C	-0.0666687	1.3091097
	-3.6732417			3.9660866	
H	1.4669733	1.2519131	C	0.7117930	2.6272936
	-4.3599188			2.0080977	
H	2.4181124	2.0012480	C	2.3590141	1.2824321
	-3.0502200			3.3194034	
H	1.2958372	2.9791276	C	0.9121300	-1.3147228
	-4.0124828			-2.7804111	
H	-0.0360413	3.8219502	C	2.3555652	-1.2895285
	-2.1120178			-3.3194973	
H	1.1705146	3.0843281	C	0.7043389	-2.6295737
	-1.0516476			-2.0082949	
H	-0.5642907	2.7395741	C	-0.0701278	-1.3091823
	-0.8025108			-3.9663874	
H	-1.0922988	1.0034624	C	0.2370686	1.7658695
	-4.1395704			-2.5243165	
H	-1.2180663	2.7284291	C	1.3495194	2.0482692
	-3.7538944			-3.5494333	
H	-1.9050801	1.5063873	C	0.1960603	2.9173815
	-2.6496428			-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	
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				

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	H	-1.6839472	3.3020541
	0.1869441			3.6107130	
C	-1.4561313	2.9104927	H	-2.7003813	2.1260216
	-1.0753132			2.7689438	
C	-2.0122552	2.1640784	H	-2.4248614	3.7350426
	-2.3031694			2.0624048	
H	-2.9595521	1.6471045	C	-0.6677120	-2.3900130
	-2.0972344			-1.9456089	
H	-1.2847805	1.4444758	C	0.3549802	-3.5303895
	-2.6999768			-1.8015228	
H	-2.2124735	2.9016285	H	0.6755939	-3.8413772
	-3.0962517			-2.8084773	
C	-0.2564725	3.7468436	H	-0.0740659	-4.4124314
	-1.5535162			-1.3089174	
H	-0.6210333	4.4530514	H	1.2476122	-3.2121404
	-2.3181189			-1.2443822	
H	0.5279777	3.1205956	C	-0.0605261	-1.3109346
	-1.9918108			-2.8628195	
H	0.2011680	4.3345632	H	0.1785066	-1.7745700
	-0.7508171			-3.8338357	
C	-2.5434562	3.8696875	H	0.8618065	-0.8784799
	-0.5551719			-2.4510467	
H	-2.1529861	4.5636924	H	-0.7650700	-0.4915332
	0.1991941			-3.0583330	
H	-3.4216639	3.3571641	C	-1.9522544	-2.9157817
	-0.1382509			-2.6140446	
H	-2.8957181	4.4800132	H	-2.7004216	-2.1260280
	-1.4026554			-2.7689256	
C	-0.6676808	2.3900040	H	-2.4249005	-3.7350443
	1.9456042			-2.0623759	
C	0.3550154	3.5303766	H	-1.6840036	-3.3020728
	1.8015145			-3.6106971	
H	-0.0740321	4.4124242	C	-1.4561330	-2.9104662
	1.3089204			1.0753254	
H	1.2476393	3.2121273	C	-2.0122389	-2.1640303
	1.2443612			2.3031767	
H	0.6756423	3.8413555	H	-2.9595329	-1.6470503
	2.8084676			2.0972429	
C	-0.0604887	1.3109133	H	-1.2847542	-1.4444287
	2.8627963			2.6999678	
H	0.1785575	1.7745373	H	-2.2124569	-2.9015677
	3.8338145			3.0962708	
H	0.8618371	0.8784590	C	-2.5434711	-3.8696583
	2.4510079			0.5552070	
H	-0.7650337	0.4915124	H	-2.8957299	-4.4799703
	3.0583094			1.4027017	
C	-1.9522123	2.9157730	H	-2.1530144	-4.5636761
	2.6140605			-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	Br	2.2225747	-1.5333927
	-1.1969224			0.6891057	
C	-0.0103723	-1.3797221	Br	2.2225548	1.5333786
	-2.8278384			-0.6892421	
H	0.2161569	-1.8565650	Ni	0.5579148	-0.0000004
	-3.7955349			-0.0000333	
H	0.9269602	-0.9882841	P	-0.9693730	1.5732739
	-2.4090800			0.1886688	
H	-0.6757971	-0.5299601	P	-0.9693803	-1.5732769
	-3.0307356			-0.1886682	
C	-1.9648616	-2.9140606	C	-2.5780250	-0.6468528
	-2.5870740			-0.4107429	
H	-2.6745328	-2.0970932	H	-2.6643448	-0.4161017
	-2.7769229			-1.4799118	
H	-2.4826484	-3.6961320	H	-3.4406038	-1.2791391
	-2.0214700			-0.1524904	
H	-1.6976853	-3.3397615	C	-2.5780101	0.6468494
	-3.5677894			0.4107972	
C	-1.4566643	-2.8865340	H	-2.6642940	0.4160979
	1.1222035			1.4799688	
C	-2.0338864	-2.1218643	H	-3.4405975	1.2791357
	2.3290785			0.1525743	
H	-2.9851464	-1.6208326	C	-1.4469022	2.8564276
	2.1035782			-1.1829416	
H	-1.3199508	-1.3851236	C	-2.0222106	2.0647190
	2.7194988			-2.3731429	
H	-2.2330282	-2.8457397	H	-2.9757717	1.5722685
	3.1349159			-2.1389105	
C	-2.5335039	-3.8592685	H	-1.3097749	1.3163291
	0.6050062			-2.7437358	
H	-2.8850536	-4.4653467	H	-2.2163803	2.7697001
	1.4557968			-3.1967517	
H	-2.1354898	-4.5559023	C	-0.2485493	3.6645296
	-0.1429464			-1.7092279	
H	-3.4135526	-3.3557088	H	-0.6218907	4.3539306
	0.1811194			-2.4849948	
C	-0.2600256	-3.7077229	H	0.5177465	3.0172113
	1.6324492			-2.1481809	
H	0.5077430	-3.0709364	H	0.2372638	4.2647464
	2.0841768			-0.9330191	
H	0.2236624	-4.2942181	C	-2.5258840	3.8401881
	0.8444227			-0.6912865	
H	-0.6350585	-4.4122301	H	-2.1348332	4.5476060
	2.3936567			0.0500708	
			H	-3.4109366	3.3442202
				-0.2688818	
			H	-2.8682377	4.4332524
				-1.5548725	
Combination of torsional					
angles = -30					
E(BP86/def2-TZVP) =					
-8050.74247546104					

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	H	0.9584605	1.2229672
	-0.1195750			2.3867595	
C	-2.5758673	0.6562037	H	-0.6207098	0.6780256
	0.3950448			3.0040897	
H	-2.6665502	0.4505317	C	-2.0447661	2.9775490
	1.4687327			2.4624795	
H	-3.4372618	1.2828434	H	-1.8094984	3.4903719
	0.1194864			3.4089739	
C	-1.4294493	2.8188220	H	-2.6986678	2.1314263
	-1.2535653			2.7131100	
C	-1.9900603	1.9932169	H	-2.6123508	3.6806588
	-2.4274587			1.8425809	
H	-2.9468529	1.5082961	C	-0.7164418	-2.5341711
	-2.1908436			-1.8186105	
H	-1.2738196	1.2338894	C	0.1917724	-3.7608256
	-2.7670855			-1.6239105	
H	-2.1734032	2.6739873	H	0.4417955	-4.1659648
	-3.2736114			-2.6176019	
C	-0.2248397	3.6119338	H	-0.3027260	-4.5628065
	-1.7878793			-1.0607545	
H	-0.5882877	4.2780773	H	1.1294373	-3.4938868
	-2.5882660			-1.1179553	
H	0.5468005	2.9525781	C	-0.0081175	-1.5623126
	-2.1988100			-2.7826000	
H	0.2517686	4.2339071	H	0.1724709	-2.0835302
	-1.0232352			-3.7369877	
C	-2.5163886	3.8140021	H	0.9585408	-1.2229542
	-0.8039149			-2.3866957	
H	-2.1402115	4.5380611	H	-0.6206055	-0.6779942
	-0.0711433			-3.0040705	
H	-3.4090865	3.3266635	C	-2.0446974	-2.9775138
	-0.3875781			-2.4625228	
H	-2.8429572	4.3870721	H	-2.6985870	-2.1313856
	-1.6868736			-2.7131656	
C	-0.7164926	2.5341940	H	-2.6123047	-3.6806262
	1.8186120			-1.8426470	
C	0.1917384	3.7608399	H	-1.8094034	-3.4903297
	1.6239356			-3.4090144	
H	-0.3027337	4.5628212	C	-1.4295127	-2.8188235
	1.0607575			1.2535292	
H	1.1294186	3.4938900	C	-1.9901637	-1.9932307
	1.1180144			2.4274126	
H	0.4417307	4.1659835	H	-2.9469419	-1.5082966
	2.6176330			2.1907658	
C	-0.0082071	1.5623372	H	-1.2739295	-1.2339151
	2.7826311			2.7670808	
H	0.1723560	2.0835609	H	-2.1735479	-2.6740124
	3.7370201			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	H	0.1502457	4.5144586
	-0.0703746			2.3285214	
C	-2.5736016	-0.6893060	C	-0.1530486	1.9114109
	-0.3316923			2.7323545	
H	-2.6892051	-0.5828638	H	-0.0556241	2.5396469
	-1.4170762			3.6327089	
H	-3.4255132	-1.2924079	H	0.8495623	1.5840284
	0.0168262			2.4281454	
C	-2.5735800	0.6893217	H	-0.7420099	1.0284090
	0.3317838			3.0143985	
H	-2.6891353	0.5828813	C	-2.2279769	3.1765952
	1.4171730			2.1405460	
H	-3.4255014	1.2924320	H	-2.0736958	3.8251699
	-0.0166964			3.0177298	
C	-1.3288467	2.6686410	H	-2.8482163	2.3343307
	-1.4951701			2.4740387	
C	-1.7930354	1.7161565	H	-2.7975099	3.7552046
	-2.6124376			1.4039956	
H	-2.7600850	1.2428054	C	-0.8409713	-2.7366855
	-2.3947084			-1.6284252	
H	-1.0460283	0.9379390	C	0.0103343	-3.9925424
	-2.8135203			-1.3681047	
H	-1.9197654	2.3002235	H	0.1501132	-4.5144491
	-3.5376126			-2.3285743	
C	-0.0862024	3.4108653	H	-0.4789120	-4.6982759
	-2.0153629			-0.6847556	
H	-0.3810560	3.9728501	H	0.9998974	-3.7342056
	-2.9172395			-0.9711622	
H	0.7202033	2.7184149	C	-0.1531779	-1.9113991
	-2.2803914			-2.7323712	
H	0.3211984	4.1239891	H	-0.0557978	-2.5396278
	-1.2915614			-3.6327355	
C	-2.4537398	3.6896417	H	0.8494491	-1.5840308
	-1.2394755			-2.4282003	
H	-2.1497809	4.4860790	H	-0.7421407	-1.0283877
	-0.5500253			-3.0143824	
H	-3.3765114	3.2303245	C	-2.2280937	-3.1765688
	-0.8580612			-2.1404919	
H	-2.7055533	4.1699202	H	-2.8483367	-2.3342961
	-2.1988889			-2.4739569	
C	-0.8408786	2.7366947	H	-2.7976051	-3.7551759
	1.6284292			-1.4039233	
C	0.0104260	3.9925426	H	-2.0738525	-3.8251405
	1.3680628			-3.0176849	
H	-0.4788416	4.6982724	C	-1.3287942	-2.6686458
	0.6847249			1.4952017	
H	0.9999717	3.7341946	C	-1.7929132	-1.7161616
	0.9710846			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	C	-0.1293946	4.1687203
	0.1092547			1.0235537	
Ni	0.5593491	-0.0000155	H	-0.5556227	4.7657634
	-0.0000060			0.2073097	
P	-0.9630832	1.5971944	H	0.8975598	3.8845928
	-0.0349447			0.7655338	
P	-0.9630913	-1.5972166	H	-0.0950675	4.8165421
	0.0349560			1.9144687	
C	-2.5933579	-0.7223023	C	-0.4153557	2.2812254
	-0.2498800			2.6331641	
H	-2.7466416	-0.7404381	H	-0.3914594	3.0330543
	-1.3360497			3.4385535	
H	-3.4268455	-1.2891178	H	0.6068729	1.9164233
	0.1918775			2.4697827	
C	-2.5933509	0.7222895	H	-1.0410792	1.4501745
	0.2499130			2.9851194	
H	-2.7466198	0.7404257	C	-2.4225051	3.4229255
	1.3360847			1.6787506	
H	-3.4268415	1.2891097	H	-2.3512746	4.1908202
	-0.1918333			2.4655855	
C	-1.1902010	2.4573054	H	-3.0697334	2.6275706
	-1.7475291			2.0702064	
C	-1.5291013	1.3578760	H	-2.9219782	3.8841653
	-2.7693966			0.8189148	
H	-2.5083664	0.8947833	C	-0.9904886	-2.9387665
	-2.5856638			-1.3652215	
H	-0.7576308	0.5778974	C	-0.1294126	-4.1687312
	-2.7852488			-1.0235931	
H	-1.5675982	1.8111072	H	-0.0950907	-4.8165322
	-3.7726507			-1.9145233	
C	0.1060312	3.1371079	H	-0.5556316	-4.7657947
	-2.2225113			-0.2073604	
H	-0.0787642	3.5579558	H	0.8975430	-3.8846063
	-3.2246858			-0.7655754	
H	0.9371982	2.4257701	C	-0.4153897	-2.2812091
	-2.2897722			-2.6331607	
H	0.4266844	3.9538243	H	-0.3915013	-3.0330226
	-1.5679100			-3.4385647	
C	-2.3358988	3.4856511	H	0.6068410	-1.9164123
	-1.7466845			-2.4697802	
H	-2.1092952	4.3690421	H	-1.0411141	-1.4501496
	-1.1381068			-2.9850950	
H	-3.2923396	3.0630011	C	-2.4225329	-3.4229222
	-1.4075867			-1.6787580	
H	-2.4864291	3.8343122	H	-3.0697613	-2.6275580
	-2.7812656			-2.0701950	
C	-0.9904637	2.9387605	H	-2.9220033	-3.8841781
	1.3652170			-0.8189301	

H	-2.3513079	-4.1908010	C	-2.5992857	0.7309823
	-2.4656089			0.2229668	
C	-1.1901961	-2.4573236	H	-2.7662267	0.7895752
	1.7475465			1.3058844	
C	-1.5290788	-1.3578867	H	-3.4250055	1.2841940
	2.7694103			-0.2495789	
H	-2.5083402	-0.8947847	C	-1.1406536	2.3830230
	2.5856814			-1.8180887	
H	-0.7576003	-0.5779167	C	-1.4525230	1.2418878
	2.7852535			-2.8018403	
H	-1.5675738	-1.8111124	H	-2.4384540	0.7894069
	3.7726670			-2.6267751	
C	-2.3359039	-3.4856581	H	-0.6839950	0.4598318
	1.7467267			-2.7605578	
H	-2.4864267	-3.8343039	H	-1.4600156	1.6514631
	2.7813139			-3.8244423	
H	-2.1093156	-4.3690591	C	0.1761022	3.0346373
	1.1381594			-2.2768213	
H	-3.2923441	-3.0630032	H	0.0311773	3.4093011
	1.4076337			-3.3034861	
C	0.1060350	-3.1371294	H	1.0048478	2.3169571
	2.2225275			-2.2809175	
H	0.9372065	-2.4257965	H	0.4776957	3.8795332
	2.2897767			-1.6493760	
H	0.4266794	-3.9538541	C	-2.2801773	3.4146450
	1.5679340			-1.8971163	
H	-0.0787572	-3.5579656	H	-2.0685730	4.3226012
	3.2247075			-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	
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				

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	H	-0.1840140	-4.9480553
	-3.8644338			-1.6403649	
C	0.2426329	2.9307466	H	-0.5353469	-4.7618890
	-2.3218017			0.0831425	
H	0.1371044	3.2631396	H	0.8688235	-3.9190831
	-3.3675633			-0.6373838	
H	1.0630930	2.2051763	C	-0.5854787	-2.4817003
	-2.2680986			-2.5401123	
H	0.5323448	3.7984450	H	-0.6035968	-3.2978974
	-1.7202631			-3.2802306	
C	-2.2221045	3.3487840	H	0.4403882	-2.0968108
	-2.0328354			-2.4750007	
H	-2.0186982	4.2771965	H	-1.2453144	-1.6888087
	-1.4862605			-2.9172409	
H	-3.2026194	2.9641570	C	-2.5086931	-3.5575618
	-1.7173648			-1.3660737	
H	-2.3069034	3.6118856	H	-3.1909275	-2.8012273
	-3.0997092			-1.7748522	
C	-1.0654400	3.0380862	H	-2.9447279	-3.9545640
	1.1870889			-0.4422411	
C	-0.1689712	4.2301842	H	-2.4775697	-4.3842246
	0.8042208			-2.0937795	
H	-0.5353546	4.7618747	C	-1.0957460	-2.3114178
	-0.0831627			1.8803295	
H	0.8688478	3.9190785	C	-1.3906742	-1.1349068
	0.6373130			2.8266918	
H	-0.1839497	4.9480582	H	-2.3843532	-0.6965518
	1.6403286			2.6587317	
C	-0.5853722	2.4817070	H	-0.6299036	-0.3494978
	2.5401148			2.7347037	
H	-0.6034591	3.2979097	H	-1.3692247	-1.5039140
	3.2802277			3.8644718	
H	0.4404920	2.0968171	C	-2.2220195	-3.3487900
	2.4749627			2.0329162	
H	-1.2451920	1.6888183	H	-2.3067736	-3.6118862
	2.9172774			3.0997949	
C	-2.5086367	3.5575595	H	-2.0186378	-4.2772054
	1.3661473			1.4863376	
H	-2.4774836	4.3842282	H	-3.2025472	-2.9641630
	2.0938452			1.7174854	
H	-3.1908542	2.8012282	C	0.2427311	-2.9307539
	1.7749596			2.3217773	
H	-2.9447093	3.9545544	H	1.0631892	-2.2051840
	0.4423291			2.2680382	
C	-1.0654891	-3.0380895	H	0.5324183	-3.7984543
	-1.1870704			1.7202303	
C	-0.1690019	-4.2301892	H	0.1372452	-3.2631431
	-0.8042509			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	H	-2.8884923	4.0546306
	-2.8840289			-0.0775402	
H	-2.3137441	0.4774186	C	-1.1290359	-3.1390908
	-2.7218402			-0.9205356	
H	-0.5778738	0.0411457	C	-0.1435684	-4.2452996
	-2.6755959			-0.5009613	
H	-1.2043020	1.1073285	H	-0.1954408	-5.0508359
	-3.9511949			-1.2513100	
C	0.4245750	2.5907318	H	-0.4009723	-4.6908159
	-2.4437736			0.4683764	
H	0.4193104	2.8215096	H	0.8883544	-3.8754073
	-3.5214913			-0.4676148	
H	1.1873616	1.8235243	C	-0.7992229	-2.7136274
	-2.2588761			-2.3634659	
H	0.7290243	3.4954707	H	-0.8520214	-3.6050806
	-1.9068177			-3.0090002	
C	-2.0291802	3.1741818	H	0.2125723	-2.2943800
	-2.3830559			-2.4362300	
H	-1.8060577	4.1445087	H	-1.5229445	-1.9870240
	-1.9242796			-2.7574043	
H	-3.0482430	2.8762089	C	-2.5581531	-3.7241966
	-2.0966262			-0.9131965	
H	-2.0312534	3.3236794	H	-3.3074281	-3.0299421
	-3.4750462			-1.3153207	
C	-1.1289852	3.1390939	H	-2.8885052	-4.0546243
	0.9205681			0.0776422	
C	-0.1435334	4.2453022	H	-2.5592049	-4.6090533
	0.5009556			-1.5698131	
H	-0.4009758	4.6908200	C	-0.9809148	-2.1001478
	-0.4683713			2.0467100	
H	0.8883876	3.8754092	C	-1.2912533	-0.8478991
	0.4675673			2.8840669	
H	-0.1953751	5.0508377	H	-2.3136359	-0.4774077
	1.2513073			2.7219207	
C	-0.7991169	2.7136290	H	-0.5777658	-0.0411417
	2.3634853			2.6756036	
H	-0.8518887	3.6050820	H	-1.2041449	-1.1073212
	3.0090223			3.9512295	
H	0.2126802	2.2943796	C	-2.0290967	-3.1741722
	2.4362099			2.3831274	
H	-1.5228248	1.9870268	H	-2.0311248	-3.3236680
	2.7574515			3.4751180	
C	-2.5581017	3.7242020	H	-1.8059971	-4.1445006
	0.9132855			1.9243432	
H	-2.5591263	4.6090584	H	-3.0481703	-2.8761958
	1.5699025			2.0967398	
H	-3.3073620	3.0299484	C	0.4246635	-2.5907315
	1.3154388			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	Ni	0.5418932	-0.0000038
	-2.9357657			-0.0000334	
H	0.1457454	-2.3274144	P	-0.9938032	1.5478551
	-2.4266540			-0.2484855	
H	-1.6037386	-2.0580289	P	-0.9938086	-1.5478371
	-2.7066186			0.2485457	
C	-2.5542887	-3.7678568	C	-2.6606138	-0.7619193
	-0.7930576			-0.0751405	
H	-3.3278828	-3.0920223	H	-2.8995031	-1.0351444
	-1.1806582			-1.1117116	
H	-2.8480488	-4.0905830	H	-3.4371688	-1.2201090
	0.2114970			0.5560754	
H	-2.5595349	-4.6612683	C	-2.6605940	0.7619665
	-1.4380508			0.0753443	
C	-0.9525753	-2.0445423	H	-2.8993887	1.0351962
	2.0845344			1.1119358	
C	-1.2849200	-0.7816489	H	-3.4371955	1.2201698
	2.8968098			-0.5558046	
H	-2.3168782	-0.4382726	C	-0.9337260	1.9966214
	2.7346403			-2.1170853	
H	-0.5913121	0.0358246	C	-1.2923610	0.7284610
	2.6658274			-2.9094331	
H	-1.1841457	-1.0160337	H	-2.3323268	0.4111451
	3.9685659			-2.7445211	
C	-1.9659010	-3.1373936	H	-0.6173548	-0.0998803
	2.4634921			-2.6642320	
H	-1.9463052	-3.2595949	H	-1.1840521	0.9435691
	3.5587092			-3.9844959	
H	-1.7244375	-4.1126591	C	0.5080829	2.3945649
	2.0250136			-2.4901312	
H	-2.9968443	-2.8729171	H	0.5462881	2.5904167
	2.1868534			-3.5740246	
C	0.4731886	-2.4873006	H	1.2195277	1.5892851
	2.4672415			-2.2626015	
H	1.2095917	-1.7003957	H	0.8487358	3.2978928
	2.2574784			-1.9722184	
H	0.7951506	-3.3922361	C	-1.9135892	3.1083418
	1.9406067			-2.5273315	
H	0.4930107	-2.6989276	H	-1.6508950	4.0853668
	3.5486774			-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	
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				

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	H	0.2614034	0.6257818
	3.1681890			4.6131764	
C	0.9004870	-2.2690971	H	0.1286108	-1.0838871
	2.7979221			5.0491518	
C	0.0793988	-0.3766573	H	3.3366679	-1.0582635
	4.2054191			3.1488146	
C	2.5396569	-0.6882761	H	2.5457603	-1.3272882
	3.8073790			4.7051330	
C	0.9318666	2.1186825	H	2.7989499	0.3259548
	1.9949843			4.1284801	
C	-0.5100144	2.4919573	H	-1.2213237	2.2639067
	2.3924518			1.5872007	
C	1.2906496	2.9100759	H	-0.5482676	3.5759723
	0.7262704			2.5876237	
C	1.9115571	2.5298195	H	-0.8508045	1.9745947
	3.1065225			3.2960451	
C	0.9319424	-2.1186454	H	2.3306608	2.7449407
	-1.9949822			0.4092229	
C	1.9116147	-2.5297393	H	1.1822802	3.9853009
	-3.1065522			0.9405377	
C	1.2908131	-2.9100124	H	0.6157587	2.6642330
	-0.7262767			-0.1019727	
C	-0.5099335	-2.4919974	H	2.9520127	2.2596235
	-2.3923961			2.8747483	
C	1.1380579	0.7929415	H	1.6487509	2.1085917
	-3.1682067			4.0838379	
C	2.5395374	0.6883899	H	1.8766472	3.6269974
	-3.8074356			3.2055951	
C	0.9003121	2.2691286	H	1.8767553	-3.6269195
	-2.7979382			-3.2056176	
C	0.0792817	0.3766431	H	2.9520648	-2.2594911
	-4.2054038			-2.8748145	
H	3.4354098	0.5569769	H	1.6487546	-2.1085300
	1.2196614			-4.0838608	
H	2.8977060	-1.1109513	H	1.1824933	-3.9852445
	1.0360091			-0.9405337	
H	2.8976295	1.1110964	H	0.6159385	-2.6642013
	-1.0360542			0.1019890	
H	3.4354190	-0.5568034	H	2.3308268	-2.7448200
	-1.2197143			-0.4092672	
H	-0.0898201	-2.4147592	H	-0.5481366	-3.5760142
	2.3474516			-2.5875678	
H	0.9519499	-2.8690226	H	-0.8507847	-1.9746515
	3.7207354			-3.2959761	
H	1.6715302	-2.6575600	H	-1.2212248	-2.2639851
	2.1182963			-1.5871184	
H	-0.9336717	-0.4190429	H	2.7988727	-0.3258273
	3.7857384			-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	H	0.7926280	-3.0761664
	-0.7519244			3.5342021	
P	0.9901137	0.1780339	H	1.4478696	-2.8013002
	1.5748548			1.9133674	
P	0.9900297	-0.1785204	H	-0.8608522	-0.4905814
	-1.5746118			3.9053032	
C	1.1277312	-0.9850867	H	0.4721032	0.3818079
	3.1182031			4.7206953	
C	0.7471747	-2.4054964	H	0.2200325	-1.3400851
	2.6610658			5.0374546	
C	0.1759770	-0.5662602	H	3.2908595	-1.4484309
	4.2539411			2.9679471	
C	2.5653853	-1.0344944	H	2.5585104	-1.7058993
	3.6801161			4.5537231	
C	1.0300444	2.0113058	H	2.9325068	-0.0604372
	2.1553675			4.0220857	
C	-0.3533122	2.4264609	H	-1.1400956	2.2726151
	2.6906812			1.9415759	
C	1.3261200	2.8745701	H	-0.3179555	3.4988436
	0.9171893			2.9429298	
C	2.1098376	2.2990482	H	-0.6453055	1.8777811
	3.2124239			3.5923087	
C	1.0288591	-2.0118175	H	2.3381624	2.7085926
	-2.1550840			0.5213236	
C	2.1081278	-2.3001843	H	1.2583975	3.9362527
	-3.2125017			1.2034264	
C	1.3249054	-2.8752420	H	0.5934903	2.6944027
	-0.9170142			0.1205663	
C	-0.3549269	-2.4261734	H	3.1159847	2.0007454
	-2.6899118			2.8839161	
C	1.1283304	0.9844775	H	1.8995373	1.8189872
	-3.1179778			4.1753376	
C	2.5659646	1.0328911	H	2.1374803	3.3863791
	-3.6800250			3.3904660	
C	0.7488114	2.4051562	H	2.1350770	-3.3875334
	-2.6607991			-3.3905422	
C	0.1761477	0.5663314	H	3.1145545	-2.0024666
	-4.2536107			-2.8843180	
H	3.4424240	0.4250185	H	1.8977947	-1.8200071
	1.2540461			-4.1753465	
H	2.8459956	-1.2009438	H	1.2565029	-3.9368883
	0.9360180			-1.2032253	
H	2.8467213	1.1993867	H	0.5926469	-2.6946872
	-0.9357966			-0.1201398	
H	3.4421736	-0.4269405	H	2.3371781	-2.7098112
	-1.2537912			-0.5215062	
H	-0.2719774	-2.4362321	H	-0.3202480	-3.4985331
	2.2547038			-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	H	2.6807838	1.3510567
	-1.6732301			-0.7218887	
Br	-2.2366150	-0.2108315	H	3.4199906	-0.1499415
	1.6732216			-1.2776194	
C	2.5675475	-0.2574607	H	-0.1081905	-2.6857256
	0.7174490			1.8995451	
C	2.5675418	0.2575250	H	0.9376086	-3.3824308
	-0.7174345			3.1594714	
P	0.9457835	0.0795215	H	1.6521778	-2.8589014
	1.5935804			1.6321750	
P	0.9457917	-0.0795112	H	-0.9823732	-1.0592064
	-1.5935700			3.7578363	
C	1.0848168	-1.2332203	H	0.2125611	-0.2557282
	3.0263001			4.8055495	
C	0.8796175	-2.6132025	H	0.1228813	-2.0196814
	2.3732771			4.7749670	
C	0.0381077	-1.1148154	H	3.3016880	-1.3591048
	4.1513757			2.9647623	
C	2.4836030	-1.1745263	H	2.5383149	-1.9599807
	3.6727972			4.4437070	
C	1.0863891	1.8804569	H	2.6669568	-0.2164169
	2.2934098			4.1775516	
C	0.3272586	2.0408950	H	-0.6904785	1.6330408
	3.6214470			3.5642510	
C	0.4214370	2.8152813	H	0.2478568	3.1179419
	1.2674958			3.8403095	
C	2.5491667	2.3145048	H	0.8565612	1.5766135
	2.4904450			4.4623203	
C	1.0864562	-1.8804389	H	0.9274175	2.7944651
	-2.2934047			0.2964762	
C	2.5492477	-2.3144370	H	0.4707174	3.8492607
	-2.4904468			1.6473068	
C	0.4215377	-2.8152903	H	-0.6341573	2.5553149
	-1.2674934			1.1097981	
C	0.3273271	-2.0408924	H	3.1097625	2.3476532
	-3.6214411			1.5456850	
C	1.0847785	1.2332313	H	3.0950493	1.6725557
	-3.0262926			3.1947114	
C	2.4835649	1.1745817	H	2.5563091	3.3354679
	-3.6727933			2.9049463	
C	0.8795323	2.6132095	H	2.5564229	-3.3353977
	-2.3732750			-2.9049535	
C	0.0380704	1.1147822	H	3.1098472	-2.3475717
	-4.1513643			-1.5456885	
H	3.4199813	0.1500334	H	3.0951071	-1.6724661
	1.2776367			-3.1947114	
H	2.6808253	-1.3509888	H	0.4708508	-3.8492661
	0.7219036			-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	H	0.9570487	2.8192643
	-2.4222857			0.5042536	
C	2.6254925	-2.1356005	H	0.5675268	3.7828779
	-2.6077515			1.9417154	
C	0.4805355	-2.7817570	H	-0.5882551	2.5602061
	-1.4884947			1.3454731	
C	0.4334380	-1.8374344	H	3.1582132	2.2307609
	-3.7830014			1.6526406	
C	1.0294742	1.3986343	H	3.1715687	1.4312722
	-2.9294385			3.2456423	
C	2.4019617	1.3773276	H	2.6670994	3.1234078
	-3.6318027			3.0984122	
C	0.8589346	2.7321485	H	2.6704380	-3.1213047
	-2.1767645			-3.0980798	
C	-0.0674164	1.3659165	H	3.1605503	-2.2281435
	-4.0102674			-1.6522848	
H	3.4184396	0.0574687	H	3.1732681	-1.4286813
	1.2808161			-3.2453040	
H	2.6550864	-1.3945031	H	0.5713879	-3.7827913
	0.6346016			-1.9415669	
H	2.6537691	1.3966394	H	-0.5856296	-2.5612260
	-0.6343152			-1.3454525	
H	3.4186232	-0.0545766	H	0.9598487	-2.8187745
	-1.2804562			-0.5040897	
H	-0.0992062	-2.7716642	H	0.4264528	-2.8930277
	1.6467968			-4.0996315	
H	0.8755742	-3.5505981	H	0.9546185	-1.2681198
	2.9133931			-4.5628575	
H	1.6717783	-2.9335152	H	-0.6080030	-1.4972665
	1.4635684			-3.7179883	
H	-1.0701098	-1.3484710	H	2.5512898	0.4628781
	3.5721915			-4.2214348	
H	0.0271159	-0.5182811	H	3.2470268	1.4886387
	4.6937844			-2.9399255	
H	0.0384873	-2.2846156	H	2.4436239	2.2248093
	4.6112137			-4.3348275	
H	3.2481878	-1.4857547	H	0.8722703	3.5509627
	2.9403991			-2.9132834	
H	2.4453392	-2.2228376	H	1.6688314	2.9346731
	4.3351387			-1.4633141	
H	2.5511489	-0.4607881	H	-0.1019481	2.7709927
	4.2218352			-1.6468878	
H	-0.6098251	1.4962112	H	0.0273627	0.5178109
	3.7179742			-4.6939256	
H	0.4232827	2.8929293	H	0.0367249	2.2841480
	4.0997672			-4.6112216	
H	0.9529291	1.2685021	H	-1.0710109	1.3466881
	4.5629901			-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	P	0.9419200	-0.0556349
	-1.7448683			1.5895850	
H	3.1976899	-1.2769208	P	0.9418866	0.0556373
	-3.3026873			-1.5896047	
H	0.6538828	-3.7402164	C	0.9511413	-1.5620066
	-2.0871352			2.8120737	
H	-0.5238513	-2.5693223	C	0.8070881	-2.8368977
	-1.4322130			1.9585556	
H	1.0353938	-2.8283268	C	-0.2091084	-1.5848068
	-0.6147252			3.8237053	
H	0.4943524	-2.7702061	C	2.2851193	-1.6139242
	-4.2121497			3.5827521	
H	0.9619427	-1.1087671	C	1.2191145	1.6058022
	-4.6053004			2.5545127	
H	-0.5871362	-1.4302127	C	0.4905099	1.6196802
	-3.7650226			3.9096580	
H	2.4785456	0.6046167	C	0.6278943	2.7377671
	-4.2469524			1.6962547	
H	3.2088317	1.5642010	C	2.7131536	1.8936281
	-2.9338823			2.7901516	
H	2.3764047	2.3704929	C	1.2190591	-1.6058008
	-4.2723371			-2.5545367	
H	0.8162961	3.6299760	C	2.7130928	-1.8936288
	-2.7808530			-2.7902078	
H	1.6757767	2.9760926	C	0.6278564	-2.7377641
	-1.3843070			-1.6962642	
H	-0.0990966	2.8008018	C	0.4904246	-1.6196804
	-1.5024691			-3.9096660	
H	-0.0764680	0.6428385	C	0.9510891	1.5620081
	-4.6199438			-2.8120949	
H	-0.0372355	2.4083416	C	2.2850503	1.6139171
	-4.5099900			-3.5828029	
H	-1.1254395	1.4678150	C	0.8070633	2.8369015
	-3.4529095			-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	
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				

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	H	-0.5583925	1.2872158
	3.9657950			3.8312943	
C	0.7153728	2.7053846	H	0.6023168	2.5012265
	1.8025345			4.4195785	
C	2.7555037	1.7533463	H	0.9392702	0.7825547
	2.8900135			4.6749936	
C	1.2571543	-1.5206150	H	1.2480103	2.8290998
	-2.6210082			0.8525828	
C	2.7554513	-1.7533792	H	0.8580878	3.6305356
	-2.8900471			2.3846322	
C	0.7153233	-2.7053865	H	-0.3554970	2.5888270
	-1.8025338			1.5914340	
C	0.5091386	-1.5011329	H	3.3264674	1.9344911
	-3.9657965			1.9687293	
C	0.9057010	1.6437346	H	3.2291355	0.9272077
	-2.7436496			3.4367029	
C	2.2177856	1.7490242	H	2.8558013	2.6574216
	-3.5451497			3.5117394	
C	0.7653399	2.8819683	H	2.8557282	-2.6574571
	-1.8370489			-3.5117727	
C	-0.2852771	1.6818398	H	3.3264258	-1.9345302
	-3.7181408			-1.9687709	
H	3.4258219	-0.1070158	H	3.2290862	-0.9272480
	1.2729229			-3.4367448	
H	2.6168660	-1.4590540	H	0.8580192	-3.6305424
	0.4809281			-2.3846282	
H	2.6168641	1.4590435	H	-0.3555424	-2.5888145
	-0.4809611			-1.5914199	
H	3.4258082	0.1070043	H	1.2479717	-2.8291030
	-1.2729649			-0.8525882	
H	-0.1249426	-2.8148804	H	0.6022330	-2.5012397
	1.1975376			-4.4195776	
H	0.6538992	-3.7700518	H	0.9391999	-0.7825722
	2.4787164			-4.6750044	
H	1.6453604	-3.0558096	H	-0.5584547	-1.2872147
	1.2041340			-3.8312801	
H	-1.2439150	-1.6179366	H	2.3285605	0.9332601
	3.1913303			-4.2713318	
H	-0.2585244	-0.8852676	H	3.1109499	1.7709390
	4.4667553			-2.9058539	
H	-0.2429728	-2.6434317	H	2.2026071	2.6913356
	4.2554138			-4.1162536	
H	3.1109689	-1.7709649	H	0.6538995	3.7700443
	2.9058090			-2.4787517	
H	2.2026313	-2.6913639	H	1.6453688	3.0558034
	4.1162107			-1.2041751	
H	2.3285976	-0.9332901	H	-0.1249357	2.8148869
	4.2712998			-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	Br	-2.1966676	0.5712775
	3.5054462			1.6168707	
H	2.9066436	2.4685748	C	2.5592041	-0.4241046
	3.6601542			0.6369811	
H	2.9065752	-2.4686333	C	2.5592018	0.4240985
	-3.6601369			-0.6369847	
H	3.3854539	-1.8095194	P	0.9551678	-0.1696901
	-2.0917033			1.5718604	
H	3.2312108	-0.7339375	P	0.9551655	0.1696816
	-3.5054553			-1.5718633	
H	0.9647953	-3.5562428	C	0.8100686	-1.8008464
	-2.5327410			2.5935862	
H	-0.2609667	-2.5890769	C	0.6758731	-2.9577584
	-1.6673544			1.5844764	
H	1.3680633	-2.8104077	C	-0.4420608	-1.8503420
	-0.9769104			3.4875284	
H	0.6370994	-2.3527297	C	2.0689183	-2.0253404
	-4.5127621			3.4523638	
H	0.9089930	-0.6140316	C	1.3256040	1.3328790
	-4.7000384			2.7451845	
H	-0.5534145	-1.2067462	C	0.5182737	1.2570268
	-3.8516771			4.0538148	
H	2.2475564	1.1117468	C	0.9020447	2.6143255
	-4.2678400			2.0064911	
H	3.0541650	1.8944210	C	2.8224001	1.4428055
	-2.8837434			3.0927996	
H	2.1012969	2.8583940	C	1.3256085	-1.3328768
	-4.0245040			-2.7451992	
H	0.5660712	3.8335830	C	2.8224059	-1.4427934
	-2.3119606			-3.0928122	
H	1.6183697	3.0938498	C	0.9020538	-2.6143317
	-1.1018310			-2.0065182	
H	-0.1442846	2.8110079	C	0.5182812	-1.2570168
	-1.0425099			-4.0538309	
H	-0.3433306	1.0062365	C	0.8100670	1.8008468
	-4.3836032			-2.5935747	
H	-0.3628660	2.7554000	C	2.0689181	2.0253482
	-4.1045424			-3.4523480	
H	-1.3040340	1.6649485	C	0.6758716	2.9577488
	-3.0509542			-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	
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				

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	H	2.9329234	-2.1415430
	3.3613141			2.8368138	
C	1.9886310	-2.1588624	H	1.8827619	-3.1686757
	3.3995596			3.8280823	
C	1.3528671	1.2350946	H	2.0702030	-1.4575245
	2.8034974			4.2397367	
C	0.5062522	1.1358803	H	-0.5637419	1.0527835
	4.0856898			3.8584071	
C	0.9954564	2.5587652	H	0.6614241	2.0598370
	2.1051812			4.6662473	
C	2.8422765	1.2793140	H	0.8107279	0.2975186
	3.1958384			4.7250432	
C	1.3528654	-1.2350805	H	1.6166010	2.7390744
	-2.8035083			1.2189368	
C	2.8422733	-1.2792726	H	1.1795486	3.3875731
	-3.1958575			2.8080135	
C	0.9954793	-2.5587605	H	-0.0611573	2.5815065
	-2.1051969			1.8096116	
C	0.5062429	-1.1358692	H	3.4929156	1.5390183
	-4.0856962			2.3494105	
C	0.7629207	1.8723723	H	3.2031312	0.3420612
	-2.5125209			3.6386458	
C	1.9885843	2.1588707	H	2.9721921	2.0702307
	-3.3995727			3.9518687	
C	0.6366279	2.9855350	H	2.9721985	-2.0701838
	-1.4544106			-3.9518919	
C	-0.5205358	1.9219576	H	3.4929215	-1.5389690
	-3.3613117			-2.3494340	
H	3.4437418	-0.2431353	H	3.2031093	-0.3420114
	1.2553674			-3.6386629	
H	2.6147072	-1.5012471	H	1.1795809	-3.3875617
	0.3385794			-2.8080346	
H	2.6146886	1.5012691	H	-0.0611324	-2.5815202
	-0.3385974			-1.8096218	
H	3.4437293	0.2431657	H	1.6166317	-2.7390646
	-1.2553919			-1.2189569	
H	-0.1792673	-2.7823082	H	0.6614270	-2.0598186
	0.7472482			-4.6662621	
H	0.4090866	-3.9304866	H	0.8107022	-0.2974969
	1.9722323			-4.7250440	
H	1.5631978	-3.1461930	H	-0.5637514	-1.0527914
	0.8881909			-3.8584078	
H	-1.4138028	-1.7117401	H	2.0701583	1.4575293
	2.7607849			-4.2397470	
H	-0.5101026	-1.2221616	H	2.9328804	2.1415634
	4.2018011			-2.8368325	
H	-0.6105313	-2.9392007	H	1.8827025	3.1686809
	3.7756022			-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	H	-1.5277979	-1.7780375
	-1.5335879			2.2817773	
C	0.6556069	-2.0205010	H	-0.8082894	-1.3875794
	2.3168769			3.8527425	
C	0.6293820	-3.0589639	H	-0.9199648	-3.0800116
	1.1796030			3.3346500	
C	-0.7321667	-2.0516566	H	2.7550184	-2.3915231
	2.9864715			2.8903458	
C	1.7459485	-2.4192588	H	1.5591525	-3.4562754
	3.3270007			3.6501425	
C	1.3852593	1.0007488	H	1.7366526	-1.7924567
	2.9161771			4.2272470	
C	0.3941656	0.8934539	H	-0.6470197	0.9319509
	4.0898068			3.7445867	
C	1.2290135	2.3997601	H	0.5622965	1.7543141
	2.2936261			4.7571890	
C	2.8227749	0.8723103	H	0.5482800	-0.0139375
	3.4581621			4.6875862	
C	1.3855508	-1.0005591	H	1.9430853	2.5731681
	-2.9161305			1.4774118	
C	2.8230688	-0.8718737	H	1.4342428	3.1537998
	-3.4580502			3.0708334	
C	1.2295150	-2.3995999	H	0.2095127	2.5563708
	-2.2935933			1.9193190	
C	0.3944923	-0.8934263	H	3.5792814	1.1453642
	-4.0898046			2.7096977	
C	0.6553582	2.0205644	H	3.0587940	-0.1271467
	-2.3168504			3.8428079	
C	1.7456824	2.4195137	H	2.9348673	1.5807891
	-3.3269175			4.2946395	
C	0.6288992	3.0590158	H	2.9353195	-1.5803290
	-1.1795711			-4.2945263	
C	-0.7323873	2.0514865	H	3.5795878	-1.1448029
	-2.9865139			-2.7095528	
H	3.4689637	-0.2836952	H	3.0589354	0.1276256
	1.2560888			-3.8426800	
H	2.6726171	-1.5146045	H	1.4349074	-3.1536010
	0.2750108			-3.0707949	
H	2.6723691	1.5150106	H	0.2100241	-2.5563857
	-0.2749096			-1.9193326	
H	3.4689657	0.2842371	H	1.9435798	-2.5728904
	-1.2559547			-1.4773478	
H	-0.1059351	-2.7958057	H	0.5627972	-1.7542561
	0.4072965			-4.7571820	
H	0.3360839	-4.0298244	H	0.5484823	0.0139929
	1.6092422			-4.6875740	
H	1.6099501	-3.2008880	H	-0.6467021	-0.9320985
	0.7059893			-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	H	-0.9881989	3.0822302
	4.7393083			-3.2422503	
H	0.4414734	-0.0362842	H	-1.5418618	1.8117367
	4.6545263			-2.1246012	
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				