

Supporting Information

The Crucial Roles of MgCl₂ as a Non-innocent Additive in the Ni-Catalyzed Carboxylation of Benzyl Halide with CO₂

Fareed Bhasha Sayyed and Shigeyoshi Sakaki*

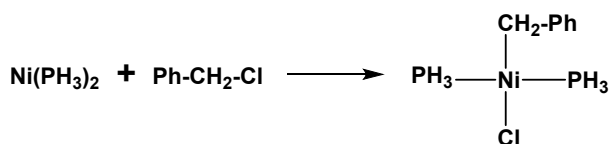
*Fukui Institute for Fundamental Chemistry, Kyoto University, Nishihiraki-cho 34-4,
Takano, Sakyo-ku, Kyoto 606-8103, Japan*

E-mail: sakaki.shigeyoshi.47e@st.kyoto-u.ac.jp

Computational Details

All the calculations were carried out using Gaussian09 suite of program.¹ All of the geometries were optimized by the DFT with the B3LYP-D functional.² For geometry optimizations and frequency calculations, BS-I basis set system was employed. In BS-I, we employed Lanl2Tz(f) basis set for Ni,³ 6-31G(d) basis sets for H, C, O, P, and Mg, and 6-31+G(d) for Cl. All the stationary structures were characterized with no imaginary frequency and the transition state structures (TSs) were characterized with a single imaginary frequency. Intrinsic reaction coordinate (IRC) calculations⁴ were performed on all the TSs. The computational method and BS-I basis set system are selected after a careful comparison between the geometrical parameters of optimized and experimentally reported structures.

The DFT(B3LYP-D)-calculated activation energy of a model system of oxidative addition reaction ((PH_3)₂Ni + PhCH₂Cl → (PH_3)₂Ni(PhCH₂)(Cl); see Scheme S1) is in excellent agreement with the activation energy calculated at the CCSD(T) level. Therefore, we selected the B3LYP-D method for the present study. The solvent effect of *N,N*-dimethylformamide (DMF) was evaluated by conductor-like polarizable continuum model (CPCM),⁵ in which a better basis system BS-II was used. In BS-II, we employed SDD basis sets⁶ for Ni and Zn with effective core potentials, 6-311G(d) basis sets for H, C, O, P, and Mg, and 6-311+G(d) for Cl, wherein optimized structures with the DFT(B3LYP-D)/BS-I were employed. The Gibbs energy was evaluated by using the electronic energy calculated by the DFT(B3LYP-D)/BS-II, where the translational entropy was corrected by the method of Whitesides et al.⁷ NBO analysis was carried out by the method of Weinhold et al.,⁸ as implemented in the Gaussian 09 at the B3LYP-D/BS-II level.



Scheme S1. The reaction employed for checking the reliability of the computational methods.

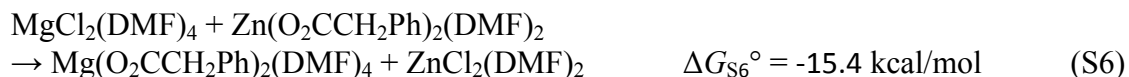
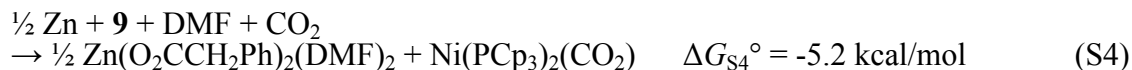
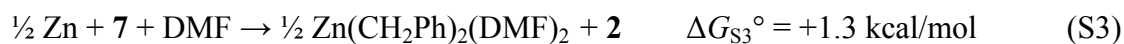
Table S1. Activation energy (E_a) and reaction energy (ΔE) for the oxidative addition of benzyl chloride to Ni(PH₃)₂. All the values in kcal/mol.^a

Method	E_a	ΔE	$E_a^{\text{err } b}$	$\Delta E^{\text{err } c}$
CCSD(T)	1.3	-46.2	-	-
B3PW91	6.4	-36.1	-5.1	-10.1
M06	4.9	-35.1	-3.6	-11.1
TPSS	-3.2	-37.8	4.5	-8.4
TPSSh	0.2	-39.2	1.2	-7.0
LC-BLYP	8.2	-42.2	-6.9	-4.0
M06L	-3.8	-44.4	5.1	-1.8
B97-1	4.5	-44.5	-3.1	-1.7
B97-2	9.1	-32.6	-7.7	-13.6
B97D	-1.1	-32.6	2.4	-13.6
PBE0	4.9	-39.7	-3.6	-6.5
B2PLYP	16.7	-4.3	-15.4	-41.9
mPW2PLYP	-0.7	-26.9	2.0	-19.3
wB97XD	5.8	-40.8	-4.5	-5.4
B3LYP-D	2.1	-43.6	-0.8	-2.6
B3LYP	7.8	-36.9	-6.4	-9.3
CAM-B3LYP	8.4	-40.4	-7.1	-5.8
M05	11.9	-25.7	-10.6	-20.5
M05-2X	6.9	-49.0	-5.6	2.8
M06-2X	9.1	-46.8	-7.8	0.7
HCTH	8.9	-19.9	-7.6	-26.3

^a The geometries were optimized with the B3PW91 method with BS-I basis set, wherein Lanl2Tz(f) was used for Ni and cc-pVDZ basis sets were used for C, H, P, and Cl. These geometries were employed in single point CCSD(T) calculations by replacing cyclopentyl group with H. ^b $E_a^{\text{err}} = E_a(\text{CCSD(T)}) - E_a(\text{DFT})$ ^c $\Delta E^{\text{err}} = \Delta E(\text{CCSD(T)}) - \Delta E(\text{DFT})$

One electron reduction process

In the experiment, NiCl₂·glyme was used as a nickel catalyst source and two equivalents of PCp₃ ligand were added. The glyme can be easily replaced with PCp₃ and the calculated ΔG_{S1}° for this process is -15.9 kcal/mol, as shown in Eq. S1. The next step is the reduction of the Ni(II) complex, Ni(PCp₃)₂Cl₂ with Zn to form Ni(PCp₃)₂ **2**. We used Zn atom as a model of zinc powder like in our previous work.⁹ The reduction process of Ni(II) to Ni(0) occurs easily, as indicated by a considerably negative ΔG_{S2}° (-13.3 kcal/mol). In the presence of DMF, Suzuki et al.¹⁰ reported that ZnCl₂ interacts with two DMF molecules. Also, Zn(O₂CCH₂Ph)₂ and Mg(O₂CCH₂Ph)₂ are likely to be associated with solvent molecules, as shown by previous reports.⁹ Hence, we calculated these species interacting with DMF.



Isomerization process

We studied the *cis-trans* isomerization reaction of *cis*-Ni(Cl)(CH₂Ph)(PCp₃)₂ **4**. As shown in Figure S1, one of the PCp₃ ligands dissociates from the Ni-center to form a monophosphine Ni(II) intermediate Ni(Cl)(CH₂Ph)(PCp₃) **4a**. From **4a**, *cis-trans* isomerization occurs to afford **4b** via a transition state **TS**_{4a-4b}. The ΔG^{\ddagger} for the isomerization reaction is 11.2 kcal/mol, indicating that this process easily occurs. Then, PCp₃ coordinates with the Ni-center to form *trans*-Ni(Cl)(CH₂Ph)(PCp₃)₂ **5**. The intermediates **9**, **11**, and **13** also isomerize to **9a**, **11a**, and **13a**, respectively, as shown Figure S2. However, these isomerizations are not important very much in the catalytic reaction (for isomerization processes see our previous work in reference 5b).

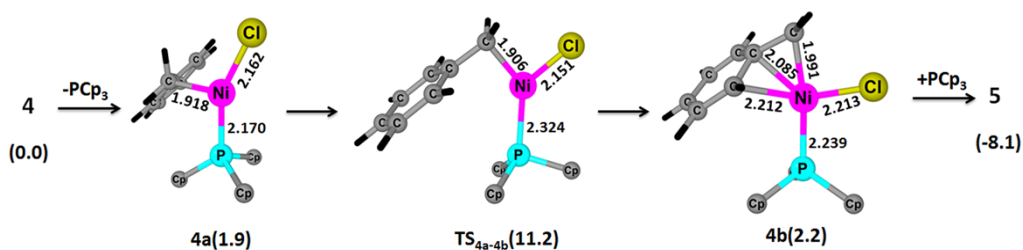


Fig. S1 *Cis-trans* isomerization between 4 and 5. In parenthesis is the Gibbs energy. Bond lengths are in Å units and the Cp on the phosphine represents a cyclopentyl group.

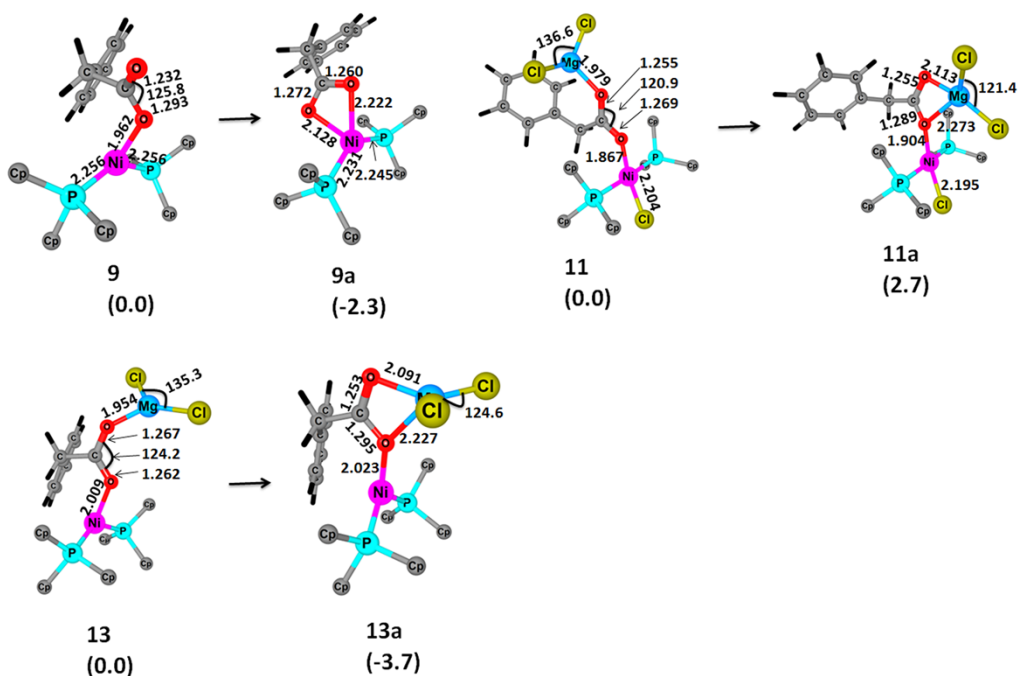


Fig. S2 Structures of 9a, 11a, and 13a. In parenthesis is the Gibbs energy. Bond lengths are in Å unit and angles are in degree. The Cp on the phosphine represents a cyclopentyl group.

The reason of the easy CO₂ insertion into the Ni^I-CH₂Ph is important for the CO₂ fixation reaction. The Ni^I-CH₂Ph bond energy of **7** is smaller than the Ni^{II}-CH₂Ph one of **5** by 14.7 kcal/mol and the Ni^I-O bond energy of **9** is larger than the Ni^{II}-O one of **6** by 30.5 kcal/mol. Also, the charge transfer (CT) to CO₂ from the Ni-CH₂Ph moiety occurs much more in the insertion reaction into the Ni^I-CH₂Ph bond than into the Ni^{II}-CH₂Ph bond (see Fig S3); note that this CT is indispensable for the CO₂ insertion. These are responsible for the easier CO₂ insertion into the Ni^I-CH₂Ph bond of **7** than that into the Ni^{II}-CH₂Ph bond of **5**.

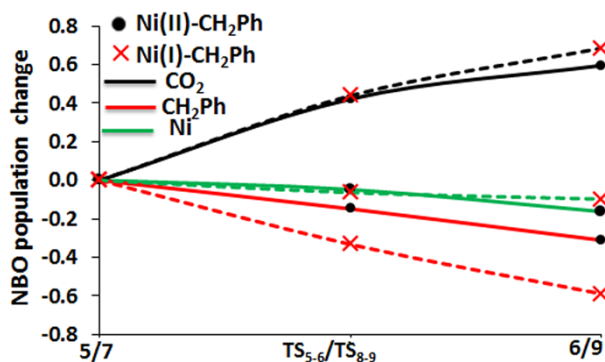


Fig. S3 Population changes by the CO₂ insertion into the Ni^{II}-CH₂Ph bond of **5** and Ni^I-CH₂Ph bond of **7**.

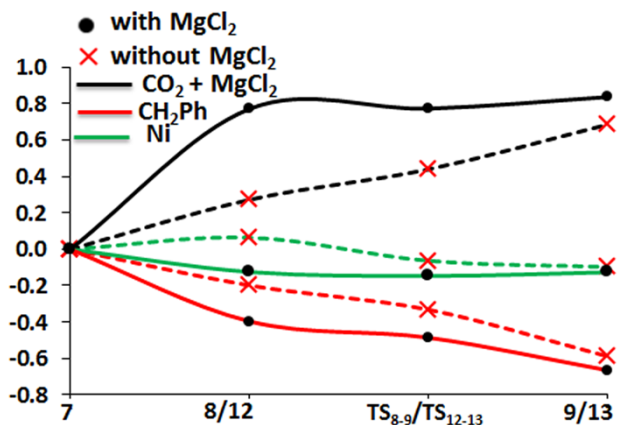


Fig. S4 Population changes in the CO₂ insertion into the Ni^I-CH₂Ph bond of **7**.

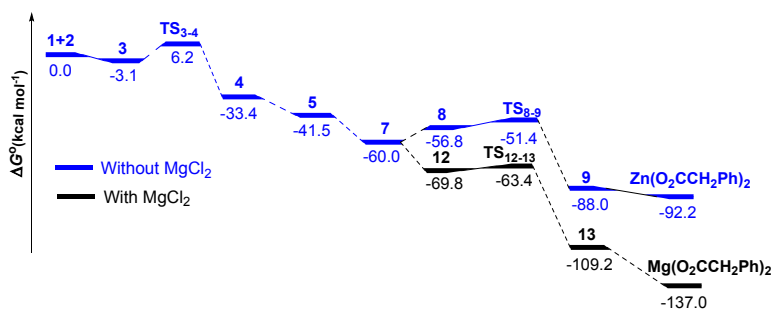


Fig. S5 Gibbs free energy profile (in kcal/mol) for the total catalytic cycle of Ni-catalyzed carboxylation of benzyl chloride with CO₂.

Table S2. Ni^I-C, Ni^{II}-C, Ni^I-O, and Ni^{II}-O bond dissociation energies, BDE (in kcal/mol).^a

Bond type	Reaction	BDE
Ni ^I -C of 7	(Cp ₃ P) ₂ Ni ^I -(CH ₂ Ph) → (Cp ₃ P) ₂ Ni ⁰ + PhCH ₂ •	43.4
Ni ^{II} -C of 5	(Cp ₃ P) ₂ Ni ^{II} -(CH ₂ Ph)(Cl) → (Cl)(Cp ₃ P) ₂ Ni ^I + PhCH ₂ •	28.7
Ni ^{II} -O of 11	(Cp ₃ P) ₂ Ni ^{II} -(Cl)(η ¹ -O ₂ CCH ₂ Ph) → (Cp ₃ P) ₂ Ni ^I (Cl) + η ² -O ₂ CCH ₂ CPhMgCl ₂ •	78.2
Ni ^{II} -O of 6	(Cp ₃ P) ₂ Ni ^{II} -(η ¹ -O ₂ CCH ₂ Ph)(Cl) → (Cl)(Cp ₃ P) ₂ Ni ^I + PhCH ₂ COO•	66.2
Ni ^I -O of 13	(Cp ₃ P) ₂ Ni ^I -(η ¹ -O ₂ CCH ₂ Ph) → (Cp ₃ P) ₂ Ni ⁰ + η ² -O ₂ CCH ₂ CPhMgCl ₂ •	116.0
Ni ^I -O of 9	(Cp ₃ P) ₂ Ni ^I -(η ¹ -O ₂ CCH ₂ Ph) → (Cp ₃ P) ₂ Ni ⁰ + PhCH ₂ COO•	96.7

^aCalculated at B3LYP-D/BS-II level.

Table S3. B3LYP-D/BSII calculated electronic energies (E) used for calculating bond dissociation energies. All values are in atomic units.

	E
2	-2029.860709
5	-2761.209872
7	-2300.912091
6	-2949.872465
11	-4070.658167
9	-2489.599874
13	-3610.397172
PhCH ₂ COO [•]	-459.585039
(Cl)(Cp ₃ P) ₂ Ni ^I	-2490.181929
η^2 -O ₂ CCH ₂ CPhMgCl ₂ [•]	-1580.351577

Table S4. Electronic energies in vacuo (E), thermal energies (E_T), gas phase free energies (G), electronic energies in DMF (E_{sol}), and Gibbs free energies in DMF (G_{sol}) of the all the species. All values are in atomic units.

	E	E_{sol}	E_T	G	G_{sol}
1	-731.167415	-731.265601	0.126668	-731.080323	-731.166031
2	-2027.925077	-2029.864734	0.832412	-2027.200336	-2029.127516
3	-2759.127981	-2761.156913	0.964621	-2758.282006	-2760.298461
TS₃₋₄	-2759.112299	-2761.143888	0.964015	-2758.264589	-2760.283701
4	-2759.168548	-2761.208406	0.966429	-2758.319317	-2760.346698
4a	-1829.859429	-1831.749603	0.545619	-1829.398806	-1831.276503
TS_{4a-4b}	-1829.845142	-1831.732950	0.543876	-1829.386421	-1831.261752
4b	-1829.864838	-1831.750757	0.545201	-1829.402677	-1831.276120
5	-2759.183870	-2761.218523	0.965702	-2758.337463	-2760.359639
CO₂	-188.581064	-188.643519	0.014238	-188.590192	-188.640169
TS₅₋₆	-2947.707060	-2949.807949	0.981893	-2946.844900	-2948.933313
6	-2947.788806	-2949.887979	0.983123	-2946.930028	-2949.016724
6a	-2947.805864	-2949.899028	0.982311	-2946.951837	-2949.032524
7	-2298.926611	-2300.926564	0.959381	-2298.083381	-2300.070203
8	-2487.506778	-2489.570075	0.976751	-2486.655043	-2488.705210
TS₈₋₉	-2487.496331	-2489.561037	0.975988	-2486.645067	-2488.696641
9	-2487.547369	-2489.619793	0.977353	-2486.695747	-2488.755038
9a	-2487.559012	-2489.619421	0.976700	-2486.711354	-2488.758632
MgCl₂	-1120.627987	-1120.768417	0.006955	-1120.650893	-1120.778845
10	-4068.425058	-4070.624051	0.993625	-4067.567840	-4069.754356
TS₁₀₋₁₁	-4068.403450	-4070.603679	0.992618	-4067.544844	-4069.732595
11	-4068.500942	-4070.693698	0.993377	-4067.645546	-4069.825826
11a	-4068.497786	-4070.691137	0.993564	-4067.640712	-4069.821586
12	-3608.200915	-3610.369710	0.987646	-3607.349166	-3609.504830
TS₁₂₋₁₃	-3608.190642	-3610.358729	0.986700	-3607.339668	-3609.494624
13	-3608.261440	-3610.429740	0.987271	-3607.412448	-3609.567616
13a	-3608.272647	-3610.436712	0.988056	-3607.422642	-3609.573575

Consideration of DMF coordination with MgCl₂ in TS₁₂₋₁₃:

Because DMF is a coordinating solvent, MgCl₂ interacts with DMF to afford MgCl₂(DMF)₄ in DMF solvent. Also, we must consider the DMF cluster because DMF molecule can form hydrogen bond with each other, as shown in Fig. S6. We found that the stacking geometry is more stable than the planar one in gas phase but less stable than the planar one in DMF solution.

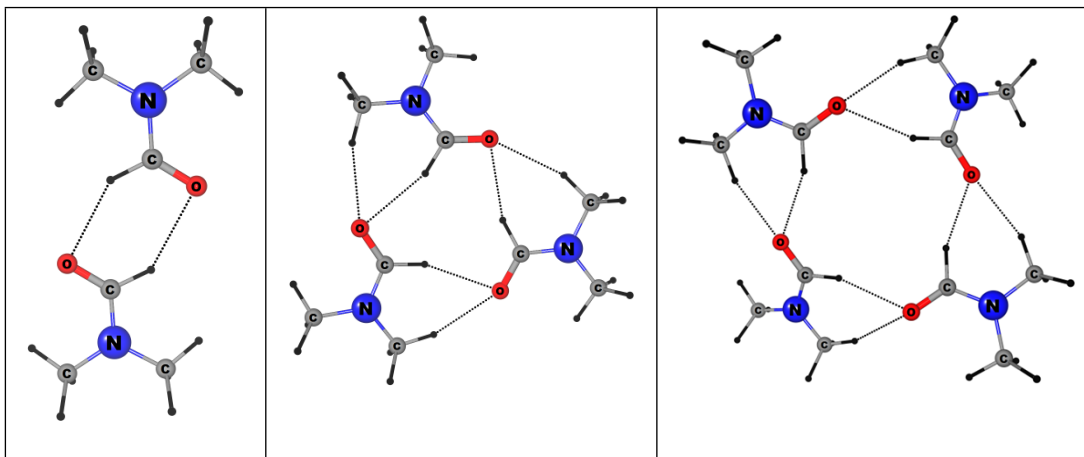
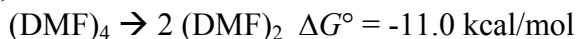
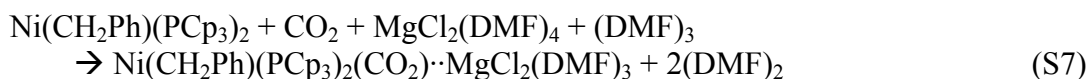


Fig. S6 The geometries of DMF dimer, trimer and tetramer.

See Table S5 for the Gibbs energies of the dimer, trimer, and tetramer. From the Gibbs energy, the tetramer is calculated to be converted to two molecules of dimer.

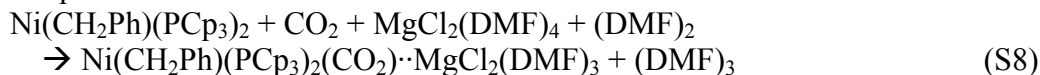


It is concluded that DMF dimer and trimer mainly exist in solution. In TS₁₂₋₁₃, the Mg centre interacts with three DMF molecules, because the Mg already interacts with the O of CO₂ coordinated with the Ni centre; see Fig. S7. Hence, we considered Eq. S7 to evaluate the energy of TS₁₂₋₁₃. The geometries of **12** and TS₁₂₋₁₃ with MgCl₂(DMF)₃ were optimized by fixing the geometry of the Ni(CH₂Ph)(PCp₃)₂(CO₂) moiety. This is not unreasonable because the interaction with DMF is not strong and does not influence very much the geometry of the Ni(CH₂Ph)(PCp₃)₂(CO₂) moiety.



The left-hand side represents **7** + CO₂ + MgCl₂(DMF)₄ and the right-hand side represents the TS₁₂₋₁₃ (or **12**) interacting with MgCl₂(DMF)₃. The ΔG° value for Eq. S7 is 1.0 kcal/mol, representing that the TS₁₂₋₁₃ is more unstable than **7** + CO₂ + MgCl₂(DMF)₄ by only 1.0 kcal/mol. We employed the same equation for the Ni(I)-CO₂ adduct **12**, but the value becomes positive, indicating that MgCl₂(DMF)₃ does not coordinate with the O of CO₂ in the Ni(I)-CO₂ adduct.

If we employ Eq. S8, the ΔG° value is 9.0 kcal/mol, indicating that DMF dimer does not participate in the reaction.



Because many dimer and trimer exist in solution, the reaction occurs via Eq. S7 but not via Eq. S8. In conclusion, MgCl_2 accelerates the reaction even if DMF molecules coordinate with MgCl_2 .

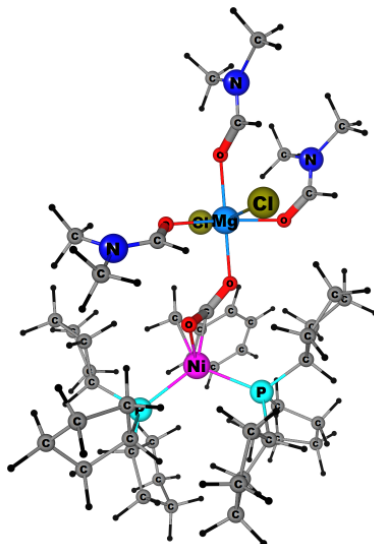


Fig. S7 The geometry of TS_{12-13} interacting with $\text{MgCl}_2(\text{DMF})_3$.

Table S5. The ΔG_{sol} (au unit) of important species for interaction with $\text{MgCl}_2(\text{DMF})_4$.

System	ΔG_{sol}
7	-2300.070203
CO_2	-188.640169
12	-2488.705210
TS_{12-13}	-3609.494624
$\text{Ni}(\text{PCp}_3)_2(\text{CH}_2\text{Ph})(\text{CO}_2) \cdot \text{MgCl}_2(\text{DMF})_3$ 12	-4355.063288
$\text{Ni}(\text{PCp}_3)_2(\text{CH}_2\text{Ph})(\text{CO}_2) \text{MgCl}_2(\text{DMF})_3 \text{TS}_{12-13}$	-4355.067884
MgCl_2	-1120.778845
$\text{MgCl}_2(\text{DMF})_4$	-2114.875860
DMF	-248.505436
$(\text{DMF})_2$	-497.023986 ($\Delta G_{\text{int}} = -8.23$) ^a
$(\text{DMF})_3$	-745.528040 ($\Delta G_{\text{int}} = -7.36$) ^a
$(\text{DMF})_4$	-994.030389 ($\Delta G_{\text{int}} = -5.42$) ^a

^aIn parenthesis is the Gibbs interaction energy (kcal/mol unit).

References

- (1) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. Montgomery, J. A. , J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian09, Revision B.01, I. Gaussian, Wallingford CT and 2010.
- (2) S. Grimme. *J. Comp. Chem.* 2006, **27**, 1787.
- (3) (a) A. W. Ehlers, M. Böhme, S. Dapprich, A. Gobbi, A. Höllwarth, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp and G. Frenking. *Chem. Phys. Lett.* 1993, **208**, 111; (b) A. Höllwarth, M. Böhme, S. Dapprich, A. W. Ehlers, A. Gobbi, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp and G. Frenking. *Chem. Phys. Lett.* 1993, **208**, 237.
- (4) (a) H. P. Hratchian and H. B. Schlegel. *J. Chem. Phys.* 2004, **120**, 9918; (b) H. P. Hratchian and H. B. Schlegel. *J. Chem. Theory and Comput.* 2005, **1**, 61.
- (5) (a) V. Barone and M. Cossi. *J. Phys. Chem. A* 1998, **102**, 1995; (b) M. Cossi, N. Rega, G. Scalmani and V. Barone. *J. Comp. Chem.* 2003, **24**, 669.
- (6) M. Dolg, U. Wedig, H. Stoll and H. Preuss. *J. Chem. Phys.* 1987, **86**, 866.
- (7) (a) M. Mammen, E. Shakhnovich, I. J. Deutch, M and G. Whitesides, *M. J. Org. Chem.* 1998, **63**, 3821; (b) A. Ishikawa, Y. Nakao, H. Sato and S. Sakaki. *Inorg. Chem.* 2009, **48**, 8154; (c) G. Zeng and S. Sakaki. *Inorg. Chem.* 2011, **50**, 5290.
- (8) E. Glendening, D, C. Landis, R and F. Weinhold. *WIREs Comput. Mol. Sci.* 2012, **2**, 1.
- (9) (a) K. M. N. Burgess, Y. Xu, M. C. Leclerc and D. L. Bryce. *J. Phys. Chem. A* 2013, **117**, 6561; (b) C. N. R. Rao, S. Natarajan and R. Vaidhyanathan. *Angew. Chem. Int. Ed.* 2004, **43**, 1466.

Table S6. B3LYP-D/BS-I optimized Cartesian coordinates of the species involved in the catalytic cycle investigated here.

1				2			
C	0.020723000	0.000067000	0.450118000	P	-2.052106000	-0.183203000	-0.394572000
C	-0.656366000	1.209353000	0.245295000	C	-2.835762000	1.077552000	-1.527943000
C	-0.656272000	-1.209292000	0.245406000	H	-2.672288000	0.667515000	-2.530692000
C	-1.991951000	1.210415000	-0.158874000	C	-4.357102000	1.326423000	-1.336004000
C	-1.991854000	-1.210496000	-0.158763000	H	-4.961300000	0.661306000	-1.962866000
C	-2.661527000	-0.000075000	-0.361530000	H	-4.656905000	1.152098000	-0.295016000
H	-0.130880000	2.148232000	0.403714000	C	-4.545095000	2.818121000	-1.664732000
H	-0.130711000	-2.148115000	0.403912000	H	-4.540137000	2.965676000	-2.753763000
H	-2.510478000	2.152814000	-0.312945000	H	-5.482535000	3.230257000	-1.271987000
H	-2.510307000	-2.152950000	-0.312750000	C	-3.289832000	3.458057000	-1.051081000
H	-3.702209000	-0.000131000	-0.674420000	H	-3.398643000	3.487022000	0.041880000
C	1.453236000	0.000145000	0.885016000	H	-3.107331000	4.482464000	-1.395616000
H	1.705047000	0.894005000	1.459130000	C	-2.157983000	2.485465000	-1.440929000
H	1.705066000	-0.893541000	1.459394000	H	-1.754229000	2.757217000	-2.423587000
Cl	2.616385000	-0.000060000	-0.547415000	H	-1.321761000	2.510450000	-0.737600000
				C	-2.477884000	0.406817000	1.323749000
				H	-3.545732000	0.653080000	1.395183000
				C	-1.626148000	1.628698000	1.766482000
				H	-0.681870000	1.628199000	1.209315000
				H	-2.136207000	2.571957000	1.546213000
				C	-1.345507000	1.443683000	3.286843000
				H	-0.266389000	1.356421000	3.457669000
				H	-1.697931000	2.295264000	3.879553000
				C	-2.054426000	0.129744000	3.690565000
				H	-3.065233000	0.345614000	4.061693000
				H	-1.519533000	-0.413439000	4.478982000
				C	-2.150900000	-0.667931000	2.381947000
				H	-1.180859000	-1.119169000	2.142029000
				H	-2.895519000	-1.470064000	2.414368000
				C	-3.206291000	-1.626757000	-0.629315000
				H	-4.195923000	-1.350804000	-0.242950000
				C	-3.341383000	-2.004642000	-2.128650000
				H	-4.135466000	-1.437382000	-2.626333000
				H	-2.398682000	-1.796005000	-2.655797000
				C	-3.575172000	-3.522730000	-2.113414000
				H	-4.606321000	-3.740176000	-1.800855000
				H	-3.409608000	-3.993361000	-3.089957000
				C	-2.587739000	-3.993773000	-1.035017000
				H	-1.570665000	-3.975654000	-1.449148000
				H	-2.785189000	-5.009624000	-0.673733000
				C	-2.706904000	-2.929067000	0.079996000
				H	-3.435051000	-3.241481000	0.837990000
				H	-1.748406000	-2.780586000	0.587248000
				P	2.114955000	-0.186022000	-0.082833000
				C	3.439031000	-0.749517000	-1.274276000
				H	3.178701000	-1.783006000	-1.533797000
				C	3.475859000	0.049013000	-2.592724000
				H	2.606970000	-0.156240000	-3.227648000
				H	3.495222000	1.126518000	-2.386385000
				C	4.818460000	-0.379873000	-3.203662000
				H	4.729782000	-1.402715000	-3.594737000

	H	5.150267000	0.266026000	-4.025149000		
	C	5.780879000	-0.354250000	-1.996360000		
	H	6.183579000	0.659048000	-1.873797000		
	H	6.634311000	-1.029315000	-2.125024000		
	C	4.906139000	-0.725024000	-0.760864000		
	H	5.177011000	-1.697442000	-0.335334000		
	H	5.038902000	0.015448000	0.036448000		
	C	2.645715000	-1.048642000	1.493601000		
	H	3.660488000	-0.726576000	1.752777000		
	C	2.592485000	-2.593386000	1.295264000		
	H	2.721221000	-2.908651000	0.254203000		
	H	3.394836000	-3.061809000	1.881456000		
	C	1.229221000	-2.998968000	1.873714000		
	H	0.440882000	-2.687054000	1.171929000		
	H	1.137666000	-4.076255000	2.056428000		
	C	1.149081000	-2.143633000	3.145245000		
	H	1.824805000	-2.553678000	3.908509000		
	H	0.143267000	-2.094509000	3.578477000		
	C	1.643468000	-0.764320000	2.662812000		
	H	0.782396000	-0.205964000	2.282604000		
	H	2.099521000	-0.167729000	3.459985000		
	C	2.604769000	1.601922000	0.181313000		
	H	3.689522000	1.684522000	0.032220000		
	C	1.882205000	2.569483000	-0.815125000		
	H	2.591473000	2.935159000	-1.566566000		
	H	1.070932000	2.057691000	-1.347061000		
	C	1.340358000	3.739774000	0.045042000		
	H	1.406680000	4.706281000	-0.467387000		
	H	0.284300000	3.563372000	0.284994000		
	C	2.162876000	3.679064000	1.343282000		
	H	1.691905000	4.211708000	2.178312000		
	H	3.160258000	4.111899000	1.181756000		
	C	2.278034000	2.167262000	1.583703000		
	H	3.028105000	1.886456000	2.331197000		
	H	1.308532000	1.797160000	1.930355000		
	Ni	0.051883000	-0.422863000	-0.511453000		
3	TS₃₋₄					
P	2.167453000	0.501389000	0.042998000	P -2.085676000	-0.333973000	0.339178000
C	2.404688000	2.346636000	0.327878000	C -2.164180000	-1.057584000	2.069272000
H	3.376503000	2.479478000	0.813426000	H -3.185002000	-0.910068000	2.433910000
C	2.371330000	3.122313000	-1.024896000	C -1.825976000	-2.581417000	2.063629000
H	3.123610000	3.922106000	-1.000421000	H -2.549170000	-3.113210000	2.695595000
H	2.592655000	2.496929000	-1.896558000	H -1.868717000	-3.036844000	1.069762000
C	0.965873000	3.735531000	-1.082938000	C -0.423955000	-2.676061000	2.683568000
H	0.881074000	4.555112000	-1.806312000	H -0.187937000	-3.677343000	3.064356000
H	0.248175000	2.954617000	-1.357695000	H 0.316713000	-2.413020000	1.923054000
C	0.729677000	4.171299000	0.369768000	C -0.447695000	-1.592720000	3.768042000
H	-0.320698000	4.392886000	0.594199000	H 0.551870000	-1.325540000	4.133076000
H	1.313585000	5.077581000	0.580136000	H -1.038909000	-1.936933000	4.627367000
C	1.275098000	2.982648000	1.190266000	C -1.153797000	-0.413947000	3.068442000
H	1.634889000	3.284606000	2.179054000	H -1.656248000	0.255104000	3.772935000
H	0.482327000	2.246801000	1.346620000	H -0.416478000	0.185201000	2.528248000
C	3.696545000	0.207178000	-1.017335000	C -3.526239000	-1.259767000	-0.440693000
H	3.394702000	0.453712000	-2.045487000	H -3.165101000	-2.272060000	-0.648046000
C	4.256347000	-1.229113000	-1.035351000	C -3.998232000	-0.607642000	-1.784985000
H	4.489257000	-1.540918000	-0.010663000	H -3.400233000	0.260216000	-2.079026000

H	3.572757000	-1.968778000	-1.463393000	H	-3.912373000	-1.342169000	-2.595775000
C	5.559266000	-1.078105000	-1.838690000	C	-5.487473000	-0.262341000	-1.575264000
H	6.259166000	-1.904743000	-1.672673000	H	-5.581892000	0.733095000	-1.120507000
H	5.321311000	-1.057705000	-2.909859000	H	-6.054507000	-0.253894000	-2.512946000
C	6.133134000	0.295865000	-1.393508000	C	-5.967501000	-1.327144000	-0.576859000
H	6.498277000	0.867447000	-2.253770000	H	-6.072391000	-2.293868000	-1.088819000
H	6.980402000	0.168122000	-0.710322000	H	-6.929487000	-1.085908000	-0.109047000
C	4.960287000	1.031506000	-0.681988000	C	-4.807668000	-1.387441000	0.430572000
H	5.120106000	1.027573000	0.403853000	H	-4.898596000	-0.540631000	1.123219000
H	4.866014000	2.076248000	-0.991649000	H	-4.797277000	-2.299923000	1.036904000
C	2.729448000	-0.237373000	1.664284000	C	-2.925652000	1.342763000	0.552133000
H	3.816057000	-0.099192000	1.760748000	H	-3.985214000	1.176097000	0.321700000
C	2.050253000	0.379716000	2.901569000	C	-2.889707000	1.998433000	1.948472000
H	2.438832000	1.373782000	3.146024000	H	-3.463006000	1.436301000	2.694138000
H	0.977069000	0.478669000	2.715849000	H	-1.862233000	2.077276000	2.313962000
C	2.305221000	-0.659248000	4.006214000	C	-3.462446000	3.401697000	1.676762000
H	3.323133000	-0.528593000	4.396126000	H	-4.558609000	3.348516000	1.668100000
H	1.612310000	-0.557020000	4.849102000	H	-3.175879000	4.126614000	2.447447000
C	2.180119000	-2.030746000	3.297035000	C	-2.938820000	3.786296000	0.264934000
H	1.190658000	-2.465997000	3.469164000	H	-2.130189000	4.521464000	0.330085000
H	2.917888000	-2.745359000	3.677996000	H	-3.735200000	4.239486000	-0.335728000
C	2.381101000	-1.745089000	1.780322000	C	-2.422560000	2.467941000	-0.377536000
H	3.155066000	-2.382225000	1.342835000	H	-2.767471000	2.332222000	-1.405158000
H	1.454005000	-1.943963000	1.231446000	H	-1.332289000	2.458717000	-0.416114000
P	-1.712447000	0.142995000	0.240585000	P	1.828965000	0.242560000	0.003187000
C	-2.042711000	-0.116021000	2.069302000	C	1.789871000	2.068850000	0.392596000
H	-3.114702000	-0.322026000	2.181368000	H	2.775808000	2.392709000	0.745945000
C	-1.262804000	-1.318402000	2.633395000	C	1.347129000	2.983673000	-0.769187000
H	-1.648996000	-2.279637000	2.279689000	H	2.166868000	3.205852000	-1.458648000
H	-0.222380000	-1.252172000	2.307313000	H	0.567397000	2.485097000	-1.348208000
C	-1.365924000	-1.131909000	4.154745000	C	0.777756000	4.262466000	-0.093866000
H	-2.349808000	-1.475893000	4.500288000	H	1.484939000	5.096520000	-0.167275000
H	-0.604436000	-1.697604000	4.704536000	H	-0.144900000	4.578436000	-0.592679000
C	-1.233630000	0.395741000	4.363553000	C	0.524221000	3.891690000	1.395035000
H	-0.192924000	0.657497000	4.579209000	H	-0.479543000	4.173470000	1.733138000
H	-1.835842000	0.743814000	5.210126000	H	1.243353000	4.408788000	2.042054000
C	-1.681757000	1.053198000	3.024510000	C	0.747768000	2.370944000	1.480733000
H	-2.538478000	1.718432000	3.158413000	H	1.056200000	2.035896000	2.476436000
H	-0.873099000	1.664497000	2.615073000	H	-0.169950000	1.838768000	1.218232000
C	-3.213156000	-0.699127000	-0.480968000	C	3.358627000	0.061945000	-1.055255000
H	-3.047724000	-0.680046000	-1.563139000	H	3.476307000	-1.018811000	-1.162207000
C	-4.621364000	-0.138368000	-0.199517000	C	4.672293000	0.689030000	-0.513842000
H	-4.756956000	0.004077000	0.879896000	H	4.696429000	0.787918000	0.574315000
H	-4.806827000	0.825011000	-0.682538000	H	5.515047000	0.041852000	-0.796014000
C	-5.576737000	-1.255310000	-0.700021000	C	4.807983000	2.033233000	-1.246934000
H	-6.452348000	-1.349522000	-0.047758000	H	4.169309000	2.787812000	-0.775749000
H	-5.948545000	-1.021388000	-1.704310000	H	5.835299000	2.416869000	-1.240858000
C	-4.722447000	-2.559172000	-0.720341000	C	4.296778000	1.717386000	-2.663236000
H	-4.541732000	-2.873689000	-1.756015000	H	5.108080000	1.258180000	-3.243355000
H	-5.213695000	-3.393246000	-0.206853000	H	3.971525000	2.612271000	-3.206540000
C	-3.381250000	-2.171381000	-0.067821000	C	3.146218000	0.697684000	-2.468270000
H	-3.464169000	-2.234780000	1.025236000	H	2.167193000	1.176727000	-2.554462000
H	-2.546884000	-2.802301000	-0.373832000	H	3.172336000	-0.076741000	-3.240394000
C	-2.102875000	1.947115000	-0.067295000	C	2.351805000	-0.462635000	1.671861000
H	-1.173949000	2.465147000	0.168111000	H	1.399285000	-0.665291000	2.160304000
C	-2.402020000	2.242539000	-1.556335000	C	3.099088000	-1.816752000	1.586046000
H	-1.508568000	2.166678000	-2.180465000	H	2.420690000	-2.639971000	1.357947000
H	-3.134040000	1.529995000	-1.954792000	H	3.864468000	-1.792815000	0.800909000

C	-3.022861000	3.644842000	-1.504999000	C	3.788938000	-1.936502000	2.952038000
H	-2.236414000	4.384257000	-1.296383000	H	3.044536000	-2.174775000	3.725631000
H	-3.522547000	3.935427000	-2.436896000	H	4.565148000	-2.710685000	2.977618000
C	-3.987615000	3.544546000	-0.308689000	C	4.336131000	-0.517548000	3.166590000
H	-4.908288000	3.042067000	-0.632702000	H	5.221884000	-0.379046000	2.531862000
H	-4.273528000	4.520901000	0.099008000	H	4.630806000	-0.309718000	4.201655000
C	-3.242548000	2.660557000	0.726569000	C	3.194666000	0.401568000	2.675597000
H	-2.800812000	3.274478000	1.518634000	H	2.553851000	0.691078000	3.517132000
H	-3.920624000	1.956927000	1.213304000	H	3.583680000	1.328971000	2.250639000
Ni	0.254603000	-0.290336000	-0.705034000	Ni	-0.156897000	-0.560959000	-0.764244000
C	0.090282000	-2.063600000	-2.040324000	C	0.176229000	-1.982336000	-2.381760000
C	-1.188147000	-2.259688000	-2.630726000	C	1.506899000	-2.220526000	-2.854730000
C	0.904413000	-0.953730000	-2.464251000	C	-0.257227000	-2.595246000	-1.143448000
C	-1.736266000	-1.314700000	-3.476614000	C	2.359429000	-3.056011000	-2.177779000
C	0.266304000	0.049510000	-3.264347000	C	0.659850000	-3.479084000	-0.487516000
C	-1.024946000	-0.118084000	-3.737088000	C	1.929430000	-3.686399000	-0.974714000
H	-1.737336000	-3.167041000	-2.392875000	H	1.813258000	-1.744131000	-3.781998000
H	1.985777000	-1.041438000	-2.488636000	H	-1.315195000	-2.797818000	-1.011910000
H	-2.723538000	-1.467428000	-3.903773000	H	3.359314000	-3.245328000	-2.559072000
H	0.834722000	0.934544000	-3.541528000	H	0.325700000	-4.005004000	0.401612000
H	-1.480978000	0.660097000	-4.343990000	H	2.609070000	-4.351758000	-0.448727000
C	0.804007000	-3.211693000	-1.375079000	C	-0.763035000	-1.278488000	-3.198340000
H	0.996678000	-4.039042000	-2.065539000	H	-0.518969000	-1.156953000	-4.248191000
H	1.741659000	-2.877171000	-0.931353000	H	-1.815201000	-1.416730000	-2.978665000
Cl	-0.128106000	-3.989778000	0.007109000	Cl	-0.747535000	0.925260000	-2.934220000
4				5			
P	-2.199963000	-0.451258000	0.374103000	P	2.506401000	-0.006575000	-0.105289000
C	-2.453417000	-0.864822000	2.178202000	C	3.333836000	-0.646008000	-1.669141000
H	-3.522306000	-0.735631000	2.376022000	H	4.369722000	-0.300063000	-1.587063000
C	-2.027412000	-2.338191000	2.452608000	C	3.286894000	-2.206917000	-1.794938000
H	-2.731920000	-2.794883000	3.159709000	H	4.293111000	-2.588788000	-2.000016000
H	-2.016802000	-2.962932000	1.552210000	H	2.955598000	-2.692653000	-0.872689000
C	-0.642211000	-2.216076000	3.101511000	C	2.319268000	-2.521356000	-2.971360000
H	-0.329108000	-3.124776000	3.628860000	H	2.894930000	-2.815325000	-3.857598000
H	0.095082000	-1.997719000	2.322990000	H	1.637080000	-3.344444000	-2.736468000
C	-0.799281000	-0.996268000	4.019577000	C	1.594588000	-1.193715000	-3.251676000
H	0.158090000	-0.579160000	4.351865000	H	0.774763000	-1.033160000	-2.539023000
H	-1.369620000	-1.279839000	4.913837000	H	1.178768000	-1.133486000	-4.263711000
C	-1.611775000	0.002441000	3.165702000	C	2.686236000	-0.153356000	-2.984283000
H	-2.252969000	0.646905000	3.774601000	H	3.445342000	-0.205441000	-3.778454000
H	-0.934633000	0.667227000	2.619697000	H	2.298070000	0.862263000	-2.941125000
C	-3.560055000	-1.484465000	-0.391543000	C	3.367638000	-1.050584000	1.184910000
H	-3.256644000	-2.524087000	-0.264888000	H	2.843495000	-2.014593000	1.209147000
C	-3.712149000	-1.171279000	-1.916324000	C	3.348972000	-0.468458000	2.614536000
H	-2.896337000	-0.562010000	-2.317969000	H	3.751259000	0.551351000	2.605118000
H	-3.697578000	-2.116029000	-2.473114000	H	2.350121000	-0.427740000	3.059135000
C	-5.099729000	-0.520314000	-2.053784000	C	4.318042000	-1.399354000	3.358302000
H	-5.040800000	0.554061000	-1.832407000	H	4.657600000	-0.989330000	4.316133000
H	-5.514788000	-0.625574000	-3.062450000	H	3.814193000	-2.352928000	3.563345000
C	-5.935393000	-1.235246000	-0.979729000	C	5.477112000	-1.613517000	2.353122000
H	-6.181620000	-2.247374000	-1.328187000	H	5.893211000	-2.624213000	2.423718000
H	-6.876198000	-0.725223000	-0.740679000	H	6.294433000	-0.912975000	2.559748000
C	-4.980422000	-1.319101000	0.229734000	C	4.873378000	-1.330877000	0.942881000
H	-5.065507000	-0.401918000	0.825241000	H	5.361116000	-0.457026000	0.494757000
H	-5.219710000	-2.150558000	0.902186000	H	5.013928000	-2.164152000	0.249419000
C	-2.964547000	1.250368000	0.175364000	C	3.342127000	1.634214000	0.201657000

H	-4.017360000	1.055829000	-0.049059000	H	4.304261000	1.386901000	0.666634000
C	-2.984772000	2.206353000	1.385101000	C	3.652606000	2.522369000	-1.029432000
H	-3.638199000	1.845316000	2.187210000	H	4.580671000	2.218219000	-1.527069000
H	-1.988288000	2.346354000	1.811462000	H	2.838561000	2.481664000	-1.753578000
C	-3.476413000	3.514875000	0.742951000	C	3.705344000	3.937467000	-0.430188000
H	-4.561764000	3.451966000	0.588547000	H	4.636945000	4.076111000	0.137667000
H	-3.280529000	4.395027000	1.366420000	H	3.652537000	4.721712000	-1.194293000
C	-2.746301000	3.571621000	-0.620888000	C	2.497523000	3.939019000	0.521790000
H	-1.824938000	4.151266000	-0.522873000	H	1.578554000	4.026507000	-0.066778000
H	-3.356165000	4.063697000	-1.386145000	H	2.520034000	4.755288000	1.253049000
C	-2.412196000	2.097393000	-0.996975000	C	2.538073000	2.544883000	1.187218000
H	-2.864869000	1.787197000	-1.943120000	H	3.050490000	2.585530000	2.155767000
H	-1.339443000	1.943946000	-1.122436000	H	1.529363000	2.158857000	1.369029000
P	1.486139000	0.572958000	0.056126000	P	-2.014718000	0.621704000	0.110390000
C	1.596115000	2.428659000	-0.050190000	C	-2.516286000	2.413949000	0.260939000
H	2.603182000	2.715015000	0.279243000	H	-3.428711000	2.406333000	0.868735000
C	1.351085000	3.043540000	-1.453134000	C	-1.452542000	3.298769000	0.988035000
H	2.268431000	3.045086000	-2.047260000	H	-1.787381000	3.515553000	2.009980000
H	0.613220000	2.454997000	-2.005558000	H	-0.485508000	2.793085000	1.053986000
C	0.830292000	4.488009000	-1.188125000	C	-1.339259000	4.589913000	0.141834000
H	1.523167000	5.245980000	-1.569465000	H	-1.183297000	5.484932000	0.755244000
H	-0.125037000	4.639346000	-1.701278000	H	-0.491456000	4.489812000	-0.543773000
C	0.656815000	4.608779000	0.347130000	C	-2.639005000	4.634594000	-0.678514000
H	-0.219972000	5.202625000	0.631325000	H	-2.569815000	5.288644000	-1.555690000
H	1.538581000	5.088055000	0.791962000	H	-3.470985000	4.992368000	-0.054465000
C	0.570284000	3.154577000	0.836260000	C	-2.862318000	3.160373000	-1.052534000
H	0.763994000	3.044713000	1.907440000	H	-3.884255000	2.947550000	-1.380044000
H	-0.422297000	2.753736000	0.623459000	H	-2.174313000	2.874915000	-1.852013000
C	3.047888000	0.011224000	-0.798784000	C	-3.000280000	-0.157615000	1.473211000
H	3.065684000	-1.070698000	-0.641130000	H	-2.665612000	-1.196324000	1.524831000
C	4.350170000	0.653364000	-0.221528000	C	-4.537723000	-0.162091000	1.379519000
H	4.217848000	1.119547000	0.758676000	H	-4.900917000	0.848814000	1.154029000
H	5.106147000	-0.134558000	-0.100301000	H	-4.910479000	-0.831776000	0.600511000
C	4.817949000	1.644959000	-1.296982000	C	-4.993829000	-0.579368000	2.800980000
H	4.232496000	2.570786000	-1.229799000	H	-5.929472000	-0.083454000	3.081543000
H	5.878399000	1.907476000	-1.202126000	H	-5.177667000	-1.659134000	2.835994000
C	4.478560000	0.910474000	-2.601351000	C	-3.817888000	-0.198520000	3.751369000
H	5.217425000	0.113776000	-2.766840000	H	-3.379918000	-1.102875000	4.190789000
H	4.487385000	1.562027000	-3.482873000	H	-4.139424000	0.441808000	4.580006000
C	3.086569000	0.301455000	-2.333524000	C	-2.774172000	0.499179000	2.852506000
H	2.300619000	0.990297000	-2.637917000	H	-2.995057000	1.571759000	2.785159000
H	2.912881000	-0.613452000	-2.900808000	H	-1.750498000	0.400427000	3.225060000
C	1.867227000	0.216652000	1.871958000	C	-2.726847000	0.013326000	-1.486923000
H	0.885384000	0.016158000	2.298662000	H	-2.086158000	0.499044000	-2.228844000
C	2.702661000	-1.064280000	2.125059000	C	-2.568031000	-1.520277000	-1.650593000
H	2.130993000	-1.973834000	1.939652000	H	-1.554136000	-1.791423000	-1.951504000
H	3.584801000	-1.099339000	1.479218000	H	-2.774284000	-2.049381000	-0.711948000
C	3.160879000	-0.901830000	3.580567000	C	-3.640138000	-1.880594000	-2.688307000
H	2.315061000	-1.069675000	4.261326000	H	-3.309590000	-1.568132000	-3.688815000
C	3.962010000	-1.597006000	3.858090000	H	-3.857203000	-2.954427000	-2.721145000
C	3.596083000	0.571262000	3.623602000	C	-4.842499000	-1.029994000	-2.247174000
H	4.581591000	0.664426000	3.148853000	H	-5.318948000	-1.505990000	-1.379596000
H	3.676724000	0.975517000	4.638930000	H	-5.608596000	-0.920552000	-3.023481000
C	2.536241000	1.312537000	2.771185000	C	-4.221008000	0.325206000	-1.835127000
H	1.772562000	1.764527000	3.414630000	H	-4.246798000	1.029297000	-2.673531000
H	2.988443000	2.128859000	2.203896000	H	-4.769247000	0.792717000	-1.015033000
Ni	-0.288165000	-0.706705000	-0.755919000	Ni	0.211589000	0.194329000	0.040152000
C	0.607274000	-2.912736000	-1.247513000	C	-0.429359000	-2.535337000	0.837729000

C	1.476528000	-2.787431000	-2.355219000	C	-1.419213000	-3.300395000	1.481168000
C	1.139753000	-3.429397000	-0.043283000	C	0.105892000	-3.049587000	-0.355188000
C	2.804680000	-3.194963000	-2.267538000	C	-1.877076000	-4.505336000	0.941833000
C	2.473600000	-3.824125000	0.045370000	C	-0.334218000	-4.257663000	-0.893290000
C	3.312208000	-3.710784000	-1.068003000	C	-1.338800000	-4.989970000	-0.252878000
H	1.086996000	-2.350107000	-3.267993000	H	-1.829091000	-2.944121000	2.424105000
H	0.478878000	-3.532738000	0.813161000	H	0.841366000	-2.456435000	-0.881007000
H	3.454274000	-3.096956000	-3.133504000	H	-2.650480000	-5.068382000	1.459271000
H	2.860168000	-4.219243000	0.981321000	H	0.092435000	-4.620975000	-1.825407000
H	4.351493000	-4.022230000	-1.002995000	H	-1.693459000	-5.925666000	-0.676955000
C	-0.803060000	-2.503860000	-1.309932000	C	0.051910000	-1.230594000	1.400200000
H	-1.244452000	-2.469052000	-2.305153000	H	-0.603105000	-0.916639000	2.217197000
H	-1.415089000	-3.056053000	-0.596809000	H	1.032956000	-1.382988000	1.848247000
Cl	-0.273732000	0.064878000	-2.988733000	Cl	0.283974000	1.822040000	-1.588833000
4a				TS_{4a-4b}			
P	0.727978000	0.221163000	0.341042000	P	0.439818000	0.467507000	0.373053000
C	0.014329000	0.018160000	2.040891000	C	-0.236192000	0.694579000	2.087623000
H	0.721070000	0.452243000	2.758122000	H	0.469582000	1.326919000	2.639532000
C	-1.380974000	0.716484000	2.156045000	C	-1.641282000	1.362199000	2.082036000
H	-1.308809000	1.674285000	2.683003000	H	-1.575314000	2.447628000	2.216804000
H	-1.806210000	0.916734000	1.168380000	H	-2.155677000	1.177853000	1.132890000
C	-2.287861000	-0.309762000	2.858421000	C	-2.419829000	0.642251000	3.195314000
H	-2.144041000	-0.275199000	3.947419000	H	-2.135864000	1.037018000	4.180555000
H	-3.345795000	-0.128956000	2.641951000	H	-3.505352000	0.751938000	3.084448000
C	-1.773295000	-1.644457000	2.305435000	C	-1.937636000	-0.808412000	3.051224000
H	-2.074048000	-1.748777000	1.255503000	H	-2.393076000	-1.248593000	2.155871000
H	-2.132915000	-2.521706000	2.854588000	H	-2.184737000	-1.442933000	3.909800000
C	-0.246425000	-1.487537000	2.377749000	C	-0.418265000	-0.669183000	2.833316000
H	0.108635000	-1.691937000	3.395727000	H	0.102978000	-0.628564000	3.797174000
H	0.264637000	-2.185028000	1.707267000	H	-0.008256000	-1.517662000	2.275310000
C	0.634383000	2.042116000	0.029335000	C	0.143722000	2.113820000	-0.433942000
H	-0.429016000	2.277325000	0.110078000	H	-0.942713000	2.234221000	-0.419358000
C	1.172128000	2.456227000	-1.377970000	C	0.661983000	2.154345000	-1.907327000
H	1.690916000	1.626782000	-1.867667000	H	1.317349000	1.304029000	-2.120919000
H	0.351745000	2.747675000	-2.041383000	H	-0.168961000	2.102740000	-2.617793000
C	2.154268000	3.620044000	-1.119672000	C	1.460612000	3.470026000	-2.022797000
H	2.940043000	3.681309000	-1.880863000	H	2.236195000	3.424396000	-2.795519000
H	1.611858000	4.574652000	-1.122467000	H	0.785296000	4.299273000	-2.273496000
C	2.695261000	3.349494000	0.292531000	C	2.020767000	3.682702000	-0.607904000
H	3.171346000	4.225178000	0.747849000	H	2.384616000	4.701587000	-0.432962000
H	3.436575000	2.541484000	0.260717000	H	2.853272000	2.990008000	-0.432079000
C	1.446784000	2.884825000	1.059478000	C	0.830797000	3.309633000	0.291530000
H	1.688980000	2.337401000	1.977212000	H	1.127382000	3.079823000	1.321176000
H	0.849899000	3.757049000	1.354262000	H	0.129015000	4.152327000	0.338170000
C	2.530827000	-0.162343000	0.522310000	C	2.272468000	0.387621000	0.654971000
H	2.974368000	0.572061000	1.208739000	H	2.598015000	1.347617000	1.078470000
C	2.799151000	-1.575731000	1.081264000	C	2.659678000	-0.736320000	1.642137000
H	2.545186000	-1.671912000	2.141840000	H	2.413319000	-0.488229000	2.680247000
H	2.208285000	-2.315104000	0.521828000	H	2.137680000	-1.663705000	1.372625000
C	4.292706000	-1.770624000	0.781743000	C	4.161857000	-0.907943000	1.377942000
H	4.883735000	-1.193022000	1.505128000	H	4.711596000	-0.061373000	1.812992000
H	4.606838000	-2.817453000	0.852938000	H	4.566357000	-1.831454000	1.806835000
C	4.468660000	-1.187119000	-0.639812000	C	4.250128000	-0.876543000	-0.161052000
H	4.378830000	-1.981430000	-1.388629000	H	4.059468000	-1.880343000	-0.555306000
H	5.452267000	-0.723861000	-0.771308000	H	5.232596000	-0.551146000	-0.520435000
C	3.310268000	-0.158399000	-0.820935000	C	3.105199000	0.071878000	-0.623516000

H	3.672827000	0.842905000	-1.072298000	H	3.481386000	0.994954000	-1.077167000
H	2.645266000	-0.480048000	-1.631934000	H	2.489176000	-0.438111000	-1.373166000
Ni	-0.167467000	-1.284002000	-0.939388000	Ni	-0.009449000	-1.536349000	-0.715688000
C	-2.317383000	0.399806000	-1.401775000	C	-2.350038000	-1.078809000	-1.468558000
C	-3.253077000	-0.499093000	-0.850300000	C	-3.270308000	-1.227130000	-0.406048000
C	-2.532106000	1.777275000	-1.216715000	C	-2.286215000	0.172112000	-2.122142000
C	-4.338666000	-0.034454000	-0.111153000	C	-4.108005000	-0.180025000	-0.032985000
C	-3.622296000	2.244582000	-0.479541000	C	-3.120529000	1.222550000	-1.743473000
C	-4.524215000	1.339761000	0.086421000	C	-4.037754000	1.049773000	-0.700929000
H	-3.091304000	-1.565020000	-0.989518000	H	-3.318821000	-2.181869000	0.110979000
H	-1.833292000	2.482151000	-1.660313000	H	-1.575114000	0.300046000	-2.933441000
H	-5.040768000	-0.744820000	0.317825000	H	-4.812657000	-0.315703000	0.783054000
H	-3.767578000	3.313943000	-0.347447000	H	-3.060081000	2.175087000	-2.263828000
H	-5.368750000	1.699988000	0.667689000	H	-4.691266000	1.866789000	-0.407724000
C	-1.119557000	-0.105812000	-2.115197000	C	-1.429613000	-2.158661000	-1.824526000
H	-1.354836000	-0.834054000	-2.899305000	H	-1.726723000	-3.161687000	-1.511425000
H	-0.480373000	0.693827000	-2.497777000	H	-1.041527000	-2.139740000	-2.847291000
Cl	-0.646684000	-3.316748000	-1.498309000	Cl	1.176406000	-3.311809000	-0.978642000
4b							
P	0.624427000	0.225741000	0.371895000				
C	0.126221000	0.045170000	2.152703000				
H	0.959857000	0.397745000	2.770819000				
C	-1.174949000	0.865932000	2.445707000				
H	-0.968255000	1.734789000	3.080713000				
H	-1.619919000	1.240311000	1.519218000				
C	-2.165555000	-0.129567000	3.082747000				
H	-2.022012000	-0.174402000	4.170820000				
H	-3.207691000	0.150649000	2.889029000				
C	-1.766796000	-1.470243000	2.453738000				
H	-2.092185000	-1.502186000	1.404706000				
H	-2.186140000	-2.341963000	2.968927000				
C	-0.233623000	-1.432339000	2.499833000				
H	0.115665000	-1.653518000	3.516803000				
H	0.207224000	-2.162970000	1.820166000				
C	0.712878000	2.065950000	0.132126000				
H	-0.297097000	2.431400000	0.328372000				
C	1.118792000	2.442099000	-1.325424000				
H	1.681868000	1.632063000	-1.801324000				
H	0.242171000	2.633571000	-1.952523000				
C	2.036120000	3.668710000	-1.172673000				
H	2.682740000	3.826049000	-2.043440000				
H	1.434013000	4.576828000	-1.029583000				
C	2.811707000	3.357087000	0.116446000				
H	3.342376000	4.222299000	0.529640000				
H	3.552286000	2.571655000	-0.087980000				
C	1.720748000	2.816083000	1.060254000				
H	2.129665000	2.185750000	1.858146000				
H	1.205240000	3.652644000	1.547857000				
C	2.413440000	-0.268040000	0.303509000				
H	2.979817000	0.577752000	0.711717000				
C	2.814709000	-1.512354000	1.130363000				
H	2.867201000	-1.296252000	2.203748000				
H	2.103586000	-2.324850000	0.968509000				
C	4.162228000	-1.899217000	0.503045000				
H	4.937207000	-1.178337000	0.801818000				
H	4.497300000	-2.899980000	0.798790000				

C	3.87377000	-1.78469300	-1.00469100
H	3.33462700	-2.67922800	-1.33474300
H	4.78224300	-1.68788900	-1.60987000
C	2.93447000	-0.55612500	-1.14078900
H	3.46739700	0.32084400	-1.52721800
H	2.10966300	-0.78047500	-1.82450900
Ni	-0.79107700	-0.87467300	-0.96878800
C	-2.72893500	-0.40030800	-1.57486900
C	-3.73794500	-0.40097500	-0.55271500
C	-1.98179900	0.80790500	-1.77008000
C	-4.06149200	0.75372900	0.11826000
C	-2.36306800	1.99397800	-1.08371200
C	-3.38411800	1.97233600	-0.16030900
H	-4.25872800	-1.33186300	-0.34678400
H	-1.31649700	0.89388800	-2.62850700
H	-4.85006600	0.74029500	0.86587900
H	-1.84682600	2.92243500	-1.30883800
H	-3.67273900	2.87959000	0.36281600
C	-2.21097300	-1.58541000	-2.16915500
H	-2.63605400	-2.54777300	-1.89800000
H	-1.74966900	-1.53526600	-3.15586000
Cl	0.19885300	-2.85218300	-0.89926800

Table S7. B3LYP-D/BS-I optimized Cartesian coordinates of the species involved in the CO₂ insertion of Ni^{II}-CH₂Ph bond.

TS ₅₋₆				6			
P	2.085340000	-0.650910000	-0.123427000	P	-1.787333000	1.288736000	-0.234784000
C	2.413178000	-1.478021000	1.524046000	C	-2.686571000	1.172036000	1.379426000
H	3.382971000	-1.979452000	1.413282000	H	-3.704519000	1.552239000	1.217074000
C	2.506813000	-0.475609000	2.710514000	C	-2.746754000	-0.317821000	1.803285000
H	3.503896000	-0.039104000	2.793196000	H	-3.560985000	-0.858832000	1.315812000
H	1.818482000	0.356192000	2.562041000	H	-1.820557000	-0.812989000	1.501906000
C	2.113489000	-1.281306000	3.983446000	C	-2.852285000	-0.320845000	3.353938000
H	2.902591000	-1.258941000	4.742845000	H	-3.755820000	-0.832580000	3.701377000
H	1.213489000	-0.850190000	4.434655000	H	-1.993516000	-0.851521000	3.781619000
C	1.819971000	-2.714915000	3.490325000	C	-2.824267000	1.167903000	3.771684000
H	1.055804000	-3.223227000	4.090149000	H	-2.341850000	1.330094000	4.742398000
H	2.732425000	-3.324905000	3.529443000	H	-3.848629000	1.558763000	3.839765000
C	1.395282000	-2.517757000	2.029050000	C	-2.086012000	1.865285000	2.616880000
H	1.389633000	-3.439354000	1.444675000	H	-2.216163000	2.950797000	2.608830000
H	0.389016000	-2.094736000	1.983943000	H	-1.013355000	1.656410000	2.672377000
C	3.497891000	0.584257000	-0.193510000	C	-2.828387000	0.219493000	-1.322334000
H	3.232758000	1.436675000	0.430545000	H	-2.641942000	-0.802373000	-0.989897000
C	3.829068000	1.088397000	-1.641689000	C	-2.473075000	0.330504000	-2.841619000
H	3.216971000	0.623898000	-2.413966000	H	-1.754800000	1.127410000	-3.053658000
H	3.619910000	2.156768000	-1.693323000	H	-2.008250000	-0.603547000	-3.165847000
C	5.332397000	0.809173000	-1.854720000	C	-3.822812000	0.577873000	-3.555747000
H	5.473352000	-0.177449000	-2.319187000	H	-3.996535000	1.657234000	-3.673289000
H	5.806178000	1.551575000	-2.506870000	H	-3.858658000	0.125640000	-4.553125000
C	5.909678000	0.782346000	-0.434905000	C	-4.873096000	0.005638000	-2.590706000
H	5.972884000	1.804127000	-0.036110000	H	-4.861527000	-1.092347000	-2.632818000
H	6.904455000	0.325452000	-0.369452000	H	-5.894153000	0.345115000	-2.801740000
C	4.840287000	-0.004790000	0.334450000	C	-4.353814000	0.466842000	-1.220036000
H	4.936051000	-1.069108000	0.081630000	H	-4.579027000	1.534734000	-1.088313000
H	4.939076000	0.086348000	1.418366000	H	-4.796818000	-0.075753000	-0.378599000
C	2.680519000	-1.829996000	-1.447162000	C	-2.034189000	2.981440000	-0.948452000
H	3.717358000	-1.525828000	-1.625536000	H	-2.989664000	2.939539000	-1.485989000
C	2.722217000	-3.337959000	-1.109544000	C	-2.107590000	4.144345000	0.071206000
H	3.582650000	-3.592047000	-0.478377000	H	-3.104253000	4.233498000	0.519071000
H	1.810476000	-3.647843000	-0.597312000	H	-1.379512000	3.994104000	0.871991000
C	2.764861000	-3.988859000	-2.501693000	C	-1.687021000	5.363314000	-0.764863000
H	3.763688000	-3.861895000	-2.943845000	H	-2.500810000	5.652860000	-1.445096000
H	2.540901000	-5.061863000	-2.475033000	H	-1.432948000	6.233537000	-0.148535000
C	1.726362000	-3.171440000	-3.291064000	C	-0.491133000	4.819765000	-1.565232000
H	0.719999000	-3.507930000	-3.017313000	H	0.383694000	4.764567000	-0.907509000
H	1.837627000	-3.271887000	-4.376615000	H	-0.234079000	5.437950000	-2.432967000
C	1.919830000	-1.712646000	-2.808880000	C	-0.911810000	3.384750000	-1.964057000
H	2.529086000	-1.138596000	-3.515720000	H	-1.313146000	3.355910000	-2.983428000
H	0.963337000	-1.195366000	-2.711325000	H	-0.059298000	2.698189000	-1.925126000
P	-2.543801000	0.010557000	-0.010522000	P	2.540133000	-0.158824000	0.019025000
C	-3.528627000	-1.173324000	-1.079909000	C	3.768994000	1.037298000	-0.747099000
H	-2.855848000	-1.306355000	-1.931750000	H	3.190309000	1.463876000	-1.574095000
C	-3.843869000	-2.544482000	-0.427434000	C	4.295892000	2.166319000	0.172364000
H	-3.970374000	-3.261917000	-1.249259000	H	4.619588000	2.980313000	-0.489880000
H	-3.054527000	-2.929847000	0.213806000	H	3.545390000	2.581528000	0.842900000
C	-5.187517000	-2.351431000	0.296801000	C	5.530851000	1.571338000	0.889348000
H	-5.727199000	-3.297994000	0.410948000	H	6.301557000	2.334856000	1.040249000
H	-5.018724000	-1.955727000	1.303973000	H	5.259623000	1.190179000	1.878219000

C	-5.968114000	-1.321296000	-0.560143000	C	6.028537000	0.413627000	-0.024256000
H	-6.405752000	-0.539290000	0.071122000	H	5.938281000	-0.546522000	0.497218000
H	-6.799269000	-1.792069000	-1.096492000	H	7.080429000	0.524407000	-0.308703000
C	-4.939307000	-0.740087000	-1.566471000	C	5.102756000	0.442713000	-1.258296000
H	-5.084154000	-1.214260000	-2.545274000	H	5.502501000	1.153401000	-1.994791000
H	-5.061548000	0.329720000	-1.720140000	H	5.014654000	-0.520169000	-1.760522000
C	-3.240615000	1.715786000	-0.288622000	C	2.755140000	-1.758545000	-0.897694000
H	-2.531422000	2.383689000	0.205806000	H	1.863930000	-2.326845000	-0.631170000
C	-4.609337000	2.017900000	0.370472000	C	3.952166000	-2.666069000	-0.523288000
H	-5.324361000	1.204716000	0.217880000	H	4.885575000	-2.103345000	-0.432097000
H	-4.509498000	2.174213000	1.449959000	H	3.785413000	-3.184213000	0.427247000
C	-5.071342000	3.274015000	-0.385731000	C	4.028535000	-3.614229000	-1.731120000
H	-6.136898000	3.490346000	-0.246845000	H	4.968613000	-4.176254000	-1.777610000
C	-4.501623000	4.143263000	-0.029392000	H	3.203632000	-4.337808000	-1.679053000
H	-4.700853000	2.966013000	-1.848118000	C	3.823437000	-2.673182000	-2.931969000
H	-4.623090000	3.867328000	-2.465619000	H	3.502075000	-3.201772000	-3.835603000
H	-5.480128000	2.334602000	-2.293888000	H	4.773211000	-2.173309000	-3.164300000
C	-3.359443000	2.188938000	-1.773277000	C	2.770489000	-1.635958000	-2.456303000
H	-3.318454000	1.361984000	-2.484136000	H	3.028739000	-0.627749000	-2.794597000
H	-2.513103000	2.834554000	-2.022488000	H	1.776574000	-1.859559000	-2.848820000
C	-2.945855000	-0.245943000	1.794922000	C	3.073977000	-0.641071000	1.746718000
H	-4.030894000	-0.154552000	1.904243000	H	4.101785000	-1.006384000	1.652596000
C	-2.438236000	-1.603297000	2.384702000	C	2.970842000	0.453836000	2.849166000
H	-3.270989000	-2.278055000	2.605080000	H	3.809445000	0.313192000	3.541613000
H	-1.783943000	-2.110117000	1.673050000	H	3.039307000	1.465709000	2.455618000
C	-1.612470000	-1.236896000	3.635267000	C	1.620297000	0.230783000	3.589734000
H	-2.259953000	-1.131016000	4.516208000	H	1.800279000	0.012334000	4.648839000
H	-0.850528000	-1.989401000	3.861733000	H	0.988667000	1.121203000	3.529880000
C	-1.026655000	0.129198000	3.262830000	C	0.957050000	-0.975900000	2.896029000
H	-0.257054000	-0.006246000	2.491944000	H	0.297180000	-0.611328000	2.099067000
H	-0.577958000	0.671010000	4.103555000	H	0.350119000	-1.588304000	3.573291000
C	-2.233402000	0.850139000	2.653148000	C	2.134713000	-1.751831000	2.286121000
H	-2.912703000	1.170102000	3.453578000	H	2.667650000	-2.292024000	3.080774000
H	-1.951000000	1.749183000	2.097183000	H	1.833373000	-2.488907000	1.536084000
Ni	-0.202003000	-0.162146000	-0.326609000	Ni	0.381919000	0.603794000	-0.146964000
C	1.111306000	2.797773000	0.224725000	C	-1.967043000	-3.143716000	0.282507000
C	1.346269000	2.675916000	1.606154000	C	-2.231587000	-3.426091000	1.630364000
C	1.930409000	3.673687000	-0.505654000	C	-3.010239000	-3.255195000	-0.644458000
C	2.403266000	3.337574000	2.229524000	C	-3.512705000	-3.776950000	2.054138000
C	2.989581000	4.339481000	0.115576000	C	-4.299324000	-3.594116000	-0.220430000
C	3.244877000	4.163528000	1.478561000	C	-4.557989000	-3.851082000	1.127869000
H	0.685267000	2.044372000	2.193735000	H	-1.427845000	-3.331687000	2.358114000
H	1.757712000	3.795362000	-1.567144000	H	-2.805434000	-3.066849000	-1.692646000
H	2.568664000	3.207390000	3.296169000	H	-3.698378000	-3.977232000	3.106326000
H	3.624162000	4.996727000	-0.473877000	H	-5.101633000	-3.660647000	-0.951177000
H	4.076117000	4.678523000	1.952957000	H	-5.561435000	-4.111873000	1.454093000
C	-0.025370000	2.047451000	-0.381680000	C	-0.561641000	-2.699106000	-0.091647000
H	-0.560250000	1.560253000	0.460956000	H	-0.157313000	-2.096530000	0.724288000
H	-0.793269000	2.709626000	-0.786021000	H	0.074894000	-3.591614000	-0.183026000
Cl	-0.515205000	-2.343144000	-0.604557000	Cl	0.907293000	2.466228000	0.946682000
C	0.182713000	1.383439000	-2.153620000	C	-0.423315000	-1.941426000	-1.420641000
O	-0.792927000	0.716302000	-2.500460000	O	-0.006632000	-0.708618000	-1.396900000
O	1.179614000	1.857153000	-2.650631000	O	-0.669545000	-2.527797000	-2.475601000
6a				10			
Ni	0.512184000	-0.592717000	0.274813000	P	1.545632000	1.338124000	0.240233000
P	-1.569191000	-1.343048000	0.783665000	C	1.260514000	3.074364000	-0.371821000

P	2.508657000	0.161102000	-0.488223000	H	2.160506000	3.634615000	-0.087767000
C	-1.917122000	-2.994005000	0.030875000	C	1.060236000	3.170579000	-1.904030000
C	-3.377738000	-3.504001000	0.021201000	H	2.004988000	3.139393000	-2.449913000
C	-3.364043000	-4.551378000	-1.103973000	H	0.476188000	2.316806000	-2.243098000
C	-2.565179000	-3.837299000	-2.209062000	C	0.266726000	4.488441000	-2.146360000
C	-1.428700000	-3.103556000	-1.455935000	H	0.822528000	5.194752000	-2.771955000
C	-2.965541000	-0.206866000	0.335793000	H	-0.673859000	4.265214000	-2.660822000
C	-4.256584000	-0.359347000	1.178067000	C	-0.020936000	5.057113000	-0.739224000
C	-5.306397000	0.346681000	0.308132000	H	-0.973571000	5.595293000	-0.681198000
C	-4.967642000	-0.115927000	-1.120462000	H	0.771504000	5.756631000	-0.442076000
C	-3.422559000	-0.258822000	-1.155330000	C	0.028958000	3.822267000	0.172502000
C	-1.772656000	-1.525172000	2.619434000	H	0.092649000	4.066475000	1.232594000
C	-0.683923000	-2.432185000	3.254718000	H	-0.862153000	3.205852000	0.030073000
C	0.387477000	-1.443727000	3.729869000	C	3.053495000	0.824765000	-0.740882000
C	-0.443541000	-0.296698000	4.318929000	H	2.719412000	0.539817000	-1.737019000
C	-1.596125000	-0.122001000	3.302856000	C	3.851871000	-0.372612000	-0.123749000
C	2.637343000	1.997612000	-0.668675000	H	3.581656000	-0.551576000	0.922211000
C	2.655232000	2.770267000	0.670160000	H	3.641151000	-1.264159000	-0.725637000
C	3.176650000	4.152634000	0.251255000	C	5.350209000	0.008797000	-0.216904000
C	4.330780000	3.805592000	-0.708432000	H	5.694854000	0.382595000	0.755206000
C	3.840089000	2.561069000	-1.495418000	H	5.980572000	-0.844950000	-0.485742000
C	2.857752000	-0.478410000	-2.194384000	C	5.389514000	1.147598000	-1.246235000
C	1.575942000	-0.876335000	-2.954993000	H	5.308859000	0.740298000	-2.262596000
C	2.116660000	-1.633706000	-4.186206000	H	6.301045000	1.752632000	-1.186920000
C	3.473168000	-2.258347000	-3.733517000	C	4.116619000	1.942278000	-0.919677000
C	3.708875000	-1.760464000	-2.283868000	H	4.266255000	2.509952000	0.008585000
C	3.888235000	-0.382033000	0.613767000	H	3.839766000	2.650312000	-1.703403000
C	5.270672000	0.296613000	0.495374000	C	2.331585000	1.555007000	1.927728000
C	5.926975000	-0.056223000	1.839869000	H	3.402564000	1.586598000	1.692210000
C	4.790079000	0.205844000	2.845302000	C	2.026468000	2.863999000	2.690430000
C	3.504604000	-0.279135000	2.127013000	H	2.514125000	3.734045000	2.235301000
H	-1.312597000	-3.684261000	0.628811000	H	0.950572000	3.040622000	2.728939000
H	-4.070832000	-2.704541000	-0.256994000	C	2.522932000	2.539163000	4.106956000
H	-3.689253000	-3.899410000	0.994973000	H	3.621801000	2.521807000	4.128889000
H	-4.369308000	-4.852752000	-1.421533000	H	2.179556000	3.266580000	4.851466000
H	-2.827521000	-5.450464000	-0.770870000	C	1.958315000	1.126555000	4.333514000
H	-3.220045000	-3.111117000	-2.709197000	H	0.890374000	1.202619000	4.567710000
H	-2.184308000	-4.520646000	-2.976187000	H	2.452229000	0.585691000	5.147464000
H	-0.495644000	-3.671064000	-1.479880000	C	2.129420000	0.411399000	2.970104000
H	-1.207331000	-2.126311000	-1.897680000	H	3.000981000	-0.242852000	2.982786000
H	-2.587285000	0.798849000	0.535181000	H	1.255900000	-0.204734000	2.751766000
H	-4.144163000	0.090181000	2.169795000	P	-2.829029000	-0.367225000	0.039093000
H	-4.524438000	-1.412142000	1.319829000	C	-3.562168000	-0.689806000	1.739637000
H	-5.171048000	1.430246000	0.385553000	H	-2.689677000	-1.013327000	2.298674000
H	-6.335688000	0.108090000	0.602594000	C	-4.203225000	0.537524000	2.441777000
H	-5.331502000	0.585602000	-1.878724000	H	-4.115156000	0.352266000	3.520445000
H	-5.437001000	-1.089996000	-1.313729000	H	-3.704108000	1.481467000	2.244558000
H	-3.138492000	-1.190297000	-1.646625000	C	-5.688355000	0.524702000	2.039716000
H	-2.944859000	0.552025000	-1.706572000	H	-6.316562000	1.004010000	2.798440000
H	-2.775244000	-1.926675000	2.801451000	H	-5.834526000	1.084303000	1.109526000
H	-0.283851000	-3.185688000	2.570615000	C	-6.045763000	-0.971081000	1.835757000
H	-1.118315000	-2.951773000	4.119603000	H	-6.581819000	-1.120595000	0.891374000
H	0.952256000	-1.089362000	2.860548000	H	-6.705494000	-1.335845000	2.630570000
H	1.096730000	-1.885343000	4.439811000	C	-4.698626000	-1.742923000	1.863128000
H	0.128611000	0.628313000	4.457025000	H	-4.573340000	-2.215652000	2.845055000
H	-0.841214000	-0.595379000	5.298351000	H	-4.658362000	-2.544169000	1.127249000
H	-2.527213000	0.205056000	3.777878000	C	-3.248449000	-1.823420000	-1.041587000
H	-1.315528000	0.640795000	2.568770000	H	-2.674950000	-1.658490000	-1.959768000

H	1.723583000	2.271789000	-1.201910000	C	-4.721877000	-1.951372000	-1.502053000
H	3.364934000	2.315494000	1.371016000	H	-5.422163000	-1.794502000	-0.680500000
H	1.669402000	2.775861000	1.141060000	H	-4.962242000	-1.224278000	-2.286886000
H	3.495352000	4.771564000	1.097968000	C	-4.786835000	-3.410276000	-1.984389000
H	2.387134000	4.695296000	-0.287546000	H	-5.811874000	-3.775567000	-2.106037000
H	5.218913000	3.543571000	-0.118525000	H	-4.280904000	-3.494223000	-2.955890000
H	4.608669000	4.635152000	-1.367830000	C	-3.995502000	-4.179229000	-0.910927000
H	3.495135000	2.837116000	-2.497809000	H	-3.633171000	-5.150915000	-1.262399000
H	4.645303000	1.832725000	-1.627886000	H	-4.646024000	-4.366478000	-0.047224000
H	3.368554000	0.321363000	-2.747114000	C	-2.837428000	-3.230796000	-0.499614000
H	0.937683000	-0.021971000	-3.194688000	H	-2.678573000	-3.238653000	0.581960000
H	0.993455000	-1.551518000	-2.317725000	H	-1.890143000	-3.536577000	-0.957497000
H	2.282388000	-0.934322000	-5.014810000	C	-3.840139000	0.981571000	-0.774438000
H	1.407378000	-2.390650000	-4.538910000	H	-4.879518000	0.663486000	-0.663737000
H	4.284625000	-1.923256000	-4.390295000	C	-3.613820000	2.405031000	-1.263216000
H	3.456366000	-3.352833000	-3.773577000	H	-4.506247000	2.753002000	0.368929000
H	3.327308000	-2.494761000	-1.567929000	H	-2.794558000	2.389300000	0.556242000
H	4.766869000	-1.580781000	-2.059723000	C	-3.230149000	3.318712000	-1.348229000
H	4.008354000	-1.442916000	0.375361000	H	-4.127528000	3.743049000	-1.817870000
H	5.172961000	1.384378000	0.426912000	H	-2.586073000	4.149360000	-1.038790000
H	5.832715000	-0.049510000	-0.379891000	C	-2.556849000	2.350798000	-2.328084000
H	6.829830000	0.530652000	2.046476000	H	-1.575182000	2.052697000	-1.933531000
H	6.202479000	-1.119611000	1.849784000	H	-2.412733000	2.761136000	-3.334482000
H	4.725287000	1.285538000	3.036764000	C	-3.506973000	1.148731000	-2.288894000
H	4.946082000	-0.290347000	3.809446000	H	-4.433942000	1.406592000	-2.819511000
H	3.177928000	-1.261141000	2.477216000	H	-3.106900000	0.250643000	-2.769903000
H	2.668096000	0.406050000	2.300109000	Ni	-0.502923000	0.208061000	0.116677000
Cl	1.388378000	-2.651081000	0.387710000	C	0.830191000	-0.720286000	-2.556865000
C	-2.499427000	3.419035000	-0.417688000	C	1.004313000	0.224786000	-3.588461000
C	-3.106260000	3.175720000	-1.658995000	C	1.783556000	-1.745675000	-2.444245000
C	-3.294632000	3.850715000	0.650959000	C	2.141954000	0.205372000	-4.401542000
C	-4.478437000	3.367819000	-1.824957000	C	2.915352000	-1.777095000	-3.253830000
C	-4.667835000	4.052678000	0.484209000	C	3.117612000	-0.786496000	-4.219748000
C	-5.263576000	3.813550000	-0.756477000	H	0.236220000	0.970040000	-3.758562000
H	-2.489824000	2.821850000	-2.478998000	H	1.645611000	-2.526550000	-1.708073000
H	-2.829448000	4.040399000	1.615756000	H	2.260444000	0.952112000	-5.180761000
H	-4.935617000	3.174913000	-2.792129000	H	3.636299000	-2.581529000	-3.114987000
H	-5.269906000	4.392914000	1.322870000	H	4.006499000	-0.804104000	-4.848273000
H	-6.331341000	3.966656000	-0.888873000	C	-0.365779000	-0.690132000	-1.684932000
C	-1.004791000	3.242478000	-0.238517000	H	-1.162388000	-0.175878000	-2.199707000
H	-0.471250000	3.905597000	-0.932823000	H	-0.677793000	-1.687920000	-1.472904000
H	-0.715505000	3.508701000	0.782216000	Cl	-0.930795000	1.223959000	2.121173000
C	-0.543424000	1.812736000	-0.554708000	C	0.205582000	-1.661025000	0.964114000
O	-0.122414000	1.159742000	0.485805000	O	-0.715422000	-2.128230000	1.558976000
O	-0.577685000	1.380920000	-1.710976000	O	1.376271000	-1.853314000	0.656239000
				Mg	3.040973000	-2.961047000	0.967334000
				Cl	3.919404000	-2.841616000	3.028652000
				Cl	3.438183000	-4.336272000	-0.770526000
TS₁₀₋₁₁				11			
P	1.500922000	1.382157000	0.279958000	P	-0.016739000	2.424764000	-0.262933000
C	1.239598000	3.140571000	-0.302107000	C	-0.168009000	3.451412000	1.276635000
H	2.130096000	3.683707000	0.038639000	H	-0.452317000	4.459743000	0.943227000
C	1.120534000	3.286090000	-1.843954000	C	-1.228972000	2.957975000	2.279996000
H	2.095701000	3.301383000	-2.334627000	H	-2.250720000	3.058846000	1.905505000
H	0.581563000	2.434897000	-2.255027000	H	-1.050835000	1.900049000	2.508738000
				C	-0.959866000	3.807721000	3.542370000

C	0.313582000	4.594964000	-2.088803000	H	-1.569308000	4.718142000	3.512176000
H	0.877342000	5.317963000	-2.687705000	H	-1.229498000	3.267343000	4.455949000
H	-0.608205000	4.366238000	-2.634405000	C	0.555600000	4.167173000	3.484233000
C	-0.024414000	5.140855000	-0.684523000	H	1.105238000	3.787507000	4.352219000
H	-0.984646000	5.668632000	-0.652320000	H	0.686899000	5.255060000	3.469450000
H	0.751012000	5.843221000	-0.351407000	C	1.083833000	3.543481000	2.170948000
C	-0.004155000	3.892858000	0.208772000	H	1.899384000	4.111208000	1.718456000
H	0.030683000	4.121506000	1.274347000	H	1.458584000	2.530740000	2.349868000
H	-0.896677000	3.288664000	0.030936000	C	-1.769635000	2.159360000	-0.816995000
C	3.062492000	0.907630000	-0.653904000	H	-2.219762000	1.432068000	-0.136123000
H	2.779635000	0.641960000	-1.671385000	C	-1.830601000	1.609529000	-2.283129000
C	3.880608000	-0.278765000	-0.033367000	H	-0.858406000	1.291139000	-2.666887000
H	3.546859000	-0.523439000	0.979826000	H	-2.486876000	0.735943000	-2.292947000
H	3.757963000	-1.151880000	-0.681201000	C	-2.469467000	2.737268000	-3.110702000
C	5.360080000	4.121506000	-0.005936000	H	-1.709280000	3.470181000	-3.417927000
H	5.617304000	0.541701000	0.995608000	H	-2.957093000	2.358648000	-4.015312000
H	6.045795000	-0.645408000	-0.244724000	C	-3.454463000	3.377948000	-2.122593000
C	5.417807000	1.334886000	-1.006331000	H	-4.310641000	2.707106000	-1.986010000
H	5.420625000	0.949092000	-2.034596000	H	-3.823612000	4.359634000	-2.441928000
H	6.295433000	1.978333000	-0.877153000	C	-2.645326000	3.450758000	-0.813612000
C	4.095262000	2.066627000	-0.740513000	H	-2.023725000	4.355826000	-0.814128000
H	4.167421000	2.605762000	0.213987000	H	-3.284623000	3.499221000	0.073588000
H	3.843006000	2.793108000	-1.515555000	C	0.637873000	3.569648000	-1.568349000
C	2.210300000	1.500023000	2.005592000	H	-0.241572000	4.098078000	-1.952069000
H	3.293801000	1.498471000	1.837494000	C	1.654346000	4.639951000	-1.103276000
C	1.907759000	2.768702000	2.837359000	H	1.159677000	5.498151000	-0.634146000
H	2.494995000	3.632029000	2.501391000	H	2.363537000	4.213357000	-0.391027000
H	0.848890000	3.023109000	2.784934000	C	2.394579000	4.990147000	-2.403766000
C	2.236294000	2.308493000	4.267222000	H	1.750776000	5.604508000	-3.048956000
H	3.324896000	2.231913000	4.397726000	H	3.323945000	5.543181000	-2.225995000
H	1.850790000	2.995498000	5.029575000	C	2.626316000	3.610070000	-3.042079000
C	1.593758000	0.911517000	4.325723000	H	3.458284000	3.113762000	-2.529209000
H	0.511036000	1.018311000	4.461192000	H	2.862671000	3.663203000	-4.110627000
H	1.983446000	0.292628000	5.140619000	C	1.320716000	2.825982000	-2.762339000
C	1.879776000	0.290470000	2.938015000	H	0.648968000	2.834000000	-3.627767000
H	2.734680000	-0.387050000	2.987436000	H	1.534941000	1.778614000	-2.523981000
H	1.025281000	-0.287401000	2.581223000	P	2.395898000	-1.477145000	0.040755000
P	-2.863771000	-0.411048000	0.056216000	C	3.797401000	-1.593845000	-1.200135000
C	-3.653841000	-0.683975000	1.734306000	H	3.392125000	-1.059488000	-2.066463000
H	-2.795385000	-1.006550000	2.330447000	C	5.145867000	-0.965332000	-0.767431000
C	-4.311944000	0.568729000	2.371903000	H	5.687855000	-0.730580000	-1.692907000
H	-4.289560000	0.412996000	3.458656000	H	5.047179000	-0.034120000	-0.212046000
C	-3.792664000	1.503505000	2.173381000	C	5.894890000	-2.083226000	-0.004831000
H	-5.769363000	0.560504000	1.880989000	H	6.972879000	-2.027834000	-0.189074000
H	-6.432449000	1.092201000	2.571917000	H	5.748723000	-1.980179000	1.074448000
H	-5.842957000	1.068578000	0.913478000	C	5.284574000	-3.421131000	-0.514422000
C	-6.142035000	-0.936809000	1.733740000	H	4.785636000	-3.948327000	0.307149000
H	-6.648267000	-1.122928000	0.779606000	H	6.041854000	-4.102376000	-0.916247000
H	-6.832367000	-1.256680000	2.521573000	C	4.259532000	-3.017096000	-1.594793000
C	-4.807126000	-1.721775000	1.840175000	H	4.770794000	-2.922147000	-2.562370000
H	-4.726757000	-2.168796000	2.838404000	H	3.456670000	-3.741406000	-1.728996000
H	-4.748856000	-2.540315000	1.126989000	C	1.290579000	-2.936685000	-0.284692000
C	-3.252999000	-1.904522000	-0.999473000	H	0.367011000	-2.689057000	0.244046000
H	-2.624172000	-1.785850000	-1.884749000	C	1.724486000	-4.318553000	0.265206000
C	-4.703131000	-1.986553000	-1.541693000	H	2.781020000	-4.525245000	0.071596000
H	-5.440058000	-1.780354000	-0.760571000	H	1.567186000	-4.393695000	1.346348000
H	-4.871317000	-1.272422000	-2.354467000	C	0.843973000	-5.281323000	-0.548790000
C	-4.807654000	-3.452257000	-1.990663000	H	1.179863000	-6.322573000	-0.486971000

H	-5.841139000	-3.773462000	-2.162645000	H	-0.189526000	-5.237184000	-0.179932000
H	-4.251760000	-3.586835000	-2.928614000	C	0.913847000	-4.705766000	-1.974184000
C	-4.115460000	-4.221633000	-0.852235000	H	0.084951000	-5.040430000	-2.605708000
H	-3.780662000	-5.219705000	-1.153419000	H	1.847473000	-5.031782000	-2.451483000
H	-4.821360000	-4.352145000	-0.022069000	C	0.916084000	-3.165291000	-1.786003000
C	-2.936112000	-3.316589000	-0.406738000	H	1.621185000	-2.682961000	-2.470260000
H	-2.817994000	-3.304394000	0.677138000	H	-0.067065000	-2.735730000	-1.985679000
H	-1.984711000	-3.677827000	-0.808344000	C	3.007572000	-1.841525000	1.769485000
C	-3.790734000	0.910808000	-0.889990000	H	3.533944000	-2.798757000	1.701236000
H	-4.837960000	0.595836000	-0.907662000	C	3.898889000	-0.757603000	2.440667000
C	-3.655529000	2.362935000	-0.321348000	H	4.636512000	-1.272314000	3.067438000
H	-4.607333000	2.717505000	0.085501000	H	4.446152000	-0.149461000	1.723594000
H	-2.920608000	2.397215000	0.483375000	C	2.960891000	0.117287000	3.322435000
C	-3.140836000	3.228680000	-1.492365000	H	3.270439000	0.063038000	4.372364000
H	-3.974169000	3.599756000	-2.103536000	H	2.998212000	1.164843000	3.013145000
H	-2.563977000	4.091224000	-1.145698000	C	1.546211000	-0.474976000	3.151381000
C	-2.316618000	2.229436000	-2.311164000	H	1.022200000	0.049038000	2.340696000
H	-1.404457000	1.974795000	-1.754496000	H	0.929777000	-0.390911000	4.053650000
H	-2.025269000	2.589935000	-3.304255000	C	1.805594000	-1.933056000	2.744248000
C	-3.242177000	1.010108000	-2.348616000	H	2.127372000	-2.506497000	3.624246000
H	-4.081222000	1.211631000	-3.026885000	H	0.930709000	-2.443787000	2.331556000
H	-2.751911000	0.104120000	-2.715780000	Ni	1.221312000	0.493962000	-0.153195000
Ni	-0.539226000	0.197838000	0.181828000	C	-2.915663000	-0.948158000	1.643863000
C	0.952871000	-0.925761000	-2.414302000	C	-3.684886000	0.173835000	1.970417000
C	0.880954000	0.160165000	-3.304245000	C	-3.523351000	-2.215740000	1.661337000
C	2.042091000	-1.800711000	-2.524319000	C	-5.033602000	0.038918000	2.303814000
C	1.906743000	0.420614000	-4.212129000	C	-4.882781000	-2.350314000	1.974501000
C	3.075232000	-1.542471000	-3.426037000	C	-5.638037000	-1.219710000	2.298792000
C	3.023826000	-0.420350000	-4.259000000	H	-3.226980000	1.156443000	1.946228000
H	0.001125000	0.797528000	-3.283193000	H	-2.942305000	-3.101012000	1.414786000
H	2.106416000	-2.678739000	-1.896418000	H	-5.619889000	0.922257000	2.539007000
H	1.833802000	1.275546000	-4.879318000	H	-5.338660000	-3.334772000	1.947359000
H	3.919050000	-2.225655000	-3.463727000	H	-6.693452000	-1.319625000	2.533260000
H	3.832762000	-0.216936000	-4.955560000	C	-1.485291000	-0.800942000	1.198288000
C	-0.169197000	-1.145164000	-1.464675000	H	-1.064843000	0.161256000	1.496050000
H	-0.984551000	-0.465291000	-1.742678000	H	-0.852500000	-1.566851000	1.665235000
H	-0.600628000	-2.144482000	-1.530654000	Cl	3.054180000	1.675434000	0.166373000
Cl	-1.102531000	1.369208000	1.976600000	C	-1.282276000	-0.950121000	-0.313616000
C	0.327618000	-1.791617000	0.372308000	O	-0.226002000	-0.471997000	-0.829776000
O	-0.584094000	-2.258629000	1.020224000	O	-2.113912000	-1.578756000	-1.011933000
O	1.561655000	-1.941141000	0.359135000	Mg	-4.045529000	-1.992599000	-0.899720000
Mg	3.141992000	-2.969781000	0.935748000	Cl	-5.155758000	-0.060678000	-1.379482000
Cl	3.850783000	-2.844367000	3.068542000	Cl	-4.439843000	-4.220017000	-1.109494000
Cl	3.957405000	-4.218955000	-0.767158000				
11a							
P	-1.818987000	-1.235991000	0.557597000				
C	-2.475776000	-2.569227000	-0.552712000				
H	-3.522707000	-2.692331000	-0.247360000				
C	-2.450339000	-2.112192000	-2.043783000				
H	-3.413868000	-1.675714000	-2.322345000				
H	-1.703068000	-1.333190000	-2.213469000				
C	-2.110040000	-3.380354000	-2.871221000				
H	-2.735549000	-3.476071000	-3.765746000				
H	-1.065618000	-3.333632000	-3.199421000				
C	-2.282061000	-4.554991000	-1.890874000				
H	-1.711687000	-5.443475000	-2.184791000				

H	-3.341138000	-4.840637000	-1.825398000
C	-1.818607000	-3.965105000	-0.549578000
H	-2.119403000	-4.563264000	0.313869000
H	-0.730390000	-3.876172000	-0.530380000
C	-2.982714000	0.148787000	0.168994000
H	-2.695548000	0.507041000	-0.820178000
C	-2.880376000	1.322109000	1.191746000
H	-2.146597000	1.144083000	1.986968000
H	-2.604217000	2.238739000	0.662063000
C	-4.291381000	1.492602000	1.784654000
H	-4.410549000	0.836110000	2.657672000
H	-4.471370000	2.521594000	2.108425000
C	-5.209604000	1.012829000	0.650411000
H	-5.242954000	1.767575000	-0.145515000
H	-6.236144000	0.808242000	0.975752000
C	-4.486894000	-0.242703000	0.133763000
H	-4.696455000	-1.080319000	0.812832000
H	-4.796245000	-0.544562000	-0.871978000
C	-2.262600000	-1.682324000	2.300529000
H	-3.296418000	-1.337487000	2.428248000
C	-2.219049000	-3.189458000	2.655162000
H	-3.119085000	-3.716882000	2.317771000
H	-1.348033000	-3.663233000	2.196059000
C	-2.039173000	-3.174963000	4.180913000
H	-2.982277000	-2.888230000	4.667595000
H	-1.733618000	-4.149417000	4.579291000
C	-0.980476000	-2.077651000	4.381043000
H	0.006381000	-2.476088000	4.117970000
H	-0.933906000	-1.701030000	5.408165000
C	-1.364676000	-0.973530000	3.367050000
H	-1.930116000	-0.168739000	3.849794000
H	-0.470207000	-0.522393000	2.931672000
P	2.599511000	-0.147215000	-0.280531000
C	3.798033000	-0.422831000	1.134593000
H	3.221195000	-0.060967000	1.991647000
C	4.268999000	-1.881462000	1.367071000
H	4.572733000	-1.937424000	2.420579000
H	3.497678000	-2.633969000	1.219976000
C	5.510910000	-2.071335000	0.466820000
H	6.237533000	-2.743741000	0.935180000
H	5.229296000	-2.521060000	-0.490123000
C	6.090061000	-0.644740000	0.248495000
H	6.076931000	-0.387037000	-0.817630000
H	7.130270000	-0.559532000	0.580658000
C	5.167420000	0.297673000	1.051110000
H	5.534819000	0.370626000	2.083160000
H	5.139123000	1.312431000	0.657154000
C	2.917701000	1.596135000	-0.883936000
H	2.046506000	1.834884000	-1.501052000
C	4.143162000	1.810561000	-1.812610000
H	5.031592000	1.303033000	-1.428095000
H	3.963881000	1.437721000	-2.825421000
C	4.344604000	3.332184000	-1.754098000
H	5.317026000	3.648600000	-2.148318000
H	3.562699000	3.828207000	-2.345936000
C	4.158608000	3.652726000	-0.262074000
H	3.914316000	4.703845000	-0.077402000
H	5.089783000	3.434274000	0.275876000

C	3.032034000	2.699314000	0.216515000
H	3.236868000	2.290893000	1.205544000
H	2.084482000	3.237566000	0.291341000
C	3.151773000	-1.123384000	-1.782705000
H	4.208153000	-0.875562000	-1.920737000
C	2.945691000	-2.663028000	-1.722671000
H	3.777701000	-3.135566000	-2.257609000
H	2.943940000	-3.053001000	-0.707141000
C	1.601694000	-2.967626000	-2.445220000
H	1.770879000	-3.631141000	-3.301179000
H	0.897801000	-3.462523000	-1.773127000
C	1.064222000	-1.603068000	-2.925093000
H	0.390176000	-1.189686000	-2.163239000
H	0.504300000	-1.662343000	-3.865550000
C	2.316369000	-0.722829000	-3.025541000
H	2.888123000	-0.993421000	-3.923914000
H	2.093044000	0.345664000	-3.093933000
Ni	0.369447000	-0.601210000	0.272837000
C	-1.847544000	1.908959000	-2.675415000
C	-2.339760000	0.902527000	-3.513216000
C	-2.732706000	2.872322000	-2.169241000
C	-3.700018000	0.839145000	-3.825135000
C	-4.092666000	2.804941000	-2.475969000
C	-4.582172000	1.785373000	-3.298429000
H	-1.656642000	0.154931000	-3.907285000
H	-2.360306000	3.658653000	-1.519809000
H	-4.067964000	0.045971000	-4.470443000
H	-4.770140000	3.549445000	-2.067259000
H	-5.642417000	1.732452000	-3.529780000
C	-0.370606000	1.915498000	-2.300005000
H	0.077908000	0.951504000	-2.551506000
H	0.162228000	2.709150000	-2.837610000
Cl	0.923244000	-2.568924000	1.071194000
C	-0.212152000	2.174950000	-0.820355000
O	-0.167041000	1.209762000	0.033383000
O	-0.208045000	3.345220000	-0.366160000
Mg	-0.269818000	2.783950000	1.670038000
Cl	-1.749089000	4.253314000	2.579241000
Cl	1.229023000	1.634215000	2.973554000

Table S8. B3LYP-D/BS-I optimized Cartesian coordinates of the species involved in the CO₂ insertion of Ni^I-CH₂Ph bond.

7				8			
P	1.271970000	1.062249000	-0.628719000	P	-1.615491000	-1.193689000	0.002102000
C	1.408682000	1.030096000	-2.493487000	C	-2.788331000	-2.107586000	-1.116863000
H	1.873568000	1.969917000	-2.813211000	H	-3.389136000	-2.724429000	-0.434546000
C	2.241214000	-0.187044000	-2.994495000	C	-3.751950000	-1.162946000	-1.904303000
H	2.806843000	0.116374000	-3.885848000	H	-4.739952000	-1.170747000	-1.429511000
H	2.956812000	-0.567522000	-2.261492000	H	-3.399536000	-0.130270000	-1.907485000
C	1.190235000	-1.234317000	-3.387033000	C	-3.804901000	-1.725451000	-3.347560000
H	1.594797000	-2.030065000	-4.024042000	H	-4.809309000	-1.669979000	-3.782303000
H	0.778288000	-1.692501000	-2.478850000	H	-3.125067000	-1.146051000	-3.979757000
C	0.109870000	-0.386881000	-4.070060000	C	-3.281706000	-3.166654000	-3.230172000
H	-0.847980000	-0.909177000	-4.179261000	H	-2.923985000	-3.573522000	-4.182991000
H	0.450661000	-0.088954000	-5.071000000	H	-4.074225000	-3.829764000	-2.854933000
C	-0.004280000	0.846455000	-3.149850000	C	-2.168491000	-3.051633000	-2.175569000
H	-0.329077000	1.746607000	-3.682192000	H	-1.893459000	-4.020225000	-1.745991000
H	-0.751091000	0.634245000	-2.377731000	H	-1.268615000	-2.617290000	-2.623159000
C	3.036699000	0.984667000	-0.067179000	C	-2.845713000	-0.411730000	1.154291000
H	3.317143000	-0.067437000	-0.175222000	H	-3.505599000	0.149279000	0.484074000
C	3.269477000	1.341784000	1.414439000	C	-2.221055000	0.611442000	2.129002000
H	2.834143000	2.318256000	1.657150000	H	-1.258368000	0.255550000	2.505492000
H	2.844316000	0.591134000	2.087223000	H	-2.060455000	1.572549000	1.641687000
C	4.801632000	1.430001000	1.481012000	C	-3.231557000	0.668602000	3.281630000
H	5.168450000	1.925831000	2.387623000	H	-2.823762000	1.128250000	4.189860000
H	5.210360000	0.413420000	1.454575000	H	-4.106571000	1.253513000	2.967542000
C	5.181973000	2.190079000	0.189422000	C	-3.617355000	-0.808525000	3.472028000
H	6.178033000	1.914350000	-0.174203000	H	-4.543459000	-0.949176000	4.040958000
H	5.195182000	3.269859000	0.382837000	H	-2.813816000	-1.321873000	4.017435000
C	4.062345000	1.851152000	-0.842194000	C	-3.711323000	-1.372548000	2.031771000
H	3.604705000	2.773347000	-1.220900000	H	-3.376579000	-2.414382000	1.990707000
H	4.442752000	1.305475000	-1.711800000	H	-4.747748000	-1.359344000	1.675487000
C	0.804699000	2.845899000	-0.325177000	C	-0.836842000	-2.581186000	0.953712000
H	1.676192000	3.453512000	-0.603392000	H	-1.611789000	-3.312178000	1.222671000
C	-0.392974000	3.325191000	-1.176839000	C	0.278040000	-3.287559000	0.154788000
H	-0.105090000	3.542894000	-2.210105000	H	-0.111983000	-3.962011000	-0.610641000
H	-1.167998000	2.554788000	-1.207568000	H	0.878984000	-2.531649000	-0.356214000
C	-0.909975000	4.552845000	-0.413347000	C	1.110923000	-4.025800000	1.226912000
H	-0.243313000	5.406540000	-0.595622000	H	0.743876000	-5.051734000	1.346236000
H	-1.922736000	4.847448000	-0.714125000	H	2.165924000	-4.090517000	0.938774000
C	-0.824160000	4.124479000	1.064374000	C	0.909476000	-3.229609000	2.550401000
H	-1.734994000	3.583681000	1.348479000	H	1.850971000	-2.811106000	2.925378000
H	-0.736942000	4.979021000	1.744444000	H	0.517776000	-3.884212000	3.336883000
C	0.409437000	3.182207000	1.145585000	C	-0.106406000	-2.108416000	2.223034000
H	1.241234000	3.676119000	1.657009000	H	-0.792806000	-1.897236000	3.049050000
H	0.179989000	2.277367000	1.713740000	H	0.420647000	-1.176950000	1.993574000
P	-2.019644000	-0.490230000	0.529412000	P	2.073533000	0.403619000	0.069266000
C	-3.111938000	-1.808384000	-0.209513000	C	3.213818000	1.385940000	-1.052271000
H	-4.150057000	-1.452898000	-0.168769000	H	4.207126000	0.936782000	-0.939771000
C	-2.727049000	-2.062292000	-1.692212000	C	2.848155000	1.323467000	-2.552389000
H	-3.172450000	-1.331655000	-2.375264000	H	3.113820000	0.366278000	-3.009612000
H	-1.635532000	-2.002995000	-1.793381000	H	1.772290000	1.459725000	-2.673883000
C	-3.187414000	-3.503940000	-1.951521000	C	3.589442000	2.531653000	-3.140764000
H	-4.281030000	-3.536110000	-2.060742000	H	4.668678000	2.326381000	-3.188493000
H	-2.744882000	-3.936942000	-2.856652000	H	3.249665000	2.792885000	-4.149600000

C	-2.758014000	-4.228206000	-0.666007000	C	3.302451000	3.632925000	-2.106017000
H	-1.681380000	-4.427265000	-0.709027000	H	2.289539000	4.019383000	-2.270493000
H	-3.274469000	-5.183055000	-0.514706000	H	3.999211000	4.476713000	-2.163571000
C	-3.040709000	-3.215657000	0.471978000	C	3.358426000	2.911457000	-0.734738000
H	-3.997375000	-3.429259000	0.963268000	H	4.314105000	3.091824000	-0.228924000
H	-2.266128000	-3.277225000	1.235744000	H	2.575763000	3.281595000	-0.069348000
C	-3.014719000	1.051728000	0.173821000	C	3.081411000	-1.153548000	0.308772000
H	-2.335728000	1.884223000	0.385303000	H	2.466832000	-1.818613000	0.924386000
C	-4.305107000	1.266645000	0.993061000	C	4.463569000	-1.035654000	0.984825000
H	-4.881463000	0.332603000	1.019693000	H	5.064517000	-0.270810000	0.476752000
H	-4.092402000	1.547386000	2.029159000	H	4.408564000	-0.765124000	2.041748000
C	-5.093748000	2.363527000	0.216921000	C	5.084347000	-2.433504000	0.760412000
H	-6.140549000	2.067452000	0.085334000	H	6.178854000	-2.396629000	0.728161000
H	-5.094997000	3.314607000	0.760759000	H	4.807251000	-3.093116000	1.591946000
C	-4.375610000	2.504363000	-1.155503000	C	4.463548000	-2.958534000	-0.569364000
H	-3.713957000	3.380583000	-1.145677000	H	3.963826000	-3.919966000	-0.404210000
H	-5.074367000	2.625926000	-1.990692000	H	5.222074000	-3.120008000	-1.343091000
C	-3.515782000	1.234113000	-1.270258000	C	3.434731000	-1.886765000	-1.003030000
H	-4.145852000	0.381564000	-1.550961000	H	3.906718000	-1.173858000	-1.688691000
H	-2.714088000	1.317116000	-2.009966000	H	2.567128000	-2.297967000	-1.521177000
C	-2.222717000	-0.594728000	2.392512000	C	2.259144000	1.280790000	1.727324000
H	-3.287460000	-0.713546000	2.619888000	H	3.185481000	1.861245000	1.666238000
C	-1.374841000	-1.745837000	3.031660000	C	1.076883000	2.247958000	1.990134000
H	-2.009980000	-2.524858000	3.466354000	H	1.233410000	3.227673000	1.530082000
H	-0.746563000	-2.212429000	2.270634000	H	0.153806000	1.844369000	1.562439000
C	-0.452634000	-1.074955000	4.072132000	C	0.945227000	2.312406000	3.518024000
H	-0.953810000	-0.999116000	5.046700000	H	1.713877000	2.976610000	3.936970000
H	0.481134000	-1.630651000	4.217225000	H	-0.035218000	2.684037000	3.838347000
C	-0.244571000	0.327865000	3.489846000	C	1.212791000	0.862512000	3.951819000
H	0.405601000	0.261489000	2.605441000	H	0.312350000	0.258495000	3.795483000
H	0.195488000	1.043385000	4.194492000	H	1.489526000	0.771732000	5.008383000
C	-1.667057000	0.704833000	3.053115000	C	2.337865000	0.380795000	3.009616000
H	-2.267347000	0.937835000	3.943109000	H	3.314412000	0.531052000	3.483332000
H	-1.701494000	1.584173000	2.404395000	H	2.258524000	-0.687926000	2.800350000
Ni	0.109494000	-0.792850000	-0.048137000	Ni	-0.170698000	0.522755000	-0.695339000
C	1.878702000	-2.623634000	0.274853000	C	-1.440225000	2.853369000	-0.763124000
C	2.886588000	-2.719210000	-0.717107000	C	-2.653430000	2.356737000	-1.298911000
C	2.309871000	-2.283877000	1.584366000	C	-1.536113000	3.686929000	0.374767000
C	4.230489000	-2.499228000	-0.421107000	C	-3.879865000	2.627085000	-0.694886000
C	3.653291000	-2.064318000	1.878353000	C	-2.765514000	3.968839000	0.969900000
C	4.630645000	-2.169551000	0.880195000	C	-3.947708000	3.425463000	0.453704000
H	2.591857000	-2.982037000	-1.729553000	H	-2.600459000	1.752740000	-2.198551000
H	1.560610000	-2.193365000	2.367708000	H	-0.627028000	4.112397000	0.789159000
H	4.974345000	-2.592730000	-1.209958000	H	-4.790400000	2.217860000	-1.127967000
H	3.943764000	-1.805494000	2.894500000	H	-2.801978000	4.613347000	1.845636000
H	5.678981000	-2.004347000	1.113112000	H	-4.904538000	3.640540000	0.921934000
C	0.448114000	-2.784170000	-0.042874000	C	-0.142299000	2.440346000	-1.336917000
H	0.284143000	-3.263830000	-1.014256000	H	-0.150965000	2.437287000	-2.430326000
H	-0.101510000	-3.333736000	0.726419000	H	0.690947000	3.038989000	-0.965132000
				C	-0.176651000	-0.283033000	-2.688160000
				O	-1.133963000	0.155585000	-3.274109000
				O	0.773010000	-1.028676000	-2.683241000
TS_{8,9}				9			
P	-1.710865000	0.688353000	0.516669000	P	-2.004211000	0.520385000	0.642613000
C	-2.738576000	0.508465000	2.061814000	C	-2.728560000	-0.486815000	2.010547000
H	-3.540182000	1.250137000	1.950539000	H	-3.714428000	-0.059536000	2.242242000

C	-3.395926000	-0.886817000	2.263244000	C	-2.891722000	-1.986290000	1.606343000
H	-4.440150000	-0.851666000	1.928894000	H	-3.953256000	-2.214254000	1.455125000
H	-2.891798000	-1.658699000	1.683121000	H	-2.372750000	-2.224479000	0.676837000
C	-3.281792000	-1.188299000	3.782355000	C	-2.288627000	-2.802500000	2.776094000
H	-4.202698000	-1.615791000	4.195754000	H	-2.857067000	-3.715813000	2.986289000
H	-2.469184000	-1.902876000	3.941323000	H	-1.263879000	-3.081013000	2.515742000
C	-2.906407000	0.155522000	4.435024000	C	-2.253669000	-1.826229000	3.964089000
H	-2.412961000	0.035454000	5.406413000	H	-1.545763000	-2.128880000	4.744061000
H	-3.806083000	0.769450000	4.586190000	H	-3.250831000	-1.741695000	4.420769000
C	-2.002778000	0.821182000	3.383386000	C	-1.867405000	-0.495441000	3.298045000
H	-1.885156000	1.898702000	3.543248000	H	-2.057027000	0.381816000	3.927492000
H	-1.014932000	0.351160000	3.391056000	H	-0.805032000	-0.525736000	3.035210000
C	-3.034779000	0.377987000	-0.756366000	C	-3.275166000	0.357536000	-0.694918000
H	-3.257964000	-0.689232000	-0.629744000	H	-3.420645000	-0.725067000	-0.773779000
C	-2.691388000	0.570212000	-2.248384000	C	-2.789691000	0.849270000	-2.077650000
H	-2.269866000	1.561450000	-2.439003000	H	-2.284871000	1.818897000	-2.000057000
H	-1.986064000	-0.178613000	-2.607278000	H	-2.083960000	0.145560000	-2.530196000
C	-4.074412000	0.458351000	-2.905354000	C	-4.100184000	1.012201000	-2.859918000
H	-4.090870000	0.809777000	-3.943714000	H	-3.988299000	1.591427000	-3.783808000
H	-4.380433000	-0.595727000	-2.897388000	H	-4.492905000	0.020402000	-3.125761000
C	-4.990423000	1.286649000	-1.976852000	C	-5.027339000	1.687730000	-1.831991000
H	-6.026091000	0.929768000	-1.988610000	H	-6.090002000	1.589223000	-2.079630000
H	-5.004807000	2.332757000	-2.306684000	H	-4.796211000	2.760559000	-1.796151000
C	-4.347181000	1.185961000	-0.561193000	C	-4.665573000	1.029533000	-0.472277000
H	-4.133808000	2.186290000	-0.166424000	H	-4.648299000	1.774933000	0.329377000
H	-5.002641000	0.689911000	0.161887000	H	-5.403639000	0.271523000	-0.188139000
C	-1.487460000	2.544527000	0.571518000	C	-2.171922000	2.259748000	1.274634000
H	-2.358118000	2.956882000	1.099640000	H	-3.117223000	2.321758000	1.830974000
C	-0.203975000	2.938438000	1.337960000	C	-1.007203000	2.668039000	2.220149000
H	-0.343055000	2.893854000	2.421411000	H	-1.234514000	2.405663000	3.257458000
H	0.584457000	2.222247000	1.093833000	H	-0.094377000	2.122849000	1.947566000
C	0.172107000	4.360249000	0.839880000	C	-0.811927000	4.201278000	2.019363000
H	0.002971000	5.111194000	1.619030000	H	-0.904153000	4.754135000	2.960271000
H	1.235557000	4.407340000	0.578407000	H	0.188771000	4.402593000	1.621952000
C	-0.727671000	4.636676000	-0.397418000	C	-1.886087000	4.633933000	0.993176000
H	-0.168463000	5.074396000	-1.231983000	H	-1.556103000	5.465680000	0.359708000
H	-1.521525000	5.344480000	-0.130044000	H	-2.797403000	4.954626000	1.514703000
C	-1.359395000	3.280914000	-0.773931000	C	-2.187715000	3.357355000	0.192613000
H	-2.326837000	3.393915000	-1.273536000	H	-3.138776000	3.398896000	-0.348073000
H	-0.706501000	2.728069000	-1.452582000	H	-1.397379000	3.182286000	-0.544478000
P	2.110017000	0.059701000	-0.426074000	P	2.152769000	0.591868000	-0.464468000
C	3.442641000	-1.126194000	-0.956478000	C	3.412754000	-0.349196000	-1.445743000
H	4.281781000	-0.489274000	-1.263143000	H	4.178195000	0.378104000	-1.747179000
C	3.962414000	-2.117360000	0.104248000	C	4.131260000	-1.493919000	-0.698045000
H	4.660014000	-1.640992000	0.802432000	H	4.903203000	-1.113557000	-0.021103000
H	3.143337000	-2.526732000	0.698876000	H	3.439828000	-2.089230000	-0.094409000
C	4.617230000	-3.214849000	-0.750360000	C	4.697360000	-2.338921000	-1.851186000
H	5.575377000	-2.853836000	-1.150509000	H	5.575301000	-1.835226000	-2.279329000
H	4.811212000	-4.135712000	-0.188868000	H	5.005590000	-3.340596000	-1.532037000
C	3.609392000	-3.415416000	-1.898050000	C	3.550742000	-2.368514000	-2.881992000
H	2.800044000	-4.071216000	-1.555550000	H	2.858667000	-3.180117000	-2.632096000
H	4.055324000	-3.877620000	-2.785712000	H	3.906354000	-2.543339000	-3.903329000
C	3.045051000	-1.998561000	-2.190771000	C	2.827631000	-0.998110000	-2.737367000
H	3.477223000	-1.572687000	-3.103137000	H	3.002820000	-0.348423000	-3.601928000
H	1.962010000	-2.032703000	-2.343780000	H	1.742042000	-1.137091000	-2.660384000
C	3.009179000	1.187797000	0.754878000	C	3.061534000	1.194672000	1.033930000
H	2.508308000	2.159429000	0.673150000	H	2.406832000	1.975151000	1.439944000
C	4.510102000	1.449469000	0.538680000	C	4.451013000	1.824623000	0.784841000

H	5.056023000	0.499574000	0.503273000	H	5.015177000	1.241772000	0.045916000
H	4.723527000	2.000589000	-0.385212000	H	4.378804000	2.854540000	0.414989000
C	4.888905000	2.224768000	1.815407000	C	5.139149000	1.698681000	2.153397000
H	5.964288000	2.195357000	2.023922000	H	6.223379000	1.856106000	2.106442000
H	4.607269000	3.278435000	1.691822000	H	4.718613000	2.440108000	2.847373000
C	4.037117000	1.575243000	2.945608000	C	4.745924000	0.278297000	2.596501000
H	3.598034000	2.343935000	3.591124000	H	4.876879000	0.110233000	3.670911000
H	4.652437000	0.932484000	3.584427000	H	5.378225000	-0.449933000	2.071618000
C	2.938867000	0.737796000	2.228867000	C	3.272949000	0.111576000	2.146828000
H	3.152906000	-0.330855000	2.308662000	H	3.059396000	-0.908619000	1.823141000
H	1.937773000	0.888993000	2.646689000	H	2.583030000	0.310256000	2.973205000
C	2.017199000	1.079420000	-1.998563000	C	1.944012000	2.135885000	-1.482100000
H	2.897817000	0.840102000	-2.610106000	H	2.910303000	2.432977000	-1.912138000
C	0.736767000	0.771967000	-2.797980000	C	0.893382000	1.962240000	-2.608442000
H	0.794153000	-0.184897000	-3.328741000	H	1.335006000	1.543186000	-3.518748000
H	-0.096678000	0.693694000	-2.094089000	H	0.117493000	1.259416000	-2.274444000
C	0.534470000	1.979867000	-3.742885000	C	0.260096000	3.366712000	-2.829867000
H	0.870100000	1.743301000	-4.758725000	H	0.514647000	3.776509000	-3.813163000
H	-0.526798000	2.245659000	-3.810092000	H	-0.833035000	3.297510000	-2.785966000
C	1.387587000	3.138856000	-3.144175000	C	0.805044000	4.268243000	-1.689296000
H	0.798824000	4.050289000	-2.992097000	H	0.035006000	4.923780000	-1.266506000
H	2.208062000	3.392655000	-3.825283000	H	1.610502000	4.908677000	-2.069345000
C	1.958423000	2.606677000	-1.811079000	C	1.378586000	3.296066000	-0.645472000
H	2.936661000	3.033456000	-1.564129000	H	2.131052000	3.757467000	0.003460000
H	1.283847000	2.852644000	-0.989261000	H	0.580989000	2.908113000	-0.002543000
Ni	0.123953000	-0.806495000	0.432041000	Ni	0.090568000	-0.123147000	0.106682000
C	-0.839342000	-2.962147000	-0.569029000	C	-0.465956000	-3.392447000	-0.809426000
C	-2.010348000	-3.373325000	0.106848000	C	-1.249739000	-4.450438000	-0.326118000
C	-0.963473000	-2.608334000	-1.929982000	C	-1.052015000	-2.481493000	-1.698650000
C	-3.238351000	-3.435962000	-0.545804000	C	-2.579536000	-4.596362000	-0.721151000
C	-2.192024000	-2.688596000	-2.587325000	C	-2.381132000	-2.630430000	-2.108472000
C	-3.339183000	-3.096604000	-1.901400000	C	-3.150627000	-3.687141000	-1.618360000
H	-1.932725000	-3.634226000	1.158328000	H	-0.806169000	-5.159078000	0.369234000
H	-0.079999000	-2.294055000	-2.477448000	H	-0.451884000	-1.658455000	-2.082709000
H	-4.121437000	-3.754963000	0.002574000	H	-3.171358000	-5.420926000	-0.331996000
H	-2.255244000	-2.423253000	-3.639880000	H	-2.813211000	-1.921327000	-2.810011000
H	-4.294439000	-3.157551000	-2.415743000	H	-4.183700000	-3.805202000	-1.934828000
C	0.453141000	-2.930009000	0.143946000	C	0.966672000	-3.247458000	-0.373591000
H	0.548033000	-3.782787000	0.816718000	H	1.483625000	-4.212209000	-0.398918000
H	1.330508000	-2.891015000	-0.494344000	H	1.482875000	-2.572342000	-1.064138000
C	0.679011000	-2.030293000	2.078294000	C	1.173690000	-2.641301000	1.041865000
O	-0.458449000	-1.748353000	2.459944000	O	0.436744000	-1.618210000	1.329207000
O	1.781371000	-2.303541000	2.489126000	O	2.043411000	-3.129784000	1.765013000
9a				12			
P	1.187186000	1.462820000	-0.330617000	P	-0.739479000	1.326622000	1.129487000
C	2.047060000	1.832575000	-1.933549000	C	-2.402764000	0.972615000	1.882031000
H	2.582599000	2.785037000	-1.830193000	H	-2.562989000	1.800643000	2.586517000
C	3.043556000	0.703363000	-2.317379000	C	-3.573603000	0.979576000	0.881840000
H	4.060560000	0.914174000	-1.969492000	H	-3.773387000	1.975278000	0.471099000
H	2.728180000	-0.243480000	-1.870409000	H	-3.364198000	0.309836000	0.044809000
C	2.911725000	0.573283000	-3.842880000	C	-4.732135000	0.418660000	1.718731000
H	3.457922000	1.382453000	-4.349145000	H	-5.114168000	1.199998000	2.389431000
C	3.295581000	-0.383681000	-4.216490000	H	-5.557581000	0.062708000	1.095577000
H	1.398888000	0.739063000	-4.052138000	C	-4.082763000	-0.712301000	2.548665000
H	0.895260000	-0.168349000	-3.701460000	H	-4.211143000	-1.690835000	2.065599000

H	1.116232000	0.921459000	-5.095817000	H	-4.553620000	-0.822421000	3.530758000
C	1.034087000	1.917264000	-3.125324000	C	-2.569902000	-0.357109000	2.668974000
H	1.164022000	2.873017000	-3.648821000	H	-2.275936000	-0.222060000	3.713883000
H	-0.010617000	1.864800000	-2.796550000	H	-1.944318000	-1.157115000	2.265391000
C	2.564099000	1.028244000	0.828418000	C	-1.055261000	3.028097000	0.461985000
H	3.126701000	0.233489000	0.323245000	H	-1.784687000	2.853384000	-0.340085000
C	2.073530000	0.463303000	2.187149000	C	0.121535000	3.785529000	-0.182296000
H	1.149662000	0.956452000	2.503761000	H	0.979434000	3.838706000	0.494923000
H	1.851515000	-0.600783000	2.088183000	H	0.442737000	3.327107000	-1.118683000
C	3.217983000	0.771525000	3.197759000	C	-0.479404000	5.185075000	-0.379817000
H	2.843611000	1.399679000	4.015243000	H	0.272707000	5.952417000	-0.595717000
H	3.617354000	-0.143146000	3.649520000	H	-1.178773000	5.147061000	-1.224687000
C	4.308374000	1.527096000	2.397522000	C	-1.246423000	5.448971000	0.935889000
H	5.043550000	0.812857000	2.010416000	H	-2.109925000	6.105426000	0.785793000
H	4.841299000	2.270177000	3.002801000	H	-0.586959000	5.941383000	1.660289000
C	3.549240000	2.146747000	1.212019000	C	-1.662076000	4.043538000	1.467296000
H	2.999666000	3.037771000	1.544807000	H	-1.261145000	3.883727000	2.475563000
H	4.202143000	2.440785000	0.381593000	H	-2.748080000	3.922595000	1.530869000
C	0.614125000	3.142695000	0.210620000	C	0.330469000	1.488506000	2.635043000
H	1.463742000	3.839328000	0.188348000	H	-0.204316000	2.084948000	3.386441000
C	-0.504638000	3.695915000	-0.693093000	C	0.669670000	0.095624000	3.212257000
H	-0.137533000	4.025958000	-1.670615000	H	-0.157740000	-0.344763000	3.771212000
H	-1.247063000	2.906935000	-0.866519000	H	0.893716000	-0.580858000	2.383905000
C	-1.117034000	4.835941000	0.141581000	C	1.918353000	0.323810000	4.088924000
H	-0.532618000	5.751869000	-0.009450000	H	1.621055000	0.511964000	5.126658000
H	-2.150206000	5.053614000	-0.151000000	H	2.565783000	-0.560545000	4.093089000
C	-1.002618000	4.370940000	1.619809000	C	2.631400000	1.575991000	3.502155000
H	-1.980090000	4.077647000	2.018083000	H	3.632470000	1.339580000	3.121834000
H	-0.626578000	5.180051000	2.255521000	H	2.761007000	2.342590000	4.273848000
C	-0.029426000	3.157224000	1.615074000	C	1.717485000	2.102243000	2.366823000
H	0.723683000	3.213092000	2.408274000	H	1.694387000	3.195010000	2.330445000
H	-0.588789000	2.225592000	1.765716000	H	2.075134000	1.749879000	1.394162000
P	-2.516805000	-0.526254000	-0.053855000	P	2.359560000	-0.707178000	-0.420956000
C	-2.756476000	-1.047765000	1.714588000	C	2.748074000	-2.171337000	-1.524435000
H	-3.812236000	-0.901120000	1.988918000	H	3.643865000	-2.629011000	-1.084934000
C	-2.352975000	-2.500504000	2.035056000	C	1.656926000	-3.264871000	-1.607183000
H	-3.049495000	-3.237586000	1.623655000	H	1.622628000	-3.903078000	-0.721118000
H	-1.357147000	-2.690678000	1.621149000	H	0.674575000	-2.803758000	-1.711691000
C	-2.301865000	-2.516450000	3.576424000	C	2.010666000	-4.012965000	-2.899993000
H	-3.306996000	-2.702104000	3.976048000	H	2.905665000	-4.632115000	-2.745606000
H	-1.646745000	-3.307207000	3.958466000	H	1.202995000	-4.666485000	-3.247868000
C	-1.821930000	-1.093433000	3.986628000	C	2.320103000	-2.864600000	-3.873574000
H	-0.809992000	-1.112709000	4.406079000	H	1.375661000	-2.432068000	-4.226423000
H	-2.481084000	-0.667596000	4.751987000	H	2.894091000	-3.178533000	-4.752115000
C	-1.855343000	-0.248372000	2.685204000	C	3.077573000	-1.820183000	-3.016011000
H	-2.207526000	0.775037000	2.847682000	H	4.159653000	-1.885364000	-3.176770000
H	-0.849435000	-0.189383000	2.254478000	H	2.782743000	-0.803659000	-3.287946000
C	-3.281027000	-1.858456000	-1.095844000	C	3.220770000	-1.212532000	1.156283000
H	-3.463914000	-1.368010000	-2.061729000	H	3.031977000	-0.405837000	1.866993000
C	-4.623848000	-2.481551000	-0.595745000	C	4.773772000	-1.388023000	1.009369000
H	-4.837427000	-2.230651000	0.448893000	H	5.108598000	-1.354938000	-0.033198000
H	-5.460158000	-2.100549000	-1.192904000	H	5.280262000	-0.566514000	1.526155000
C	-4.460515000	-4.014926000	-0.777417000	C	5.107634000	-2.744609000	1.671952000
H	-4.181177000	-4.472470000	0.180324000	H	5.120658000	-3.536283000	0.910862000
H	-5.383957000	-4.498961000	-1.115363000	H	6.085571000	-2.741644000	2.166011000
C	-3.292234000	-4.174106000	-1.768367000	C	3.931546000	-2.992253000	2.628175000
H	-3.645193000	-3.999860000	-2.794799000	H	4.031662000	-2.359082000	3.521807000
H	-2.836667000	-5.170744000	-1.733966000	H	3.851361000	-4.033812000	2.958599000

C	-2.329890000	-3.051504000	-1.353944000	C	2.726147000	-2.534762000	1.794934000
H	-1.805240000	-3.328685000	-0.433591000	H	2.520407000	-3.283332000	1.024218000
H	-1.565820000	-2.805295000	-2.096289000	H	1.807554000	-2.410271000	2.368687000
C	-3.762283000	0.836744000	-0.247590000	C	3.507746000	0.625086000	-1.096311000
H	-4.767486000	0.412015000	-0.113102000	H	4.249223000	0.111271000	-1.715387000
C	-3.577477000	1.992096000	0.751872000	C	2.734478000	1.632523000	-1.978275000
H	-3.918954000	1.738377000	1.761204000	H	2.582170000	1.269906000	-3.000086000
H	-2.516308000	2.254070000	0.810363000	H	1.742674000	1.807595000	-1.544675000
C	-4.367554000	3.143010000	0.110686000	C	3.545067000	2.932163000	-1.897734000
H	-5.440393000	2.990932000	0.287564000	H	4.439877000	2.857944000	-2.530499000
H	-4.096952000	4.122800000	0.521304000	H	2.973009000	3.810471000	-2.219337000
C	-4.054910000	3.021577000	-1.399375000	C	3.942468000	2.979490000	-0.414691000
H	-3.209012000	3.666917000	-1.659677000	H	3.080767000	3.314570000	0.174358000
H	-4.903845000	3.333097000	-2.017496000	H	4.774537000	3.661486000	-0.208364000
C	-3.673403000	1.527587000	-1.635347000	C	4.279271000	1.513904000	-0.058787000
H	-4.326468000	1.038976000	-2.366343000	H	5.352794000	1.327119000	-0.167194000
H	-2.647043000	1.461406000	-2.021872000	H	4.032968000	1.288132000	0.979776000
Ni	-0.351226000	-0.167021000	-0.454401000	Ni	0.055361000	-0.029833000	-0.605888000
C	3.371554000	-2.726181000	-0.200174000	C	-1.092408000	0.637362000	-2.677459000
C	4.295705000	-2.263329000	-1.144404000	C	-2.478828000	0.594501000	-2.388835000
C	3.640244000	-2.532857000	1.161948000	C	-0.548021000	1.879932000	-3.085450000
C	5.468111000	-1.620017000	-0.739331000	C	-3.269263000	1.736540000	-2.487747000
C	4.813401000	-1.898066000	1.570344000	C	-1.343867000	3.018869000	-3.188050000
C	5.731070000	-1.436905000	0.620303000	C	-2.707979000	2.957683000	-2.879967000
H	4.084713000	-2.398402000	-2.202244000	H	-2.932208000	-0.343868000	-2.095502000
H	2.913673000	-2.870634000	1.895268000	H	0.502392000	1.930844000	-3.348845000
H	6.173846000	-1.263792000	-1.485404000	H	-4.328954000	1.661614000	-2.260501000
H	5.008418000	-1.752662000	2.629321000	H	-0.900109000	3.957271000	-3.510890000
H	6.643434000	-0.940130000	0.939795000	H	-3.327272000	3.847041000	-2.961185000
C	2.060360000	-3.341010000	-0.642615000	C	-0.244780000	-0.556188000	-2.502781000
H	2.149001000	-3.759826000	-1.649303000	H	-0.769633000	-1.499326000	-2.638057000
H	1.752175000	-4.125962000	0.056954000	H	0.699052000	-0.528354000	-3.048799000
C	1.003205000	-2.237477000	-0.643680000	C	-0.868212000	-1.649471000	-0.012182000
O	0.706640000	-1.652664000	-1.723376000	O	-2.061350000	-1.784816000	-0.396154000
O	0.518984000	-1.871963000	0.474194000	O	-0.155018000	-2.277437000	0.748993000
				Mg	-3.717699000	-2.758621000	-0.057479000
				Cl	-3.704669000	-4.553606000	1.294489000
				Cl	-5.295887000	-1.676919000	-1.273781000
TS₁₂₋₁₃				13			
P	-0.672755000	1.434607000	1.022571000	P	0.040215000	1.960746000	0.999256000
C	-2.394317000	1.366306000	1.722712000	C	-1.613247000	2.232923000	1.784985000
H	-2.468593000	2.250374000	2.371345000	H	-1.467991000	2.958701000	2.595101000
C	-3.517211000	1.465907000	0.672470000	C	-2.654491000	2.786423000	0.771618000
H	-3.584519000	2.463629000	0.225091000	H	-2.669509000	3.882121000	0.757254000
H	-3.355193000	0.749028000	-0.135262000	H	-2.421973000	2.446346000	-0.242994000
C	-4.768911000	1.088027000	1.479743000	C	-3.985062000	2.149920000	1.201822000
H	-5.089021000	1.950564000	2.078916000	H	-4.394059000	2.663437000	2.082195000
H	-5.602654000	0.792091000	0.836175000	H	-4.739883000	2.159883000	0.409679000
C	-4.297697000	-0.045694000	2.422411000	C	-3.546148000	0.730391000	1.576212000
H	-4.538173000	-1.044232000	2.030351000	H	-3.315791000	0.209896000	0.637189000
H	-4.807469000	-0.002146000	3.390354000	H	-4.299685000	0.173109000	2.144320000
C	-2.755942000	0.117965000	2.571692000	C	-2.233234000	0.913869000	2.357810000
H	-2.472407000	0.267439000	3.617507000	H	-2.438167000	1.038624000	3.426877000
H	-2.232810000	-0.774909000	2.220734000	H	-1.585236000	0.042908000	2.238257000
C	-0.766279000	3.078376000	0.167594000	C	0.394898000	3.573625000	0.162162000
H	-1.481450000	2.899336000	-0.646535000	H	-0.511053000	3.791829000	-0.418274000

C	0.509482000	3.636122000	-0.487513000	C	1.583329000	3.538328000	-0.818485000
H	1.335488000	3.683577000	0.228841000	H	2.452264000	3.074416000	-0.340141000
H	0.823419000	3.040350000	-1.343526000	H	1.353326000	2.955141000	-1.714738000
C	0.066853000	5.053576000	-0.879437000	C	1.871978000	5.031227000	-1.123560000
H	0.904425000	5.716423000	-1.124805000	H	2.948729000	5.219577000	-1.195313000
H	-0.579018000	4.982752000	-1.764209000	H	1.431030000	5.316600000	-2.085516000
C	-0.751145000	5.544828000	0.339134000	C	1.213293000	5.841830000	0.035748000
H	-1.561806000	6.218406000	0.041932000	H	0.358018000	6.411105000	-0.346255000
H	-0.105283000	6.100885000	1.028582000	H	1.904618000	6.559308000	0.490758000
C	-1.286542000	4.255182000	1.033016000	C	0.719208000	4.786673000	1.050180000
H	-0.893181000	4.183694000	2.054325000	H	1.527190000	4.524264000	1.745056000
H	-2.378250000	4.237534000	1.105883000	H	-0.137713000	5.126268000	1.642546000
C	0.328964000	1.661761000	2.571389000	C	1.192352000	1.873108000	2.451389000
H	-0.184260000	2.373058000	3.232571000	H	1.030404000	2.733576000	3.114400000
C	0.503764000	0.302342000	3.290437000	C	0.989390000	0.554721000	3.231362000
H	-0.376048000	0.016943000	3.870792000	H	0.118783000	0.586803000	3.892486000
H	0.653749000	-0.476843000	2.536303000	H	0.819303000	-0.255335000	2.511616000
C	1.767321000	0.454039000	4.169399000	C	2.320171000	0.313686000	3.984570000
H	1.491530000	0.643635000	5.212321000	H	2.236626000	0.627066000	5.030691000
H	2.360864000	-0.467329000	4.159337000	H	2.574349000	-0.752689000	3.989509000
C	2.556210000	1.662667000	3.590202000	C	3.394568000	1.165702000	3.247091000
H	3.594608000	1.407204000	3.347637000	H	4.258119000	0.568248000	2.930917000
H	2.592634000	2.477230000	4.322325000	H	3.775840000	1.951838000	3.908585000
C	1.778422000	2.122293000	2.336384000	C	2.673013000	1.799459000	2.037599000
H	1.859101000	3.201286000	2.177058000	H	3.087500000	2.773802000	1.757797000
H	2.166997000	1.628094000	1.440246000	H	2.758277000	1.143043000	1.162701000
P	2.463237000	-0.795416000	-0.289700000	P	2.143533000	-1.414622000	-0.461756000
C	2.899792000	-2.237445000	-1.389099000	C	1.951219000	-2.908761000	-1.543038000
C	3.930146000	-2.507085000	-1.128090000	H	2.869879000	-3.500187000	-1.432504000
C	2.018944000	-3.497296000	-1.235778000	C	0.742437000	-3.817889000	-1.233569000
H	2.312026000	-4.099252000	-0.371240000	H	0.906431000	-4.458765000	-0.363407000
H	0.968072000	-3.220815000	-1.100545000	H	-0.143826000	-3.211045000	-1.029616000
C	2.233899000	-4.240046000	-2.565010000	C	0.565758000	-4.604724000	-2.540863000
H	3.213063000	-4.738181000	-2.548313000	H	1.351577000	-5.368768000	-2.615566000
H	1.472643000	-5.004771000	-2.754302000	H	-0.403533000	-5.110478000	-2.606682000
C	2.232333000	-3.118727000	-3.619800000	C	0.759013000	-3.535578000	-3.633720000
H	1.199185000	-3.884765000	-3.902417000	H	-0.193314000	-3.024451000	-3.813426000
H	2.765202000	-3.396166000	-4.535503000	H	1.088935000	-3.960051000	-4.587689000
C	2.876519000	-1.893422000	-2.915123000	C	1.790577000	-2.528374000	-3.049237000
H	3.896580000	-1.712914000	-3.270800000	H	2.757754000	-2.585937000	-3.559860000
H	2.308234000	-0.983986000	-3.131304000	H	1.433780000	-1.498522000	-3.171829000
C	3.086646000	-1.357665000	1.383648000	C	2.675208000	-2.078768000	1.191735000
H	2.975764000	-0.479550000	2.022362000	H	2.928106000	-1.188246000	1.773984000
C	4.578971000	-1.814977000	1.374641000	C	3.884329000	-3.053139000	1.144848000
H	5.133775000	-1.479890000	0.492277000	H	4.502475000	-2.925985000	0.248510000
H	5.084407000	-1.388115000	2.250565000	H	4.529002000	-2.861568000	2.012642000
C	4.530552000	-3.345531000	1.505471000	C	3.268613000	-4.457276000	1.260614000
H	4.316075000	-3.800623000	0.530648000	H	2.901386000	-4.787516000	0.282829000
H	5.472620000	-3.768230000	1.872906000	H	3.988734000	-5.204349000	1.613021000
C	3.348977000	-3.573763000	2.458148000	C	2.091640000	-4.257438000	2.232469000
H	3.667281000	-3.355224000	3.486384000	H	2.468852000	-4.272342000	3.262864000
H	2.969306000	-4.601350000	2.440170000	H	1.332505000	-5.042867000	2.150720000
C	2.285818000	-2.548127000	2.006540000	C	1.519957000	-2.855200000	1.906306000
H	1.595704000	-2.991254000	1.289825000	H	0.624847000	-2.924420000	1.281976000
H	1.673687000	-2.212692000	2.847273000	H	1.214177000	-2.332224000	2.817412000
C	3.808495000	0.405492000	-0.838786000	C	3.682660000	-0.649113000	-1.208801000
H	4.561643000	-0.222976000	-1.326740000	H	4.163390000	-1.437134000	-1.800074000
C	3.297101000	1.448212000	-1.864952000	C	3.316802000	0.523194000	-2.155745000

H	3.301445000	1.058008000	-2.888387000	H	3.007958000	0.175075000	-3.147114000
H	2.268359000	1.723528000	-1.620025000	H	2.480945000	1.092891000	-1.728321000
C	4.204738000	2.671089000	-1.667864000	C	4.571873000	1.406728000	-2.170524000
H	5.180408000	2.501239000	-2.143381000	H	5.344340000	0.952913000	-2.806142000
H	3.776289000	3.587568000	-2.090017000	H	4.374785000	2.417615000	-2.546197000
C	4.362769000	2.723653000	-0.141284000	C	5.014515000	1.388191000	-0.698471000
H	3.444202000	3.126136000	0.301525000	H	4.386743000	2.080873000	-0.125931000
H	5.198206000	3.349922000	0.190631000	H	6.057681000	1.690608000	-0.555985000
C	4.535368000	1.245865000	0.268556000	C	4.750824000	-0.061725000	-0.224707000
H	5.597040000	0.975165000	0.269832000	H	5.663753000	-0.663417000	-0.289709000
H	4.169767000	1.060302000	1.279466000	H	4.439093000	-0.084829000	0.821506000
Ni	0.145619000	-0.324646000	-0.292973000	Ni	0.452918000	0.047402000	-0.171493000
C	-0.968573000	0.108992000	-2.574977000	C	-1.928579000	0.397149000	-2.483964000
C	-2.307325000	0.556546000	-2.551631000	C	-3.261902000	0.832329000	-2.428276000
C	0.020260000	0.995780000	-3.045132000	C	-0.909422000	1.338212000	-2.679395000
C	-2.631882000	1.844039000	-2.969521000	C	-3.566584000	2.183717000	-2.597544000
C	-0.310131000	2.283360000	-3.474900000	C	-1.216164000	2.693432000	-2.849092000
C	-1.636036000	2.717576000	-3.429058000	C	-2.546049000	3.117112000	-2.815484000
H	-3.091589000	-0.110261000	-2.212547000	H	-4.058784000	0.116717000	-2.239462000
H	1.048961000	0.659232000	-3.088585000	H	0.125920000	1.002545000	-2.715933000
H	-3.670746000	2.161604000	-2.942639000	H	-4.602838000	2.506400000	-2.550591000
H	0.470672000	2.945500000	-3.840456000	H	-0.416794000	3.412059000	-3.010661000
H	-1.895621000	3.718813000	-3.762484000	H	-2.787567000	4.168051000	-2.950469000
C	-0.595018000	-1.236284000	-2.074238000	C	-1.601083000	-1.071024000	-2.289325000
H	-1.347607000	-1.995450000	-2.273135000	H	-2.177498000	-1.694415000	-2.979783000
H	0.371903000	-1.589759000	-2.420835000	H	-0.532462000	-1.235838000	-2.451449000
C	-1.351660000	-1.567546000	-0.088309000	C	-1.949138000	-1.461083000	-0.855312000
O	-2.588926000	-1.551835000	-0.239327000	O	-3.052136000	-2.056111000	-0.672088000
O	-0.601030000	-2.141637000	0.709409000	O	-1.162562000	-1.122189000	0.072145000
Mg	-4.415179000	-2.196705000	-0.063084000	Mg	-4.481705000	-1.895074000	0.650493000
Cl	-4.801372000	-3.952556000	1.284209000	Cl	-4.274296000	-2.907042000	2.660887000
Cl	-5.657671000	-0.955216000	-1.492263000	Cl	-6.183277000	-0.770325000	-0.364140000
13a							
P	2.131140000	-0.412134000	-0.838722000				
C	2.323863000	-2.120531000	-1.552900000				
H	2.942631000	-2.007831000	-2.451404000				
C	2.994393000	-3.126461000	-0.568325000				
H	4.057765000	-3.267570000	-0.792981000				
H	2.922838000	-2.768306000	0.462154000				
C	2.159077000	-4.413936000	-0.680994000				
H	2.469752000	-5.002642000	-1.554568000				
H	2.257429000	-5.046651000	0.209216000				
C	0.740164000	-3.872870000	-0.891083000				
H	0.381996000	-3.447173000	0.054056000				
H	0.013016000	-4.613111000	-1.233498000				
C	0.942701000	-2.746604000	-1.916191000				
H	0.975635000	-3.168769000	-2.926087000				
H	0.116900000	-2.031372000	-1.906708000				
C	3.812842000	-0.098709000	-0.111529000				
H	3.913514000	-0.860192000	0.668678000				
C	4.010725000	1.303164000	0.545169000				
H	3.206598000	1.993748000	0.300983000				
H	4.019559000	1.205460000	1.636615000				
C	5.368874000	1.825743000	0.017912000				
H	5.198735000	2.480485000	-0.847915000				
H	5.917826000	2.406368000	0.767229000				
C	6.114658000	0.563583000	-0.446917000				

H	6.519389000	0.024177000	0.420680000
H	6.944934000	0.778441000	-1.129193000
C	4.995549000	-0.264109000	-1.097477000
H	4.751943000	0.171303000	-2.074939000
H	5.252805000	-1.316433000	-1.253958000
C	2.040770000	0.632344000	-2.367394000
H	2.860366000	0.364039000	-3.047012000
C	0.689725000	0.445794000	-3.091223000
H	0.643279000	-0.482174000	-3.668145000
H	-0.111737000	0.400478000	-2.343568000
C	0.522985000	1.714787000	-3.959353000
H	0.846529000	1.520445000	-4.987598000
H	-0.528627000	2.019076000	-4.005109000
C	1.422149000	2.807382000	-3.307279000
H	0.850904000	3.698369000	-3.019595000
H	2.194041000	3.137357000	-4.011535000
C	2.074682000	2.141652000	-2.074244000
H	3.085622000	2.511809000	-1.873090000
H	1.472525000	2.332782000	-1.181123000
P	-0.976883000	1.811648000	0.488526000
C	-2.446886000	1.865276000	1.631719000
H	-2.868099000	2.875505000	1.532115000
C	-3.578606000	0.849228000	1.411455000
H	-4.187769000	1.047648000	0.529704000
H	-3.166687000	-0.153897000	1.286250000
C	-4.368495000	0.940368000	2.723816000
H	-4.960470000	1.865556000	2.728042000
H	-5.058459000	0.101217000	2.859134000
C	-3.274305000	1.007456000	3.811388000
H	-3.023988000	-0.005419000	4.150470000
H	-3.594188000	1.570710000	4.694468000
C	-2.038008000	1.656794000	3.119689000
H	-1.745676000	2.602982000	3.586865000
H	-1.170870000	0.991160000	3.194950000
C	-1.626286000	2.459190000	-1.128410000
H	-0.737690000	2.598384000	-1.749292000
C	-2.422646000	3.792907000	-1.030987000
H	-2.217844000	4.356436000	-0.113267000
H	-2.136269000	4.436939000	-1.872870000
C	-3.899074000	3.385756000	-1.172104000
H	-4.281568000	3.026738000	-0.209776000
H	-4.535319000	4.218131000	-1.494038000
C	-3.855575000	2.231979000	-2.187237000
H	-3.752117000	2.645128000	-3.199593000
H	-4.745957000	1.596046000	-2.166831000
C	-2.588130000	1.433428000	-1.812692000
H	-2.860090000	0.613244000	-1.143475000
H	-2.122208000	0.979113000	-2.692466000
C	-0.018407000	3.245406000	1.236148000
H	-0.730804000	3.752108000	1.895555000
C	1.166363000	2.747257000	2.099280000
H	0.838935000	2.452850000	3.103275000
H	1.620209000	1.865129000	1.634670000
C	2.159518000	3.920573000	2.105914000
H	1.840067000	4.673218000	2.838926000
H	3.178700000	3.610494000	2.365508000
C	2.058684000	4.499372000	0.681722000
H	2.693682000	3.925659000	-0.001367000

H	2.387214000	5.543112000	0.627899000
C	0.573666000	4.332392000	0.278535000
H	0.024120000	5.268219000	0.425568000
H	0.471788000	4.084870000	-0.780587000
Ni	0.072836000	-0.209528000	0.222745000
C	0.220720000	-2.208980000	2.672773000
C	0.864622000	-3.454902000	2.691584000
C	0.994588000	-1.046255000	2.793843000
C	2.247020000	-3.537605000	2.854673000
C	2.384258000	-1.126781000	2.944678000
C	3.011671000	-2.371655000	2.985485000
H	0.272129000	-4.360825000	2.591572000
H	0.512558000	-0.074151000	2.812531000
H	2.729790000	-4.510490000	2.877039000
H	2.965148000	-0.213545000	3.038090000
H	4.088696000	-2.438200000	3.113948000
C	-1.287765000	-2.141222000	2.555694000
H	-1.756603000	-2.894056000	3.195448000
H	-1.639152000	-1.151591000	2.871002000
C	-1.814417000	-2.347221000	1.144861000
O	-2.627673000	-3.262434000	0.878962000
O	-1.468186000	-1.519558000	0.211542000
Mg	-3.028818000	-2.510965000	-1.030376000
Cl	-4.951949000	-1.282527000	-0.980590000
Cl	-2.212873000	-3.553525000	-2.874968000

Table S9. B3LYP-D/BS-I optimized Cartesian coordinates of the species involved in the one-electron reduction process.

DMF				ZnCl₂(DMF)₂			
C	-0.874811000	-0.641489000	-0.000009000	Zn	-0.000023000	0.953072000	0.126904000
O	-1.958903000	-0.081983000	-0.000013000	C	2.468138000	-0.642932000	0.110347000
H	-0.772233000	-1.745552000	0.000005000	O	1.619596000	-0.125279000	-0.645516000
N	0.343019000	-0.023589000	-0.000008000	H	2.315302000	-0.662091000	1.196820000
C	1.584714000	-0.769443000	0.000027000	N	3.601670000	-1.207282000	-0.317583000
H	2.183314000	-0.529732000	-0.890690000	C	4.548187000	-1.802355000	-0.615585000
H	2.183269000	-0.529722000	0.890772000	H	4.684198000	-2.866849000	0.385569000
H	1.370369000	-1.843544000	0.000028000	H	5.519690000	-1.298321000	0.536692000
C	0.441464000	1.425595000	-0.000007000	H	4.174182000	-1.701729000	1.638525000
O	0.983237000	1.771270000	-0.891672000	C	3.955798000	-1.248889000	-1.732344000
H	-0.569209000	1.839009000	-0.000059000	H	4.040374000	-2.292221000	-2.061875000
H	0.983145000	1.771279000	0.891711000	H	3.182912000	-0.738435000	-2.308490000
				H	4.921284000	-0.750161000	-1.882012000
				C	-2.467756000	-0.643336000	0.110210000
				O	-1.619403000	-0.125556000	-0.645775000
				H	-2.314699000	-0.662612000	1.196652000
				N	-3.601329000	-1.207753000	-0.317537000
				C	-4.547812000	-1.802615000	0.615791000
				H	-5.519107000	-1.298086000	0.537438000
				H	-4.684434000	-2.866962000	0.385476000
				H	-4.173388000	-1.702514000	1.638631000
				C	-3.955827000	-1.249105000	-1.732208000
				H	-4.920429000	-0.748658000	-1.881899000
				H	-3.182128000	-0.740229000	-2.308656000
				H	-4.042367000	-2.292395000	-2.061344000
				Cl	0.000028000	0.199702000	2.321433000
				Cl	-0.000558000	3.051854000	-0.672420000
Zn(CH₂Ph)₂(DMF)₂				Zn(CO₂CH₂Ph)₂(DMF)₂			
Zn	-0.313955000	-0.056319000	0.248435000	Zn	-0.049937000	-0.039261000	-0.550299000
C	-2.893479000	-1.634057000	0.488761000	C	-4.171072000	-1.676560000	0.178475000
O	-1.774362000	-1.541347000	1.010823000	C	-3.973335000	-1.019670000	1.402884000
H	-3.268583000	-0.861771000	-0.197327000	C	-5.375076000	-1.479241000	-0.507744000
N	-3.749942000	-2.650605000	0.699815000	C	-4.969125000	-0.199528000	1.934640000
C	-5.051249000	-2.695520000	0.055178000	C	-6.377184000	-0.664104000	0.027395000
H	-5.135752000	-3.594745000	-0.569354000	C	-6.178432000	-0.023545000	1.253164000
H	-5.849751000	-2.717901000	0.808879000	H	-3.025152000	-1.146069000	1.916339000
H	-5.182333000	-1.811221000	-0.576139000	H	-4.802850000	0.298749000	2.886539000
C	-3.407541000	-3.765228000	1.573945000	H	-7.311166000	-0.531240000	-0.513280000
H	-3.440241000	-4.704406000	1.006896000	H	-6.959019000	0.605133000	1.674891000
H	-2.402786000	-3.607764000	1.969040000	C	-3.085079000	-2.574004000	-0.394773000
H	-4.127536000	-3.826052000	2.400472000	H	-2.902831000	-3.419829000	0.277923000
C	-1.897520000	2.492238000	-0.242495000	H	-3.388178000	-2.949586000	-1.376457000
O	-2.147800000	1.282829000	-0.325543000	C	-1.803202000	-1.761742000	-0.523190000
H	-1.007899000	2.850908000	0.295268000	O	-1.038885000	-1.666266000	0.484691000
N	-2.643463000	3.477760000	-0.776267000	O	-1.599422000	-1.102665000	-1.590740000
C	-2.271869000	4.876311000	-0.628636000	C	4.286266000	1.672989000	0.199968000
H	-2.110863000	5.331937000	-1.614455000	C	4.413204000	0.937005000	1.388370000
H	-3.067789000	5.429528000	-0.112743000	C	5.367254000	1.706977000	-0.688904000
H	-1.349025000	4.955019000	-0.045962000	C	5.605955000	0.276534000	1.687367000
C	-3.847809000	3.193594000	-1.542809000	C	6.561387000	1.040578000	-0.394633000

H	-3.751817000	3.610348000	-2.553676000	C	6.687420000	0.327480000	0.799512000
H	-3.979111000	2.112041000	-1.602545000	H	3.564736000	0.886583000	2.062617000
H	-4.720233000	3.648637000	-1.055544000	H	5.697480000	-0.270880000	2.622842000
C	0.518761000	1.040789000	1.827806000	H	7.391137000	1.084018000	-1.095685000
H	-0.101885000	1.924971000	2.031356000	H	7.617286000	-0.182495000	1.038254000
H	0.529661000	0.425327000	2.735533000	C	3.017491000	2.446085000	-0.104888000
C	0.293766000	-0.748940000	-1.618455000	H	2.816591000	3.146636000	0.717012000
H	-0.506572000	-1.318525000	-2.110070000	H	3.134362000	3.021033000	-1.027262000
H	0.511186000	0.134351000	-2.234973000	C	1.791338000	1.545447000	-0.233970000
C	1.895794000	1.427033000	1.418108000	O	1.438988000	0.841049000	0.761765000
C	3.023012000	0.686350000	1.824051000	O	1.164072000	1.508206000	-1.336375000
C	2.125771000	2.500661000	0.532910000	H	5.273116000	2.269207000	-1.614991000
C	4.302666000	0.989113000	1.361572000	H	-5.529972000	-1.977632000	-1.461807000
C	3.403910000	2.808642000	0.066829000	C	-2.678070000	1.436533000	-0.560465000
C	4.506668000	2.050692000	0.474444000	O	-1.624806000	1.309155000	0.086803000
H	2.878811000	-0.154600000	2.499085000	H	-2.845025000	0.874735000	-1.486752000
H	1.276187000	3.096938000	0.197467000	N	-3.694567000	2.233208000	-0.200237000
H	5.146287000	0.386651000	1.691135000	C	-4.890634000	2.352378000	-1.017680000
H	3.540421000	3.641909000	-0.619775000	H	-5.767706000	2.040920000	-0.440542000
H	5.503158000	2.283967000	0.108752000	H	-5.019642000	3.392027000	-1.348082000
C	1.516177000	-1.580827000	-1.432497000	H	-4.803672000	1.703922000	-1.894153000
C	2.760954000	-0.984396000	-1.140134000	C	-3.671263000	2.985490000	1.044986000
C	1.470435000	-2.988017000	-1.474450000	H	-4.493486000	2.647624000	1.687813000
C	3.897465000	-1.756200000	-0.908699000	H	-2.716727000	2.811074000	1.544083000
C	2.607999000	-3.763518000	-1.238094000	H	-3.792828000	4.056404000	0.836627000
C	3.833402000	-3.153924000	-0.955568000	C	2.071065000	-1.942568000	-0.095162000
H	2.826317000	0.098960000	-1.067821000	O	1.541581000	-1.417217000	-1.088959000
H	0.522863000	-3.473780000	-1.704502000	H	1.477603000	-2.195515000	0.794307000
H	4.835744000	-1.257638000	-0.676568000	N	3.372511000	-2.247721000	-0.005645000
H	2.536935000	-4.848963000	-1.281411000	C	3.930758000	-2.862598000	1.185688000
H	4.720512000	-3.755264000	-0.771769000	H	4.388234000	-3.829864000	0.936859000
				H	4.696970000	-2.205212000	1.612468000
				H	3.139677000	-3.021709000	1.925179000
				C	4.311834000	-1.890728000	-1.062815000
				H	4.795574000	-2.797293000	-1.450334000
				H	3.763903000	-1.392623000	-1.863616000
				H	5.072874000	-1.216058000	-0.657497000
MgCl₂(DMF)₄				Mg(CO₂CH₂Ph)₂(DMF)₄			
Mg	0.326190000	0.022871000	0.194892000	Mg	0.637895000	-1.223783000	0.518871000
Cl	0.311174000	-0.741618000	2.559688000	C	-3.443470000	0.948394000	-0.932968000
Cl	0.056392000	0.645564000	-2.257786000	C	-4.840808000	0.994601000	-1.031390000
C	2.284062000	-2.137089000	0.256349000	C	-2.829921000	1.568923000	0.170451000
O	2.084854000	-1.025180000	-0.257285000	C	-5.612850000	1.651976000	-0.067868000
H	1.676565000	-2.482272000	1.101322000	C	-3.598130000	2.237709000	1.123973000
N	3.236861000	-2.992540000	-0.154605000	C	-4.993005000	2.284650000	1.011854000
C	3.448699000	-4.262150000	0.518449000	H	-5.325336000	0.512280000	-1.877355000
H	3.317047000	-5.093387000	-0.187382000	H	-6.695384000	1.675848000	-0.167163000
H	4.466130000	-4.311563000	0.929895000	H	-3.106270000	2.721052000	1.965113000
H	2.730287000	-4.369155000	1.336575000	H	-5.587272000	2.808773000	1.756387000
C	4.109625000	-2.683769000	-1.278097000	C	-2.624908000	0.243581000	-1.995228000
H	4.059877000	-3.495586000	-2.015171000	H	-3.282843000	-0.157213000	-2.772051000
H	3.777636000	-1.750511000	-1.735993000	H	-1.936509000	0.965037000	-2.457378000
H	5.148392000	-2.582847000	-0.934770000	C	-1.763218000	-0.903935000	-1.417159000
C	-2.444438000	1.242749000	-0.230329000	O	-2.007561000	-2.074150000	-1.760660000
O	-1.545778000	0.967353000	0.573466000	O	-0.870937000	-0.509999000	-0.595396000
H	-2.248738000	1.273922000	-1.309938000	C	1.931216000	2.485215000	-2.060500000

N	-3.715429000	1.503134000	0.137149000	C	0.585770000	2.270878000	-1.715491000
C	-4.727102000	1.848249000	-0.845399000	C	2.371012000	3.797801000	-2.273340000
H	-5.562930000	1.136189000	-0.797715000	C	-0.294730000	3.349814000	-1.607936000
H	-5.120047000	2.856410000	-0.656496000	C	1.491137000	4.879281000	-2.160753000
H	-4.291003000	1.818658000	-1.848606000	C	0.152388000	4.658323000	-1.828415000
C	-4.116874000	1.503262000	1.537908000	H	0.237672000	1.261578000	-1.516382000
H	-4.950176000	0.803519000	1.684261000	H	-1.334005000	3.164818000	-1.347571000
H	-3.264377000	1.199352000	2.148659000	H	1.852351000	5.890376000	-2.333817000
H	-4.446532000	2.507785000	1.834212000	H	-0.537717000	5.494656000	-1.746637000
C	2.135920000	2.320234000	-0.269400000	C	2.894627000	1.318737000	-2.179878000
O	1.431655000	1.739927000	0.570239000	H	2.553134000	0.635307000	-2.966733000
H	2.070165000	2.066516000	-1.334995000	H	3.894250000	1.687868000	-2.431103000
N	3.011742000	3.293396000	0.038030000	C	2.952394000	0.544251000	-0.848121000
C	3.791529000	3.958050000	-0.991423000	O	2.012358000	-0.300343000	-0.677839000
H	3.568676000	5.033693000	-1.004266000	O	3.847750000	0.837360000	-0.026213000
H	4.865202000	3.827824000	-0.799282000	H	3.413688000	3.970665000	-2.530660000
H	3.548835000	3.533105000	-1.970029000	H	-1.755095000	1.492471000	0.281306000
C	3.210533000	3.735913000	1.411696000	C	-0.126700000	-3.734547000	-0.755638000
H	2.930706000	4.793539000	1.508771000	O	0.860020000	-3.005986000	-0.546015000
H	2.591406000	3.126211000	2.072105000	H	-0.912270000	-3.846941000	-0.002820000
H	4.267791000	3.625152000	1.685934000	N	-0.291649000	-4.476731000	-1.860581000
C	-1.883355000	-1.868661000	0.293204000	C	-1.599406000	-5.056241000	-2.133528000
O	-0.785524000	-1.773579000	-0.271047000	H	-2.190066000	-4.365591000	-2.746761000
H	-1.955974000	-1.968085000	1.385781000	H	-1.474665000	-6.015602000	-2.649254000
N	-3.060784000	-1.818927000	-0.357722000	H	-2.129323000	-5.223059000	-1.190961000
C	-4.323684000	-1.922503000	0.348636000	C	0.542426000	-4.215781000	-3.026286000
H	-4.902480000	-0.998797000	0.213547000	H	0.076420000	-3.433354000	-3.641308000
H	-4.914058000	-2.765543000	-0.034473000	H	1.524521000	-3.873685000	-2.696535000
H	-4.138085000	-2.071737000	1.416842000	H	0.640066000	-5.135712000	-3.613497000
C	-3.113796000	-1.570287000	-1.795289000	C	1.280217000	1.324339000	1.661725000
H	-3.834670000	-0.765150000	-1.987746000	O	0.363047000	0.487456000	1.796484000
H	-2.123120000	-1.265026000	-2.144097000	H	2.312761000	1.010563000	1.482306000
H	-3.444534000	-2.471343000	-2.328770000	N	1.107631000	2.650680000	1.698834000
				C	2.191238000	3.548661000	1.310215000
				H	1.868255000	4.144662000	0.449209000
				H	2.448686000	4.218362000	2.142105000
				H	3.061702000	2.957331000	1.011716000
				C	-0.203258000	3.246696000	1.904008000
				H	-0.564067000	3.682101000	0.965113000
				H	-0.895466000	2.471937000	2.236439000
				H	-0.128833000	4.035568000	2.663465000
				C	3.272192000	-2.044782000	1.160296000
				O	2.237009000	-1.791239000	1.804362000
				H	3.226495000	-2.627419000	0.231623000
				N	4.504262000	-1.667975000	1.519756000
				C	5.602518000	-1.761253000	0.568115000
				H	5.762365000	-0.778938000	0.107689000
				H	6.513072000	-2.090641000	1.083169000
				H	5.351971000	-2.486867000	-0.212226000
				C	4.692636000	-0.725430000	2.614785000
				H	5.625642000	-0.963728000	3.138619000
				H	4.739152000	0.287259000	2.197051000
				H	3.848229000	-0.805359000	3.301536000
				C	-1.612778000	-1.502165000	2.427103000
				O	-0.840088000	-2.174782000	1.725448000
				H	-1.239713000	-0.918037000	3.279425000
				N	-2.934225000	-1.405004000	2.240872000
				C	-3.774154000	-0.628658000	3.139399000

	H	-4.280559000	0.164020000	2.577843000
	H	-4.526186000	-1.278779000	3.606754000
	H	-3.157918000	-0.176231000	3.922939000
	C	-3.600470000	-2.011995000	1.093772000
	H	-4.132777000	-1.229553000	0.541003000
	H	-2.860061000	-2.460823000	0.432744000
	H	-4.319551000	-2.767155000	1.439481000