

Supporting Information

Crucial Role of Ni(I) Intermediate in Ni-Catalyzed Carboxylation of Aryl Chloride with CO₂: A Theoretical Study

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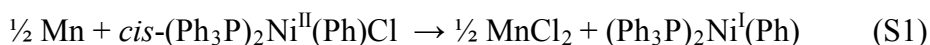
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Computational Details

All the calculations were carried out with Gaussian 09 package.¹ Dispersion corrected B3LYP-D functional² was used for all the calculations. Geometry optimizations and frequency calculations were performed with basis set system BS-I. In BS-I, we employed Lanl2Tz(f)³ for Ni and Mn, 6-31G(d) basis sets for C, H, P, and O, and 6-31+G(d) for Cl. All stationary structures were confirmed to be minima on the potential energy surface wherein no imaginary frequency was observed. The transition state (TS) was characterized with a single imaginary frequency. Intrinsic reaction coordinate (IRC)⁴ calculations were performed on all transition structures to ensure that TS connects corresponding reactant and product. Conductor-like polarizable continuum model (CPCM)⁵ was employed to consider solvent effects. 1,3-Dimethyl-2-imidazolidinone (DMI) solvent was used for all the structures. Since the data for this solvent were not internally provided in Gaussian 09, we used EPS, V_{mol} , R_{solv} and density parameters of DMI in conjunction with (CPCM, read) keyword for the estimation of electronic energy in the solvent (E_{sol}). E_{sol} was calculated with better basis set system, BS-II. In BS-II, basis sets and effective core potentials proposed by Stuttgart group were used for Ni and Mn, 6-311G(d) basis sets for C, H, P, and O, and 6-311+G(d) basis set for Cl. In calculating the Gibbs energy in solution, translational entropy corrections have been incorporated with Whitesides method;⁶ see Ref. 7 for details about this procedure. The total Gibbs energy was evaluated by incorporating E_{sol} , and thermal energies from the frequency calculations. NBO population analysis was carried out with the method of Weinhold et al. at B3LYP-D/BS-I level of theory.⁸

cis-trans* Isomerization of *cis*-NiCl(Ph)(PPh₃)₂ **4*

The *cis-trans* isomerization process from **4** to **5** is not an important event for the one-electron reduction, because one-electron reduction of **4** also affords **6**. In the Eq. S1, the one electron reduction process for **4** was shown. The Gibbs energy change (ΔG_{SI}°) for the one electron reduction of **4** is evaluated to be -24.8 kcal/mol while it is -21.1 kcal/mol for **5**. These results indicate that both of **4** and **5** undergo one-electron reduction easily.



However, we examined the *cis-trans* isomerization for the complex *cis*-NiCl(Ph)(PPh₃)₂ **4**. In the associative mechanism, solvent molecule DMI does not coordinate with the Ni centre. In Fig. S1, we have shown two possible geometries before and after geometry optimization. In Fig. S1(a), two PPh₃ groups are in *cis*-position, while in Fig. S1(b) they are *trans* to each other. In both the cases, we found that DMI does not coordinate to Ni-centre and hence the associative isomerization via Berry pseudo-rotation mechanism can be ruled out here. On the other hand, in the case of dissociative mechanism, one of the PPh₃ ligands dissociates to form a monophosphine Ni(II) intermediate Ni(PPh₃)(Ph)Cl **4A**, as shown in Fig. S2. From **4A**, *cis-trans* isomerization occurs to afford **4B**. Due to the flat potential energy surface around the transition state we were unable to locate a transition state between **4A** and **4B** but the potential surface shown in Fig. S3 indicates well that this isomerization easily occurs in both gas phase and solution phase. In the solution phase, the activation energy is about 1.5 kcal/mol, while it is barrier-less in the gas phase. Hence, the total activation barrier in the solution phase corresponds to the sum of the energy destabilization (15.1 kcal/mol) by PPh₃ dissociation and the energy barrier of 1.5

kcal/mol in the solution, which is about 16.6 kcal/mol. This result indicates that the isomerization is not a difficult process.

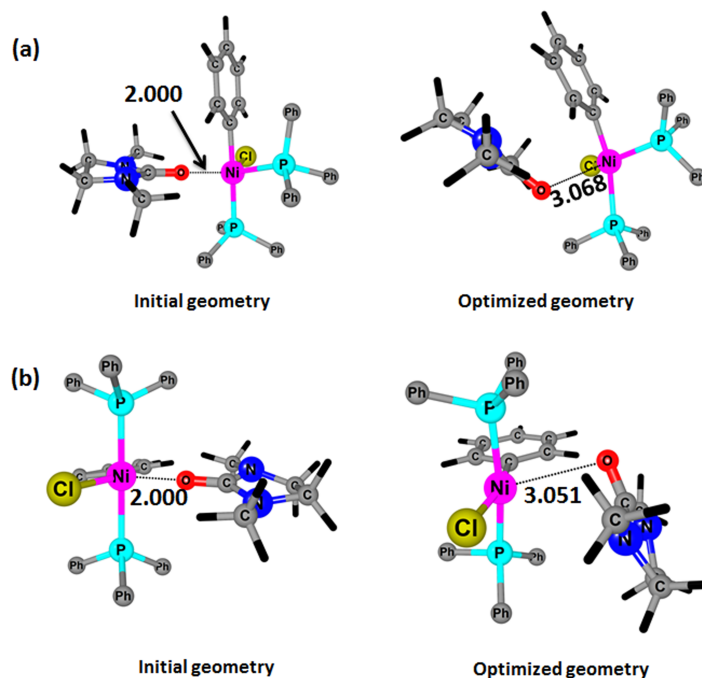


Fig. S1 Initial and optimized geometries of the complexes between DMI and **4** and **5**. (a) DMI interaction with **4** (b) DMI interaction with **5**. Bond lengths are in angstroms. Ph on the phosphine ligand represents the phenyl ring.

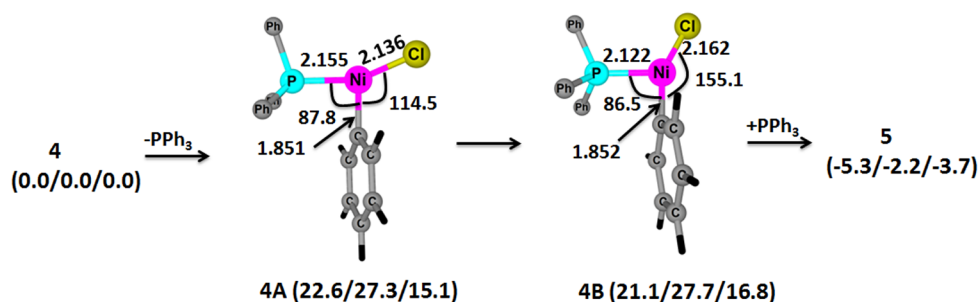


Fig. S2 Dissociative pathway for *cis-trans* isomerism between **4** and **5**. The values in the parentheses represent gas phase, solution phase and Gibbs energy in solution, respectively. Bond lengths are in angstroms and angles are in degrees. Ph on the phosphine ligand represents the phenyl ring. Note that the solvent effect somewhat changes the energy changes.

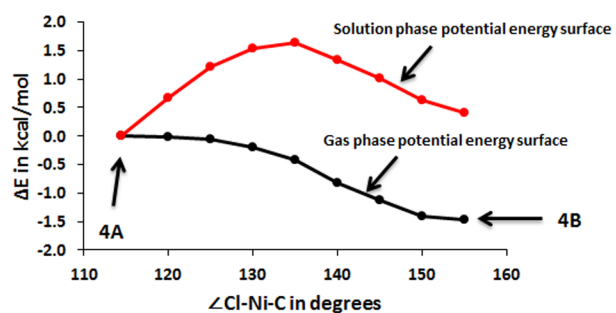


Fig. S3 Potential energy surface for the transformation of **4A** to **4B** (see Fig. S2 for $\angle\text{Cl-Ni-C}$).

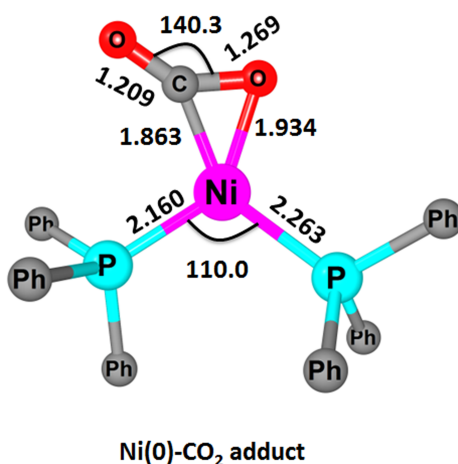


Fig. S4 Optimized structure of Ni(0)(PPh₃)₂(CO₂). Bondlengths are in angstroms and angles are degrees. Ph on the phosphine represents the phenyl ring.

Table S1. Population changes by coordination of CO₂ to (PPh₃)₂Ni(0) and Ni(I)(Ph)(PPh₃)₂.^{a, b}

	(PPh ₃) ₂ Ni ⁽⁰⁾ (CO ₂)	Ni ^(I) (Ph)(PPh ₃) ₂ (CO ₂)
CO ₂	0.4338	0.2954
Ni	0.0067	0.1165
Ni(3d)	-0.2874	-0.1514
C ₆ H ₅	-	-0.2696

^a Positive value indicate increase in population. ^b Change in population is calculated as the difference in the population of a particular group of the complex and the corresponding individual moiety.

Conformational change of **8** to **9**

The isomerization of **8** to **9** is the transformation of η^1 -O-coordinate $\text{Ni}^{\text{I}}(\text{PPh}_3)_2(\eta^1\text{-OCOPh})$ **8** to η^2 -coordinate $\text{Ni}^{\text{I}}(\text{PPh}_3)_2(\eta^1\text{-OCOPh})$ **9**. This conformational change is not important very much for this catalytic reaction because **8** can undergo one-electron reduction to afford a final product.

However, we investigated this conformational change. Shown in Fig. S5 is the potential energy surface obtained by varying the Ni-O-C angle (see Fig. 2), which suggests a smooth surface around the transition state and activation barrier is about 4kcal/mol. Our attempts to find a transition state between **8** and **9** are unsuccessful probably due to the flat energy surface. This value suggests that the conformation change easily occurs.

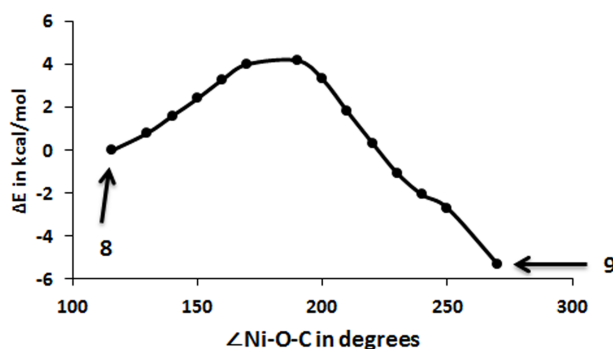


Fig. S5 Potential energy surface for the conformational change of **8** to **9** (see Fig. 2 for $\angle\text{Ni-O-C}$).

cis-trans Isomerization of **10**

This isomerization is not important in the catalytic reaction because **10** is not formed from **5** due to the very large activation energy; see Fig. 3 (b). However, we investigated the isomerization of **10**, as follows:

Similar to the *cis-trans* isomerism between **4** and **5**, the products after the CO₂ insertion reaction of **5**, complexes **10** and **11** can also exhibit *cis-trans* isomerism. All the structures of **10**, **11** and **12** are shown in Fig. S6. Initially one of the phosphine ligands dissociates from **10** to form a three coordinate Ni(II) intermediate **10A**, as shown in Fig. S7. The destabilization energy for the phosphine dissociation is 27.8 kcal/mol. **10A** isomerizes to a three-coordinate *trans*-form **10B** without transition state; see Fig. S8. Further, PPh₃ coordination leads to a product **11** which on conformational change produces **12**. But, we did not investigate this transition state because the conformation change easily occurs. A total activation barrier corresponds to the energy destabilization by the PPh₃ dissociation, which is about 28 kcal/mol; see Fig. S7.

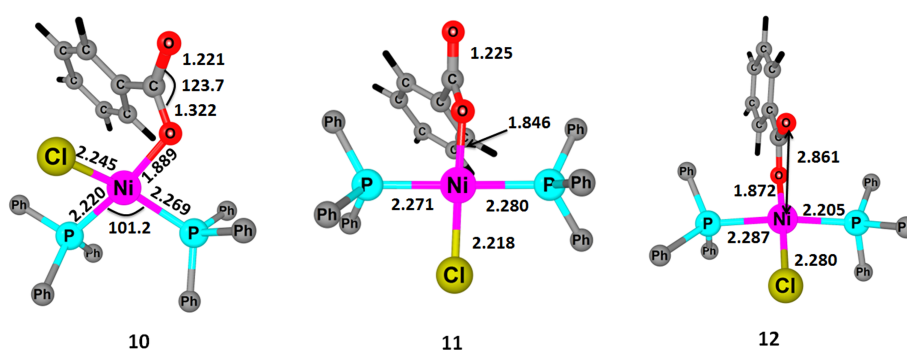


Fig. S6 Optimized structure of **10**, **11** and **12**. Bondlengths are in angstroms and angles are degrees. Ph on the phosphine ligand represents the phenyl ring.

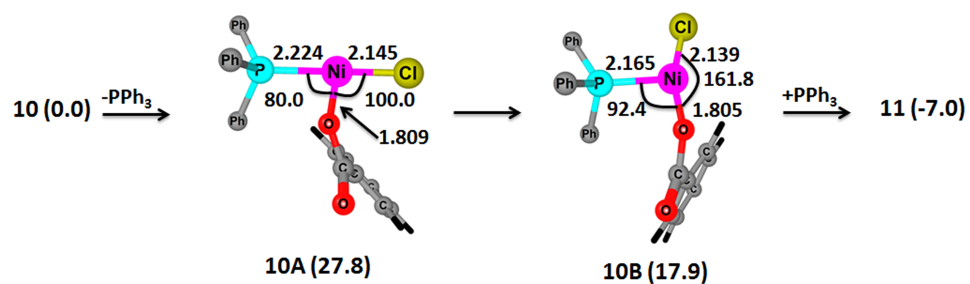


Fig. S7 Dissociative pathway for *cis-trans* isomerism between **10** and **11**. Bond lengths are in angstroms and angles are in degrees. Ph on the phosphine ligand represents the phenyl ring.

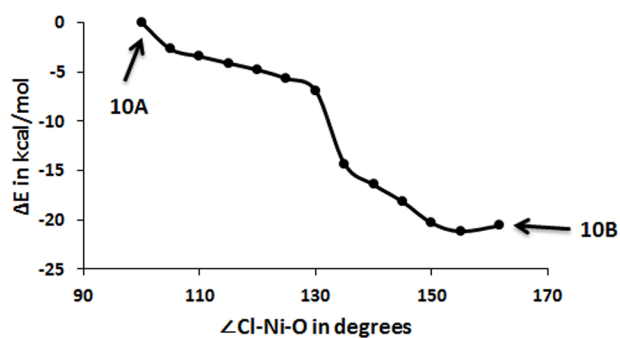


Fig. S8 Potential energy surface for the transformation of **10A** to **10B**.

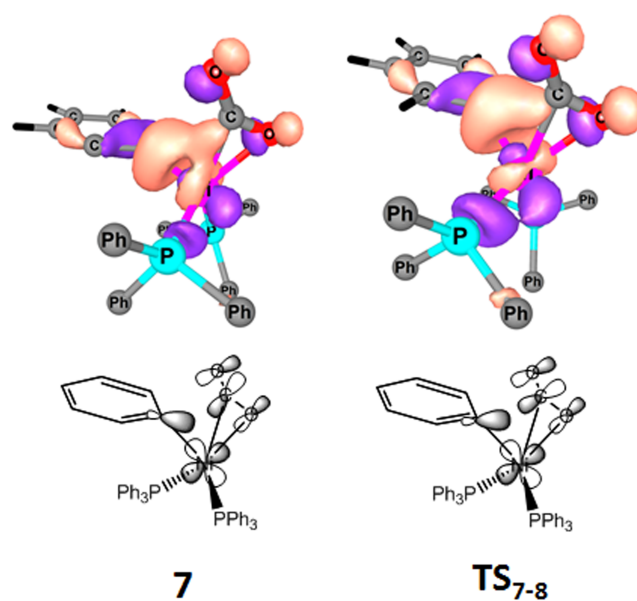


Fig. S9 Molecular orbital diagrams of **7** and **TS₇₋₈** showing the charge transfer to CO₂ from Ni and phenyl groups.

In **7**, the carbon sp² orbital mainly participates in the bonding with the Ni(I) center. In **TS₇₋₈**, the *p*-orbital somewhat mixes into the sp²-orbital. The mixing is necessary to change the sp² direction toward the carbon of CO₂.

Table S2. Ni(I)–Ph, Ni(II)–Ph, Ni(I)–O, Ni(II)–O, Mn–Ph and Mn–O bond dissociation energies, BDE (in kcal/mol).^a

Bond type	Reaction ^b	BDE
Ni(I)–Ph	$L_2Ni(I)–Ph \rightarrow NiL_2 + Ph^\bullet$	63.3
Ni(II)–Ph	$ClL_2Ni(II)–Ph \rightarrow ClNi(I)L_2 + Ph^\bullet$	54.5
Ni(I)–O ^c	$L_2Ni(I)–(\eta^2-O_2CCPh) \rightarrow NiL_2 + PhCOO^\bullet$	99.7
Ni(II)–O ^d	$ClL_2Ni(II)–\eta^1-OCOPh \rightarrow ClNi(I)L_2 + PhCOO^\bullet$	67.7
Mn–Ph	$MnPh_2 \rightarrow Mn + 2Ph^\bullet$	54.2 ^e
Mn–O ^f	$Mn(\eta^2-O_2CPh)_2 \rightarrow Mn + 2PhCOO^\bullet$	92.5 ^e

^aCalculated at B3LYP-D/BS-II level. ^bL represents PPh₃. ^cNi(I)–O represent the (PPh₃)₂Ni(I)–(η²-O₂CCPh). ^d Ni(II)–O represent (PPh₃)₂Ni–(η¹-OCOPh)(Cl). ^e Since two Mn–Ph bonds are broken in MnPh₂, average BDE is reported. ^f Mn–O represent Mn–(η²-O₂CCPh).

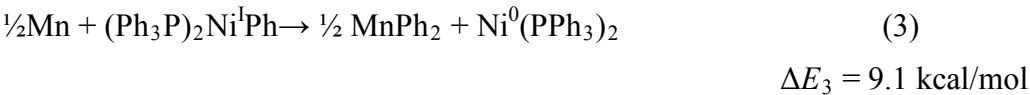
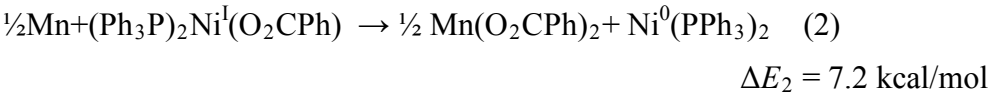


Table S3a. Population changes in the CO₂ insertion of Ni(I)(Ph)(PPh₃)₂.^a

	7	TS ₇₋₈	8	9
CO ₂ ^b	0.2954	0.3087	0.6198	0.6024
Ni(3d) ^c	-0.1514	-0.1052	-0.0666	-0.0569
Ni ^c	0.1165	0.1108	-0.1546	-0.0877
C ₆ H ₅ ^c	-0.2696	-0.2478	-0.4591	-0.5134

^a Positive value indicate increase in population. ^b Population change is relative to CO₂.
^c Population change is relative to **6**.

Table S3b. Population changes in the CO₂ insertion of Ni(II)(Ph)(Cl)(PPh₃)₂.^a

	TS ₅₋₁₀	10	11	12
CO ₂ ^b	0.1205	0.4799	0.4894	0.5178
Ni(3d) ^c	-0.2111	-0.1693	-0.1745	-0.1884
Ni ^c	-0.0416	-0.1563	-0.2155	-0.2177
C ₆ H ₅ ^c	-0.1324	-0.2165	-0.1989	-0.2366

^a Positive value indicate increase in population.

^b Population change is relative to CO₂.

^c Population change is relative to **5**.

Table S4. SCE energies in DMI (E_{sol}), thermal energies (E_{T}), entropy (S_{corr}) and Gibbs free energy (G_{sol}) for all the species involved in the catalytical cycle.

	E_{sol} (au)	E_{T} (au)	S_{corr} ^a (Cal/Mol-Kelvin)	G_{sol} (au)
CO₂	-188.643519	0.014238	22.244762	-188.638906
1	-2244.024373	0.585988	197.035828	-2243.531059
2	-691.934816	0.096432	47.357838	-691.859941
3	-2936.001484	0.684535	225.210419	-2935.423009
TS₃₋₄	-2935.989924	0.683482	226.542419	-2935.413135
4	-2936.048720	0.686300	219.853424	-2935.465935
5	-2936.052190	0.686141	224.538422	-2935.471790
6	-2475.747544	0.681653	229.491348	-2475.173985
7	-2664.398407	0.698369	235.395920	-2663.810938
TS₇₋₈	-2664.397351	0.697178	230.524918	-2663.808759
8	-2664.452505	0.700437	228.305923	-2663.859599
9	-2664.452996	0.700230	236.706924	-2663.864289
TS₅₋₁₀	-3124.652714	0.702072	232.362610	-3124.060100
10	-3124.716058	0.705068	229.685577	-3124.119177
11	-3124.721244	0.704130	240.216583	-3124.130304
12	-3124.721459	0.704341	244.893585	-3124.132530

^a Total entropy after translation entropy correction. Molar volume of DMI was calculated at B3LYP-D/BS-II method.

Table S5. Cartesian coordinates of optimized structures.

1				2			
P	1.941696000	0.036606000	-0.588665000	C	-0.178370000	-1.217707000	0.000025000
P	-1.937151000	0.013302000	-0.610204000	C	0.503452000	-0.000463000	-0.000218000
Ni	0.014977000	0.003638000	-1.424802000	C	-1.575789000	-1.208444000	0.000034000
C	-2.480797000	-1.628750000	0.030974000	C	-0.178474000	1.217620000	0.000099000
C	-1.477782000	-2.501389000	0.486422000	C	-2.276568000	0.000027000	0.000005000
C	-3.823948000	-2.019689000	0.127539000	C	-1.575321000	1.209058000	-0.000054000
C	-1.815004000	-3.735395000	1.042196000	H	-2.113625000	-2.152643000	0.000027000
C	-4.158311000	-3.263030000	0.672810000	H	0.374962000	2.151188000	0.000207000
C	-3.156295000	-4.120699000	1.134067000	H	-3.362829000	-0.000499000	0.000034000
H	-0.436741000	-2.204804000	0.413662000	H	-2.113026000	2.153212000	-0.000023000
H	-4.607498000	-1.353178000	-0.220439000	Cl	2.266309000	0.000018000	0.000018000
H	-1.026264000	-4.390209000	1.402552000	H	0.373684000	-2.152103000	0.000112000
H	-5.202498000	-3.558805000	0.739280000				
H	-3.419631000	-5.085279000	1.561092000				
C	-3.481577000	0.695966000	-1.350477000				
C	-3.677753000	0.535670000	-2.730285000				
C	-4.466281000	1.345802000	-0.590760000				
C	-4.844805000	1.001237000	-3.339283000				
C	-5.630375000	1.818969000	-1.200951000				
C	-5.822677000	1.644466000	-2.574730000				
H	-2.906093000	0.048376000	-3.322668000				
H	-4.315876000	1.481242000	0.476850000				
H	-4.987480000	0.870186000	-4.408945000				
H	-6.386815000	2.323591000	-0.604958000				
H	-6.728326000	2.014286000	-3.048712000				
C	3.499903000	-0.566534000	-1.373357000				
C	4.780194000	-0.200583000	-0.931963000				
C	3.375765000	-1.463246000	-2.444925000				
C	5.915613000	-0.727297000	-1.549931000				
C	4.511948000	-2.000309000	-3.055975000				
C	5.783383000	-1.630928000	-2.609530000				
H	4.885496000	0.503079000	-0.111129000				
H	2.381088000	-1.731745000	-2.795169000				
H	6.904170000	-0.434044000	-1.205284000				
H	4.404547000	-2.696903000	-3.883574000				
H	6.669052000	-2.040248000	-3.088781000				
C	1.828297000	-1.024943000	0.918764000				
C	2.299558000	-2.346049000	0.909185000				
C	1.082208000	-0.575033000	2.022296000				
C	2.022240000	-3.203925000	1.977604000				
C	0.814144000	-1.430842000	3.089610000				
C	1.277429000	-2.750278000	3.069397000				
H	2.875999000	-2.706289000	0.061754000				
H	0.697486000	0.438257000	2.039567000				
H	2.392061000	-4.226193000	1.956067000				
H	0.226319000	-1.066061000	3.927407000				
H	1.058445000	-3.419689000	3.897302000				
C	2.405299000	1.682593000	0.094699000				
C	2.016450000	2.819800000	-0.629724000				
C	3.078238000	1.851219000	1.313722000				
C	2.297902000	4.100290000	-0.150449000				
C	3.355152000	3.131960000	1.798705000				
C	2.965813000	4.258289000	1.068284000				
H	1.467664000	2.687970000	-1.559591000				
H	3.361269000	0.978245000	1.894252000				
H	1.988236000	4.972483000	-0.720534000				
H	3.870829000	3.250076000	2.748416000				
H	3.178485000	5.254346000	1.448194000				

C	-1.746433000	0.990290000	0.948035000	
C	-2.205769000	0.548032000	2.195670000	
C	-0.972394000	2.160695000	0.883506000	
C	-1.880687000	1.255521000	3.357971000	
C	-0.642711000	2.864484000	2.040722000	
C	-1.092365000	2.406925000	3.284952000	
H	-2.789738000	-0.364961000	2.261655000	
H	-0.578983000	2.484129000	-0.074709000	
H	-2.233592000	0.897621000	4.322260000	
H	-0.007223000	3.743059000	1.970305000	
H	-0.823339000	2.941235000	4.192633000	
3				TS₃₋₄
Ni	-0.016130000	-0.987207000	-0.437611000	P 1.636906000 -0.476943000 0.113918000
C	-0.761681000	-2.667371000	-1.191203000	P -1.814559000 0.095895000 -0.148135000
C	0.632247000	-2.835977000	-0.837933000	Ni 0.166444000 0.884312000 -0.769003000
C	-1.783223000	-3.326139000	-0.425813000	C 1.190636000 2.272649000 -1.386977000
C	0.917916000	-3.553670000	0.377413000	C -0.015399000 3.015249000 -1.343401000
C	-1.452925000	-3.968111000	0.741341000	C 2.425913000 2.844299000 -1.027530000
C	-0.089865000	-4.065513000	1.159630000	C 0.002110000 4.274192000 -0.698321000
H	1.410686000	-2.770439000	-1.595581000	C 2.406621000 4.091541000 -0.420122000
H	1.959609000	-3.695465000	0.652034000	C 1.196808000 4.798728000 -0.227757000
H	-2.234978000	-4.417565000	1.347916000	H -0.891435000 2.714619000 -1.911374000
H	0.151138000	-4.600074000	2.075168000	H -0.916346000 4.853116000 -0.638621000
Cl	-1.152026000	-2.336599000	-2.931175000	H 3.341141000 4.520315000 -0.064860000
H	-2.809042000	-3.273671000	-0.774512000	H 1.216002000 5.778772000 0.241545000
C	-1.237379000	2.128365000	-0.084984000	Cl 1.101465000 0.943622000 -3.230450000
C	-1.402314000	3.022249000	0.980299000	H 3.348182000 2.289474000 -1.150181000
C	-0.590009000	2.577113000	-1.248987000	C -1.911401000 -1.164310000 1.190401000
C	-0.949012000	4.339283000	0.873403000	C -2.106792000 -0.786921000 2.526235000
C	-0.152603000	3.896399000	-1.362427000	C -1.704739000 -2.519741000 0.887712000
C	-0.333689000	4.783620000	-0.298372000	C -2.104045000 -1.747983000 3.537981000
H	-1.858061000	2.687121000	1.904868000	C -1.701219000 -3.478289000 1.901812000
H	-0.408206000	1.883410000	-2.063412000	C -1.904258000 -3.095273000 3.229994000
H	-1.067683000	5.015112000	1.716030000	H -2.258181000 0.257738000 2.777113000
H	0.345433000	4.221583000	-2.272152000	H -1.551374000 -2.828552000 -0.139862000
H	0.018413000	5.809117000	-0.375394000	H -2.251553000 -1.439603000 4.569190000
P	-1.687680000	0.344064000	-0.034261000	H -1.541134000 -4.523437000 1.649947000
C	-3.231557000	0.257481000	-1.039346000	H -1.903044000 -3.841663000 4.020283000
C	-3.481558000	1.117741000	-2.117410000	C -2.791421000 -0.656334000 -1.502844000
C	-4.139677000	-0.782299000	-0.776426000	C -3.898278000 -1.490654000 -1.275799000
C	-4.612120000	0.938521000	-2.918765000	C -2.398094000 -0.371639000 -2.819458000
C	-5.268307000	-0.958810000	-1.576542000	C -4.610872000 -2.019714000 -2.352775000
C	-5.507070000	-0.100316000	-2.653949000	C -3.114434000 -0.903167000 -3.895489000
H	-2.801413000	1.936549000	-2.328243000	C -4.220661000 -1.724197000 -3.663711000
H	-3.963051000	-1.449891000	0.061053000	H -4.186751000 -1.734940000 -0.257541000
H	-4.794266000	1.617068000	-3.748393000	H -1.521025000 0.245970000 -2.999162000
H	-5.962612000	-1.766146000	-1.357452000	H -5.466699000 -2.664728000 -2.170747000
H	-6.385822000	-0.237969000	-3.278462000	H -2.799132000 -0.681237000 -4.911384000
C	-2.338102000	0.032568000	1.654820000	H -4.774503000 -2.140947000 -4.501073000
C	-1.735550000	-0.975705000	2.421040000	C -2.855638000 1.460617000 0.509531000
C	-3.442954000	0.723175000	2.178125000	C -2.201738000 2.481705000 1.217400000
C	-2.205026000	-1.262445000	3.705855000	C -4.246337000 1.519243000 0.345064000
C	-3.908352000	0.441078000	3.463200000	C -2.931053000 3.537008000 1.767824000
C	-3.285351000	-0.549371000	4.230861000	C -4.972518000 2.583927000 0.884088000
H	-0.914149000	-1.548197000	1.997660000	C -4.317915000 3.590693000 1.599526000
H	-3.938649000	1.476905000	1.572684000	H -1.120481000 2.453365000 1.312892000
H	-1.733096000	-2.049168000	4.288831000	H -4.758012000 0.740772000 -0.212672000
H	-4.759470000	0.986202000	3.863184000	H -2.415037000 4.322855000 2.313391000
C	-3.651383000	-0.771888000	5.230000000	H -6.049568000 2.627407000 0.744181000
H	1.758466000	1.395578000	1.257932000	H -4.885701000 4.417986000 2.017412000
C	2.264426000	2.690076000	1.087828000	C 3.424241000 -0.115014000 -0.061745000

C	1.075249000	1.086055000	2.446854000	C	3.995069000	-0.278231000	-1.336187000
C	2.116836000	3.643049000	2.098799000	C	4.188681000	0.454131000	0.965427000
C	0.942529000	2.032528000	3.462190000	C	5.309332000	0.122967000	-1.573396000
C	1.468964000	3.315716000	3.291401000	C	5.505259000	0.855878000	0.722831000
H	2.753114000	2.964860000	0.159998000	C	6.067547000	0.694627000	-0.545393000
H	0.624762000	0.106010000	2.567545000	H	3.399280000	-0.688225000	-2.146161000
H	2.503690000	4.647447000	1.947365000	H	3.756178000	0.589221000	1.951760000
H	0.411125000	1.771905000	4.373831000	H	5.737401000	-0.000238000	-2.564634000
H	1.358917000	4.060743000	4.075247000	H	6.090049000	1.295137000	1.527190000
P	1.836119000	0.059789000	-0.002314000	H	7.089529000	1.013056000	-0.733851000
C	3.185453000	-1.042517000	0.593099000	C	1.362565000	-0.508826000	1.927864000
C	3.427384000	-1.261393000	1.956194000	C	1.157787000	0.747365000	2.527716000
C	3.854761000	-1.840677000	-0.350823000	C	1.317438000	-1.659031000	2.722709000
C	4.312271000	-2.261717000	2.367450000	C	0.953557000	0.850587000	3.903569000
C	4.738866000	-2.837665000	0.060744000	C	1.097826000	-1.554034000	4.098522000
C	4.966171000	-3.056947000	1.423541000	C	0.927100000	-0.303068000	4.693502000
H	2.928294000	-0.648081000	2.699719000	H	1.157417000	1.639542000	1.904524000
H	3.679620000	-1.680912000	-1.410991000	H	1.424732000	-2.637810000	2.269912000
H	4.491073000	-2.416867000	3.428541000	H	0.806656000	1.827830000	4.356598000
H	5.248048000	-3.446051000	-0.682411000	H	1.050054000	-2.455676000	4.703036000
H	5.650694000	-3.837420000	1.744993000	H	0.759458000	-0.226685000	5.764787000
C	2.582383000	0.797041000	-1.506231000	C	1.530651000	-2.200255000	-0.497669000
C	1.873263000	0.681977000	-2.711150000	C	2.358342000	-3.228629000	-0.019812000
C	3.848548000	1.403723000	-1.511812000	C	0.617250000	-2.475233000	-1.524785000
C	2.404727000	1.195440000	-3.897215000	C	2.235969000	-4.523304000	-0.526146000
C	4.377155000	1.922313000	-2.694792000	C	0.501155000	-3.769352000	-2.038710000
C	3.652954000	1.822815000	-3.887976000	C	1.302181000	-4.795828000	-1.532211000
H	0.911873000	0.172207000	-2.713668000	H	3.101638000	-3.010042000	0.741855000
H	4.419428000	1.460838000	-0.589198000	H	0.010604000	-1.668534000	-1.925140000
H	1.848105000	1.097319000	-4.825501000	H	2.874272000	-5.316549000	-0.145579000
H	5.355743000	2.395424000	-2.689207000	H	-0.208902000	-3.969691000	-2.836675000
H	4.068146000	2.222597000	-4.809560000	H	1.212380000	-5.803497000	-1.929934000
4				5			
P	-1.386950000	0.668997000	0.170446000	P	2.260813000	0.282256000	-0.078990000
P	1.759669000	-0.426869000	-0.258979000	P	-2.205959000	0.362617000	-0.115134000
Ni	-0.434597000	-1.046128000	-0.813282000	Ni	0.027387000	0.459726000	-0.258679000
C	-2.177654000	-1.777379000	-1.055121000	C	0.008122000	-1.364900000	0.292586000
C	-2.579734000	-2.814528000	-0.201801000	C	-0.109735000	-2.302694000	-0.750816000
C	-3.084347000	-1.331618000	-2.025965000	C	0.106151000	-1.859804000	1.600603000
C	-3.863183000	-3.366641000	-0.289298000	C	-0.119824000	-3.676576000	-0.499505000
C	-4.363995000	-1.884225000	-2.125095000	C	0.104637000	-3.234798000	1.860446000
C	-4.763500000	-2.897726000	-1.248757000	C	-0.008880000	-4.149863000	0.812192000
H	-1.881015000	-3.218214000	0.529524000	H	-0.192073000	-1.956382000	-1.777938000
H	-4.153302000	-4.169874000	0.385666000	H	-0.208682000	-4.376300000	-1.327548000
H	-5.054056000	-1.514754000	-2.880752000	H	0.179415000	-3.587937000	2.886897000
H	-5.762432000	-3.321619000	-1.318379000	H	-0.012075000	-5.218751000	1.012446000
Cl	0.360739000	-2.724843000	-2.055290000	Cl	0.001892000	2.424539000	-1.354006000
H	-2.802758000	-0.525641000	-2.700273000	H	0.174438000	-1.172958000	2.437535000
C	2.125014000	0.770441000	1.103691000	C	-2.841865000	-0.386016000	-1.660316000
C	2.364619000	0.303613000	2.405520000	C	-4.040806000	-1.111896000	-1.711664000
C	2.124646000	2.156444000	0.873963000	C	-2.095886000	-0.198053000	-2.834790000
C	2.602921000	1.198905000	3.448348000	C	-4.488714000	-1.643543000	-2.923213000
C	2.361656000	3.049803000	1.919707000	C	-2.548005000	-0.730131000	-4.043469000
C	2.604788000	2.574860000	3.210261000	C	-3.742976000	-1.454296000	-4.089739000
H	2.367216000	-0.762055000	2.606136000	H	-4.613909000	-1.272321000	-0.803957000
H	1.960002000	2.543137000	-0.124121000	H	-1.173490000	0.374287000	-2.794391000
H	2.782430000	0.816895000	4.449415000	H	-5.417620000	-2.207103000	-2.954015000
H	2.361007000	4.117842000	1.717791000	H	-1.965716000	-0.578475000	-4.948465000
H	2.793715000	3.270900000	4.023622000	H	-4.091419000	-1.870977000	-5.031270000
C	2.763001000	0.234943000	-1.649992000	C	-3.079727000	1.965537000	0.043228000
C	3.934591000	0.978858000	-1.436453000	C	-4.363420000	2.157336000	-0.483155000

C	2.326175000	0.009158000	-2.965047000	C	-2.476183000	2.988024000	0.788360000
C	4.652915000	1.493402000	-2.517834000	C	-5.037282000	3.360873000	-0.264838000
C	3.044569000	0.528289000	-4.044136000	C	-3.156427000	4.185227000	1.016446000
C	4.206913000	1.272877000	-3.823629000	C	-4.436994000	4.373465000	0.488286000
H	4.273752000	1.174115000	-0.424235000	H	-4.830918000	1.370765000	-1.067911000
H	1.433383000	-0.584174000	-3.135232000	H	-1.465446000	2.852041000	1.159522000
H	5.557051000	2.069553000	-2.338746000	H	-6.029619000	3.507311000	-0.683398000
H	2.695993000	0.344987000	-5.057015000	H	-2.679863000	4.975839000	1.589769000
H	4.763928000	1.677528000	-4.664816000	H	-4.962451000	5.309962000	0.656664000
C	2.637748000	-1.918294000	0.344123000	C	-2.980154000	-0.628382000	1.227108000
C	1.879525000	-2.943577000	0.925156000	C	-2.953130000	-2.032168000	1.178115000
C	4.034309000	-2.016687000	0.322546000	C	-3.556953000	0.003621000	2.339488000
C	2.513485000	-4.050717000	1.491223000	C	-3.500499000	-2.783813000	2.216795000
C	4.666828000	-3.130596000	0.877731000	C	-4.093722000	-0.753659000	3.384039000
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H	0.796093000	-2.882314000	0.901876000	H	-2.490351000	-2.537054000	0.337861000
H	4.624894000	-1.229777000	-0.136717000	H	-3.596265000	1.087093000	2.388546000
H	1.918803000	-4.846263000	1.932101000	H	-3.465560000	-3.868500000	2.163863000
H	5.750649000	-3.206693000	0.848271000	H	-4.537756000	-0.249845000	4.238717000
H	4.401185000	-5.013132000	1.897732000	H	-4.491742000	-2.737060000	4.134721000
C	-3.207443000	0.878750000	0.133151000	C	2.717122000	0.301322000	1.695305000
C	-3.814340000	1.778225000	-0.753463000	C	1.783856000	0.784080000	2.622007000
C	-4.008424000	0.032483000	0.913800000	C	4.000235000	-0.058277000	2.132296000
C	-5.206287000	1.828113000	-0.858691000	C	2.121873000	0.892453000	3.972848000
C	-5.395570000	0.079054000	0.799536000	C	4.334798000	0.039641000	3.483295000
C	-5.998323000	0.976577000	-0.086926000	C	3.395765000	0.514992000	4.404901000
H	-3.204567000	2.432992000	-1.367486000	H	0.790589000	1.062359000	2.276834000
H	-3.547623000	-0.682177000	1.586010000	H	4.733331000	-0.412826000	1.413203000
H	-5.668274000	2.528666000	-1.549463000	H	1.391256000	1.266185000	4.685338000
H	-6.005644000	-0.593862000	1.395256000	H	5.328682000	-0.247331000	3.816527000
H	-7.080908000	1.008094000	-0.177608000	H	3.659287000	0.594472000	5.456328000
C	-1.009712000	0.563941000	1.963613000	C	2.869200000	-1.298977000	-0.763100000
C	-1.017400000	-0.738577000	2.492127000	C	3.126688000	-2.413175000	0.044027000
C	-0.754735000	1.644054000	2.815349000	C	2.900048000	-1.438739000	-2.160444000
C	-0.799856000	-0.952538000	3.853706000	C	3.421889000	-3.647320000	-0.537482000
C	-0.528344000	1.426034000	4.175089000	C	3.203602000	-2.671241000	-2.738296000
C	-0.558932000	0.132384000	4.699832000	C	3.464283000	-3.779483000	-1.926665000
H	-1.199436000	-1.581266000	1.831361000	H	3.057875000	-2.328519000	1.122217000
H	-0.685516000	2.650230000	2.424282000	H	2.686887000	-0.581682000	-2.794524000
H	-0.812726000	-1.964722000	4.249213000	H	3.605028000	-4.508547000	0.099129000
H	-0.311714000	2.271626000	4.821772000	H	3.229973000	-2.767411000	-3.820597000
H	-0.382572000	-0.030395000	5.759801000	H	3.691456000	-4.742426000	-2.376619000
C	-0.769499000	2.241537000	-0.528912000	C	3.423651000	1.545723000	-0.741092000
C	-1.033734000	3.505809000	0.021576000	C	4.607796000	1.207362000	-1.412691000
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C	-0.483872000	4.651514000	-0.554267000	C	5.498413000	2.205251000	-1.817761000
C	0.524147000	3.304345000	-2.294429000	C	4.048134000	3.888336000	-0.867069000
C	0.310566000	4.550975000	-1.702603000	C	5.220466000	3.546343000	-1.547502000
H	-1.681561000	3.598114000	0.886906000	H	4.840002000	0.168357000	-1.618796000
H	0.149174000	1.191274000	-2.170495000	H	2.236197000	3.171017000	0.041832000
H	-0.680038000	5.624431000	-0.111593000	H	6.410784000	1.929913000	-2.340681000
H	1.126448000	3.210872000	-3.193642000	H	3.823120000	4.930014000	-0.654907000
H	0.744080000	5.445450000	-2.142013000	H	5.913558000	4.321546000	-1.864104000
6				7			
P	2.019014000	0.262009000	-0.317121000	P	-1.920592000	0.238875000	-0.134300000
P	-2.118195000	0.291412000	-0.271092000	P	1.815812000	0.314257000	-0.133514000
Ni	-0.066378000	-0.410144000	-0.722140000	Ni	-0.054363000	-0.543488000	-1.259573000
C	-0.051400000	-2.350142000	-0.481003000	C	0.084968000	-2.461142000	-0.878666000
C	-0.294108000	-3.211449000	-1.574949000	C	-0.950793000	-3.175741000	-0.255313000
C	0.278505000	-2.990149000	0.735013000	C	1.325628000	-3.109811000	-1.006550000
C	-0.211717000	-4.605376000	-1.473495000	C	-0.742795000	-4.450566000	0.282327000

C	0.356489000	-4.382437000	0.856774000	C	1.543364000	-4.388083000	-0.482699000
C	0.112686000	-5.200120000	-0.250693000	C	0.510722000	-5.059552000	0.176629000
H	-0.544277000	-2.785824000	-2.548685000	H	-1.941370000	-2.734800000	-0.177013000
H	-0.403046000	-5.227781000	-2.346806000	H	-1.561292000	-4.970910000	0.777311000
H	0.614170000	-4.830385000	1.815784000	H	2.522416000	-4.853500000	-0.578778000
H	0.175008000	-6.282695000	-0.163080000	H	0.677597000	-6.050280000	0.593118000
H	0.488145000	-2.382752000	1.614164000	H	2.158417000	-2.597565000	-1.484778000
C	-2.504853000	2.052638000	-0.623130000	C	1.705888000	1.936955000	0.718304000
C	-3.763293000	2.524499000	-1.021561000	C	2.127175000	2.134233000	2.039834000
C	-1.441409000	2.961622000	-0.493400000	C	1.090269000	2.992699000	0.028312000
C	-3.952674000	3.885196000	-1.279334000	C	1.914725000	3.364849000	2.667289000
C	-1.634062000	4.320808000	-0.740232000	C	0.873444000	4.218662000	0.656112000
C	-2.892631000	4.784965000	-1.135825000	C	1.278797000	4.403944000	1.982458000
H	-4.589396000	1.829556000	-1.136645000	H	2.594401000	1.318635000	2.582348000
H	-0.457505000	2.598177000	-0.209633000	H	0.750573000	2.847261000	-0.991654000
H	-4.930264000	4.242121000	-1.593407000	H	2.238918000	3.507935000	3.695130000
H	-0.796636000	5.006231000	-0.639379000	H	0.369971000	5.014744000	0.115593000
H	-3.045298000	5.841768000	-1.339387000	H	1.100483000	5.354207000	2.479030000
C	-2.269916000	0.161297000	1.555889000	C	3.268148000	0.529147000	-1.233428000
C	-2.355494000	1.278694000	2.397557000	C	4.329640000	1.386275000	-0.900477000
C	-2.163658000	-1.122394000	2.118969000	C	3.322056000	-0.203573000	-2.428676000
C	-2.336517000	1.114554000	3.786189000	C	5.438102000	1.492608000	-1.741952000
C	-2.148125000	-1.280745000	3.503852000	C	4.434606000	-0.096880000	-3.266775000
C	-2.233607000	-0.163113000	4.341963000	C	5.493579000	0.747191000	-2.924027000
H	-2.429646000	2.274346000	1.971022000	H	4.281705000	1.970449000	0.014387000
H	-2.059617000	-1.987701000	1.472348000	H	2.485968000	-0.832241000	-2.713607000
H	-2.404024000	1.986871000	4.431353000	H	6.255929000	2.157928000	-1.477202000
H	-2.057103000	-2.277188000	3.927900000	H	4.466413000	-0.666193000	-4.191771000
H	-2.218663000	-0.288282000	5.421779000	H	6.356088000	0.832666000	-3.579919000
C	-3.552196000	-0.663232000	-0.880647000	C	2.389729000	-0.831443000	1.175004000
C	-3.375795000	-1.476789000	-2.007623000	C	1.413254000	-1.519481000	1.909059000
C	-4.803318000	-0.620962000	-0.244959000	C	3.745635000	-1.039391000	1.463524000
C	-4.445442000	-2.221368000	-2.510391000	C	1.786379000	-2.398635000	2.923679000
C	-5.871032000	-1.365049000	-0.748291000	C	4.117205000	-1.925315000	2.478097000
C	-5.692698000	-2.162946000	-1.883877000	C	3.138890000	-2.604967000	3.209006000
H	-2.393877000	-1.543005000	-2.465618000	H	0.367256000	-1.392198000	1.666682000
H	-4.931232000	-0.013141000	0.646812000	H	4.508660000	-0.522447000	0.889548000
H	-4.300626000	-2.855980000	-3.380516000	H	1.017480000	-2.931094000	3.475833000
H	-6.838112000	-1.329343000	-0.253371000	H	5.170431000	-2.088378000	2.692049000
H	-6.523290000	-2.747246000	-2.271413000	H	3.431298000	-3.299993000	3.992106000
C	2.360044000	-0.066800000	1.457041000	C	-3.609259000	-0.455840000	-0.332823000
C	1.300364000	0.078735000	2.366235000	C	-3.864862000	-1.398055000	-1.337200000
C	3.622127000	-0.455758000	1.926712000	C	-4.653918000	-0.031178000	0.505912000
C	1.502681000	-0.151029000	3.727622000	C	-5.157430000	-1.908583000	-1.499489000
C	3.822201000	-0.687838000	3.290219000	C	-5.939256000	-0.542928000	0.340011000
C	2.764652000	-0.534933000	4.191191000	C	-6.192262000	-1.484200000	-0.665318000
H	0.312487000	0.349422000	2.007057000	H	-3.063741000	-1.734568000	-1.985257000
H	4.441217000	-0.585604000	1.225347000	H	-4.455833000	0.690396000	1.293340000
H	0.667200000	-0.044517000	4.413227000	H	-5.347206000	-2.641140000	-2.279200000
H	4.802464000	-0.993900000	3.646734000	H	-6.742479000	-0.211900000	0.993276000
H	2.922270000	-0.722927000	5.250265000	H	-7.194715000	-1.884746000	-0.792844000
C	3.408185000	-0.556708000	-1.193475000	C	-1.697992000	0.202588000	1.683559000
C	3.251023000	-1.907734000	-1.546502000	C	-2.083261000	-0.957332000	2.379037000
C	4.611158000	0.102059000	-1.489621000	C	-1.003686000	1.210203000	2.368583000
C	4.293098000	-2.587916000	-2.179214000	C	-1.771668000	-1.106884000	3.730008000
C	5.647771000	-0.583031000	-2.128311000	C	-0.695936000	1.056673000	3.722265000
C	5.490890000	-1.928709000	-2.471647000	C	-1.073555000	-0.100595000	4.405148000
H	2.317246000	-2.416422000	-1.325928000	H	-2.612228000	-1.747887000	1.856899000
H	4.734592000	1.147815000	-1.223195000	H	-0.692467000	2.109306000	1.850873000
H	4.164399000	-3.633185000	-2.447644000	H	-2.072111000	-2.010452000	4.253855000
H	6.575913000	-0.065495000	-2.357670000	H	-0.147979000	1.843971000	4.231481000
H	6.298370000	-2.460293000	-2.968864000	H	-0.825139000	-0.220381000	5.456289000
C	2.383642000	2.058090000	-0.494275000	C	-2.117256000	2.008599000	-0.579384000

C	3.198298000	2.766052000	0.402673000	C	-2.689945000	2.965296000	0.270227000
C	1.781578000	2.746225000	-1.559523000	C	-1.665619000	2.399233000	-1.850203000
C	3.409060000	4.136700000	0.232291000	C	-2.793031000	4.296015000	-0.136875000
C	1.996431000	4.114710000	-1.733028000	C	-1.778390000	3.729610000	-2.260632000
C	2.810303000	4.812524000	-0.835052000	C	-2.336797000	4.680468000	-1.401997000
H	3.657091000	2.242692000	1.236786000	H	-3.032182000	2.672842000	1.257933000
H	1.123437000	2.208884000	-2.238931000	H	-1.207654000	1.668249000	-2.513995000
H	4.038205000	4.677393000	0.934752000	H	-3.228964000	5.033145000	0.532394000
H	1.520559000	4.635682000	-2.559613000	H	-1.423595000	4.021355000	-3.245355000
H	2.972714000	5.879591000	-0.963228000	H	-2.419245000	5.717254000	-1.717684000
				C	-0.692910000	-1.101986000	-3.059375000
				O	-1.571052000	-1.773883000	-3.522842000
				O	0.243372000	-0.334555000	-3.342196000
TS₇₋₈				8			
P	-1.925324000	0.261731000	-0.161975000	P	-1.624348000	0.755937000	-0.192302000
P	1.805274000	0.334388000	-0.153472000	P	1.947835000	0.171354000	-0.302225000
Ni	-0.048823000	-0.591157000	-1.193209000	Ni	-0.008107000	-0.369883000	-1.266434000
C	0.040572000	-2.540290000	-0.869382000	C	-0.982035000	-3.218537000	-0.856447000
C	-0.976947000	-3.200704000	-0.163619000	C	-2.157216000	-3.681494000	-0.249929000
C	1.294620000	-3.165514000	-0.957259000	C	0.206414000	-3.192043000	-0.113100000
C	-0.726411000	-4.398828000	0.511550000	C	-2.148108000	-4.077921000	1.089144000
C	1.551113000	-4.370056000	-0.295268000	C	0.225786000	-3.610828000	1.217980000
C	0.543453000	-4.982902000	0.454003000	C	-0.956728000	-4.045366000	1.824267000
H	-1.977060000	-2.774674000	-0.135245000	H	-3.067291000	-3.703592000	-0.839935000
H	-1.522802000	-4.882863000	1.074256000	H	-3.068867000	-4.415307000	1.559293000
H	2.537801000	-4.824417000	-0.356231000	H	1.156046000	-3.583851000	1.775606000
H	0.740556000	-5.916256000	0.976085000	H	-0.950025000	-4.361487000	2.865046000
H	2.095788000	-2.687178000	-1.516552000	H	1.116402000	-2.841274000	-0.587820000
C	1.688113000	1.964521000	0.685545000	C	2.014641000	1.871069000	0.382461000
C	2.095867000	2.168240000	2.010405000	C	2.665171000	2.228270000	1.571195000
C	1.096538000	3.022980000	-0.021150000	C	1.283154000	2.843609000	-0.314440000
C	1.895738000	3.407758000	2.624052000	C	2.559802000	3.532192000	2.062859000
C	0.893066000	4.258550000	0.592614000	C	1.173659000	4.144544000	0.175040000
C	1.285801000	4.450651000	1.921703000	C	1.808214000	4.488536000	1.372892000
H	2.544736000	1.351301000	2.566151000	H	3.225801000	1.482972000	2.125864000
H	0.763529000	2.872961000	-1.042484000	H	0.767729000	2.565924000	-1.226468000
H	2.209578000	3.555013000	3.654498000	H	3.059213000	3.798779000	2.990837000
H	0.409912000	5.057718000	0.038258000	H	0.571320000	4.870385000	-0.364380000
H	1.118123000	5.408901000	2.406559000	H	1.716370000	5.496595000	1.768912000
C	3.294859000	0.530627000	-1.207193000	C	3.303881000	0.078480000	-1.528093000
C	4.342948000	1.395734000	-0.852752000	C	4.514521000	0.767141000	-1.358873000
C	3.396993000	-0.235129000	-2.378609000	C	3.117123000	-0.746941000	-2.648848000
C	5.484448000	1.481144000	-1.651413000	C	5.533284000	0.629888000	-2.301960000
C	4.542974000	-0.148319000	-3.173293000	C	4.145639000	-0.886734000	-3.585604000
C	5.587275000	0.705765000	-2.810826000	C	5.350028000	-0.199852000	-3.413988000
H	4.260127000	2.001102000	0.045596000	H	4.650616000	1.412054000	-0.494584000
H	2.573315000	-0.873528000	-2.678020000	H	2.173120000	-1.270801000	-2.788509000
H	6.291404000	2.153205000	-1.370674000	H	6.468486000	1.168385000	-2.171800000
H	4.612810000	-0.742519000	-4.080481000	H	3.999375000	-1.526479000	-4.451686000
H	6.475751000	0.774788000	-3.433216000	H	6.145166000	-0.305569000	-4.147543000
C	2.337587000	-0.804827000	1.180050000	C	2.530159000	-0.899038000	1.070757000
C	1.334167000	-1.442646000	1.923780000	C	1.915691000	-0.791243000	2.327749000
C	3.683599000	-1.064039000	1.471680000	C	3.505192000	-1.885965000	0.867919000
C	1.670654000	-2.323169000	2.949553000	C	2.291628000	-1.634143000	3.372177000
C	4.018507000	-1.951809000	2.497697000	C	3.866958000	-2.742169000	1.911962000
C	3.013919000	-2.581488000	3.237269000	C	3.268626000	-2.613474000	3.168406000
H	0.293803000	-1.273174000	1.681387000	H	1.150190000	-0.045154000	2.494529000
H	4.466814000	-0.584619000	0.892387000	H	3.982807000	-1.984133000	-0.102174000
H	0.880688000	-2.816260000	3.508423000	H	1.806356000	-1.530028000	4.338709000
H	5.064301000	-2.154799000	2.714110000	H	4.622288000	-3.505048000	1.742873000
H	3.278076000	-3.277801000	4.029202000	H	3.556896000	-3.276644000	3.979804000

C	-3.628077000	-0.400053000	-0.361330000	C	-3.221972000	-0.108043000	-0.451711000
C	-3.888392000	-1.370259000	-1.337452000	C	-3.407988000	-0.761001000	-1.677735000
C	-4.677402000	0.079151000	0.441449000	C	-4.237074000	-0.149686000	0.516695000
C	-5.190044000	-1.855207000	-1.506977000	C	-4.587542000	-1.465212000	-1.929077000
C	-5.971759000	-0.406960000	0.268275000	C	-5.416039000	-0.850018000	0.262097000
C	-6.229347000	-1.376922000	-0.708239000	C	-5.590966000	-1.511152000	-0.959521000
H	-3.083979000	-1.751462000	-1.956909000	H	-2.623681000	-0.755582000	-2.427457000
H	-4.475564000	0.822459000	1.207490000	H	-4.093782000	0.342357000	1.474362000
H	-5.383036000	-2.610751000	-2.263666000	H	-4.693854000	-1.998283000	-2.868612000
H	-6.778713000	-0.033621000	0.893594000	H	-6.196150000	-0.886251000	1.018327000
H	-7.238807000	-1.757816000	-0.840774000	H	-6.505340000	-2.067964000	-1.147883000
C	-1.757025000	0.335334000	1.661893000	C	-1.347867000	0.662998000	1.614608000
C	-2.165979000	-0.785824000	2.406516000	C	-1.569408000	-0.570506000	2.251466000
C	-1.077470000	1.374481000	2.313272000	C	-0.778895000	1.720124000	2.342442000
C	-1.895065000	-0.865481000	3.771963000	C	-1.269627000	-0.725662000	3.604609000
C	-0.810801000	1.291535000	3.682103000	C	-0.483201000	1.559121000	3.698937000
C	-1.213446000	0.173543000	4.413955000	C	-0.737270000	0.340935000	4.335932000
H	-2.684647000	-1.600594000	1.911211000	H	-1.963945000	-1.412333000	1.690629000
H	-0.743292000	2.242972000	1.759002000	H	-0.552925000	2.661250000	1.852470000
H	-2.214723000	-1.739414000	4.333463000	H	-1.442003000	-1.687562000	4.079231000
H	-0.274445000	2.103110000	4.164708000	H	-0.041911000	2.385181000	4.249915000
H	-0.997239000	0.109072000	5.477021000	H	-0.507120000	0.219264000	5.391309000
C	-2.063125000	1.999740000	-0.734461000	C	-2.012531000	2.512672000	-0.556531000
C	-2.626435000	3.033806000	0.025042000	C	-2.663309000	3.360773000	0.350269000
C	-1.566839000	2.279844000	-2.017896000	C	-1.666334000	3.001002000	-1.825073000
C	-2.671283000	4.333951000	-0.480831000	C	-2.933444000	4.686168000	0.004559000
C	-1.620607000	3.578855000	-2.527522000	C	-1.944404000	4.323662000	-2.175094000
C	-2.166237000	4.608901000	-1.755768000	C	-2.571173000	5.170670000	-1.256157000
H	-3.006788000	2.825730000	1.020369000	H	-2.942972000	2.988075000	1.330842000
H	-1.122516000	1.482884000	-2.613303000	H	-1.165514000	2.341118000	-2.530578000
H	-3.099589000	5.132420000	0.119447000	H	-3.429275000	5.339876000	0.717392000
H	-1.231081000	3.785569000	-3.520613000	H	-1.668876000	4.692260000	-3.159541000
H	-2.202111000	5.621947000	-2.147923000	H	-2.781838000	6.202876000	-1.523285000
C	-0.576679000	-1.591970000	-2.891437000	C	-1.033442000	-2.717133000	-2.289128000
O	-1.504800000	-2.237715000	-3.294587000	O	-1.867514000	-3.175269000	-3.063735000
O	0.383104000	-0.895422000	-3.258632000	O	-0.192000000	-1.748333000	-2.582054000
9				Ni(0)-CO₂ adduct			
P	0.064902000	-1.844580000	-0.084658000	P	1.761573000	-0.068238000	-0.177659000
P	1.056416000	1.701593000	-0.036465000	P	-1.857610000	-0.204310000	-0.296825000
Ni	-0.691172000	0.292038000	-0.173115000	Ni	0.077603000	-1.121437000	-1.027355000
C	-4.552405000	1.059546000	-0.172042000	C	-1.718165000	0.053409000	1.516537000
C	-5.399009000	0.389157000	0.721824000	C	-2.268857000	1.151764000	2.189237000
C	-5.084692000	2.008683000	-1.055998000	C	-0.916224000	-0.855812000	2.224209000
C	-6.765871000	0.666831000	0.732006000	C	-2.001766000	1.347168000	3.547221000
C	-6.451696000	2.285914000	-1.044205000	C	-0.642652000	-0.657767000	3.577223000
C	-7.293538000	1.615562000	-0.150370000	C	-1.180990000	0.451041000	4.239239000
H	-4.966462000	-0.343571000	1.395137000	H	-2.875725000	1.867687000	1.643204000
H	-7.420734000	0.145337000	1.425479000	H	-0.464320000	-1.692322000	1.699874000
H	-6.862439000	3.022493000	-1.730147000	H	-2.423630000	2.207025000	4.061699000
H	-8.359126000	1.831669000	-0.141882000	H	0.014002000	-1.348768000	4.098081000
H	-4.412085000	2.514065000	-1.741433000	H	-0.958166000	0.618721000	5.289798000
C	2.199866000	1.039418000	1.242087000	C	-3.292888000	-1.332782000	-0.462303000
C	3.595840000	1.119827000	1.155750000	C	-4.289967000	-1.432994000	0.520724000
C	1.617300000	0.327202000	2.302083000	C	-3.394429000	-2.101663000	-1.632080000
C	4.395274000	0.485266000	2.110715000	C	-5.382644000	-2.281011000	0.329155000
C	2.413362000	-0.313600000	3.251305000	C	-4.491504000	-2.944570000	-1.821622000
C	3.807005000	-0.238511000	3.152700000	C	-5.486192000	-3.034503000	-0.844037000
H	4.053884000	1.650102000	0.326092000	H	-4.206001000	-0.851069000	1.434330000
H	0.536136000	0.235964000	2.353870000	H	-2.604758000	-2.057182000	-2.374499000
H	5.478090000	0.544845000	2.033034000	H	-6.150298000	-2.355047000	1.095291000
H	1.944167000	-0.894567000	4.040416000	H	-4.561622000	-3.540231000	-2.727809000

H	4.432452000	-0.748567000	3.880853000	H	-6.335563000	-3.696727000	-0.990962000
C	0.592461000	3.356397000	0.602509000	C	-2.500167000	1.405648000	-0.905400000
C	1.460447000	4.125292000	1.394070000	C	-1.571231000	2.388625000	-1.279132000
C	-0.679676000	3.854557000	0.278983000	C	-3.871453000	1.698926000	-0.966591000
C	1.066670000	5.386129000	1.845558000	C	-2.004511000	3.649742000	-1.690395000
C	-1.066474000	5.119152000	0.730862000	C	-4.302803000	2.959240000	-1.386801000
C	-0.196582000	5.885147000	1.511253000	C	-3.370710000	3.937537000	-1.745831000
H	2.437224000	3.730254000	1.660665000	H	-0.510528000	2.171773000	-1.242106000
H	-1.362111000	3.244248000	-0.307543000	H	-4.598023000	0.940988000	-0.689985000
H	1.741500000	5.976281000	2.460498000	H	-1.270491000	4.401955000	-1.965664000
H	-2.052868000	5.500704000	0.480108000	H	-5.366894000	3.176175000	-1.434619000
H	-0.503744000	6.865637000	1.866327000	H	-3.709442000	4.917664000	-2.071847000
C	2.180202000	2.050260000	-1.447860000	C	3.260748000	-0.045324000	-1.232555000
C	2.548462000	0.968813000	-2.265375000	C	3.138963000	-0.320942000	-2.599240000
C	2.700294000	3.323922000	-1.719241000	C	4.513981000	0.294966000	-0.702090000
C	3.436209000	1.156477000	-3.324479000	C	4.257725000	-0.246139000	-3.432569000
C	3.579850000	3.510888000	-2.789390000	C	5.632034000	0.361131000	-1.533012000
C	3.952448000	2.428432000	-3.590479000	C	5.503386000	0.093597000	-2.900502000
H	2.148771000	-0.019896000	-2.070606000	H	2.171768000	-0.609173000	-2.999459000
H	2.417463000	4.166967000	-1.096502000	H	4.611827000	0.497911000	0.361077000
H	3.718486000	0.306065000	-3.939039000	H	4.157113000	-0.467023000	-4.491679000
H	3.973859000	4.02960000	-2.995078000	H	6.602446000	0.618048000	-1.116289000
H	4.638368000	2.576465000	-4.420767000	H	6.375552000	0.143090000	-3.547304000
C	-1.096956000	-2.917044000	-1.014636000	C	1.539313000	1.713487000	0.221519000
C	-2.042840000	-2.307031000	-1.851107000	C	1.956785000	2.693673000	-0.693767000
C	-1.054924000	-4.315872000	-0.917386000	C	0.806922000	2.107341000	1.353609000
C	-2.932030000	-3.092293000	-2.590331000	C	1.629586000	4.036566000	-0.491125000
C	-1.946117000	-5.097019000	-1.653002000	C	0.485263000	3.449797000	1.554157000
C	-2.885002000	-4.484708000	-2.491078000	C	0.887869000	4.417448000	0.630201000
H	-2.084514000	-1.222550000	-1.917088000	H	2.530015000	2.404569000	-1.569280000
H	-0.330160000	-4.786724000	-0.258315000	H	0.484981000	1.370113000	2.078642000
H	-3.664291000	-2.614353000	-3.235562000	H	1.957651000	4.783733000	-1.209243000
H	-1.912419000	-6.180487000	-1.571798000	H	-0.090984000	3.731726000	2.430904000
H	-3.581137000	-5.094242000	-3.061620000	H	0.628455000	5.461501000	0.784336000
C	1.695439000	-2.216375000	-0.836219000	C	2.323876000	-0.832067000	1.394333000
C	1.783146000	-2.622187000	-2.177616000	C	2.847705000	-0.092144000	2.463279000
C	2.876474000	-1.907282000	-0.139318000	C	2.204710000	-2.226236000	1.515600000
C	3.025169000	-2.704673000	-2.812462000	C	3.223429000	-0.732234000	3.646947000
C	4.114278000	-1.994821000	-0.775879000	C	2.584536000	-2.863548000	2.697393000
C	4.193765000	-2.387315000	-2.115026000	C	3.086167000	-2.117161000	3.768964000
H	0.878280000	-2.864206000	-2.727079000	H	2.944345000	0.985372000	2.379360000
H	2.832417000	-1.590456000	0.896108000	H	1.824937000	-2.805415000	0.679374000
H	3.077239000	-3.018770000	-3.851836000	H	3.620524000	-0.147718000	4.472865000
H	5.014247000	-1.740978000	-0.222594000	H	2.487480000	-3.942662000	2.780890000
H	5.158999000	-2.445931000	-2.611093000	H	3.374528000	-2.614149000	4.691638000
C	0.140638000	-2.594789000	1.587925000	C	0.909292000	-2.616888000	-1.763956000
C	1.071022000	-3.575572000	1.958009000	O	1.948021000	-3.220285000	-1.903766000
C	-0.771974000	-2.112069000	2.541619000	O	-0.325812000	-2.722967000	-2.034625000
C	1.100851000	-4.059059000	3.268581000				
C	-0.742463000	-2.602133000	3.848281000				
C	0.197238000	-3.571137000	4.216275000				
H	1.786780000	-3.942805000	1.228848000				
H	-1.495212000	-1.353440000	2.253847000				
H	1.830828000	-4.814364000	3.548687000				
H	-1.449799000	-2.222601000	4.581164000				
H	0.223662000	-3.945050000	5.236657000				
C	-3.089624000	0.761594000	-0.185524000				
O	-2.606266000	-0.083040000	0.634905000				
O	-2.329197000	1.349463000	-1.022901000				
TS₅₋₁₀				10			
P	1.954634000	-0.034962000	-0.029483000	P	1.839259000	-0.291827000	0.022201000

P	-1.670131000	0.553562000	-0.100032000	P	-1.341175000	1.090408000	-0.068867000
Ni	-0.187568000	-0.739746000	-1.147749000	Ni	-0.225980000	-0.666997000	-0.840288000
C	-0.921000000	-2.517647000	-0.473975000	C	-1.544580000	-3.410251000	-0.517897000
C	-2.291548000	-2.843611000	-0.380427000	C	-2.764866000	-3.935451000	-0.960183000
C	-0.015585000	-3.198862000	0.368703000	C	-1.428900000	-2.977082000	0.810541000
C	-2.742411000	-3.785087000	0.541472000	C	-3.858290000	-3.996971000	-0.095528000
C	-0.467597000	-4.131866000	1.306503000	C	-2.515464000	-3.059319000	1.685059000
C	-1.832530000	-4.423084000	1.395267000	C	-3.735908000	-3.562360000	1.230135000
H	-3.001792000	-2.367152000	-1.047225000	H	-2.834021000	-4.281077000	-1.986435000
H	-3.801796000	-4.020342000	0.602690000	H	-4.807936000	-4.388047000	-0.452348000
H	0.244239000	-4.638717000	1.953462000	H	-2.410658000	-2.723717000	2.713833000
H	-2.186530000	-5.156662000	2.115319000	H	-4.588669000	-3.613882000	1.901962000
Cl	-0.164526000	0.767911000	-2.927423000	Cl	-1.591823000	-0.631438000	-2.621251000
H	1.047523000	-3.000841000	0.276343000	H	-0.473481000	-2.603240000	1.160649000
C	-1.137070000	2.304468000	-0.051154000	C	-1.107322000	2.652960000	-0.976732000
C	-1.418741000	3.166946000	-1.120529000	C	-1.887763000	2.877421000	-2.124505000
C	-0.359592000	2.763830000	1.023175000	C	-0.113918000	3.577128000	-0.624542000
C	-0.914753000	4.468691000	-1.116448000	C	-1.680961000	4.020906000	-2.895466000
C	0.148198000	4.063127000	1.018283000	C	0.086051000	4.720631000	-1.400512000
C	-0.124569000	4.916390000	-0.053030000	C	-0.696122000	4.946214000	-2.534620000
H	-2.005440000	2.811837000	-1.959243000	H	-2.642587000	2.153714000	-2.411819000
H	-0.150588000	2.114046000	1.863830000	H	0.502264000	3.414213000	0.248915000
H	-1.132167000	5.128788000	-1.951551000	H	-2.287796000	4.185996000	-3.781414000
H	0.762879000	4.396153000	1.849543000	H	0.860494000	5.426542000	-1.113926000
H	0.274511000	5.927370000	-0.059973000	H	-0.538513000	5.836343000	-3.138121000
C	-2.179868000	0.274216000	1.655037000	C	-0.964352000	1.404121000	1.697665000
C	-2.757552000	1.328077000	2.387687000	C	-1.062040000	2.660329000	2.309262000
C	-2.043791000	-0.971935000	2.278200000	C	-0.616447000	0.287203000	2.471885000
C	-3.196203000	1.132558000	3.697154000	C	-0.773329000	2.801623000	3.667922000
C	-2.486311000	-1.170109000	3.587386000	C	-0.337134000	0.426084000	3.832118000
C	-3.066231000	-0.120864000	4.301565000	C	-0.404249000	1.688240000	4.429763000
H	-2.842425000	2.313488000	1.943178000	H	-1.338223000	3.529088000	1.720629000
H	-1.569641000	-1.788120000	1.761865000	H	-0.543690000	-0.686399000	2.000304000
H	-3.635935000	1.961870000	4.244621000	H	-0.835682000	3.782250000	4.132400000
H	-2.367799000	-2.149520000	4.043198000	H	-0.051229000	-0.444601000	4.415524000
H	-3.408616000	-0.273880000	5.321720000	H	-0.175781000	1.803934000	5.485906000
C	-3.252134000	0.540729000	-1.033374000	C	-3.157524000	0.860694000	-0.011370000
C	-3.334898000	-0.161245000	-2.244689000	C	-3.726230000	-0.413115000	-0.123701000
C	-4.381271000	1.221765000	-0.553464000	C	-3.976802000	1.972168000	0.243261000
C	-4.533162000	-0.184485000	-2.961956000	C	-5.107095000	-0.570272000	0.015651000
C	-5.574472000	1.203121000	-1.276217000	C	-5.355626000	1.810362000	0.373194000
C	-5.652651000	0.498114000	-2.481152000	C	-5.922336000	0.536361000	0.259997000
H	-2.460632000	-0.673163000	-2.630242000	H	-3.105381000	-1.271780000	-0.338444000
H	-4.334837000	1.760936000	0.386433000	H	-3.538889000	2.963074000	0.323766000
H	-4.583274000	-0.731044000	-3.899421000	H	-5.534070000	-1.563848000	-0.076956000
H	-6.442474000	1.735646000	-0.896633000	H	-5.986009000	2.675874000	0.559568000
H	-6.583503000	0.481870000	-3.041999000	H	-6.997483000	0.410293000	0.359048000
C	1.879782000	0.481397000	1.732842000	C	2.347947000	1.433343000	0.421642000
C	1.036727000	-0.244715000	2.587741000	C	2.120645000	2.020568000	1.678811000
C	2.517200000	1.631512000	2.221892000	C	2.929441000	2.216697000	-0.590731000
C	0.812226000	0.179312000	3.897865000	C	2.484626000	3.346506000	1.920171000
C	2.293761000	2.055730000	3.533503000	C	3.282982000	3.544789000	-0.348864000
C	1.434871000	1.337616000	4.371262000	C	3.066314000	4.114153000	0.907951000
H	0.533357000	-1.130693000	2.215061000	H	1.660139000	1.452429000	2.475786000
H	3.163013000	2.208481000	1.568460000	H	3.108800000	1.788160000	-1.570734000
H	0.125577000	-0.375704000	4.529934000	H	2.297045000	3.776245000	2.899981000
H	2.785638000	2.953778000	3.898940000	H	3.727534000	4.132574000	-1.147058000
H	1.248991000	1.680750000	5.385640000	H	3.346270000	5.147169000	1.096909000
C	3.107734000	-1.464912000	-0.017278000	C	2.408742000	-1.334210000	1.422367000
C	3.470123000	-2.143812000	1.155693000	C	3.188731000	-0.856928000	2.486110000
C	3.568911000	-1.945722000	-1.255783000	C	2.077863000	-2.700478000	1.374256000
C	4.271265000	-3.287360000	1.091647000	C	3.593217000	-1.722046000	3.506591000
C	4.376861000	-3.080925000	-1.314201000	C	2.484977000	-3.558895000	2.395508000

C	4.725734000	-3.759169000	-0.141808000	C	3.234726000	-3.071030000	3.469820000
H	3.130226000	-1.778183000	2.119521000	H	3.494504000	0.181595000	2.520329000
H	3.290521000	-1.433526000	-2.170973000	H	1.524063000	-3.080066000	0.523205000
H	4.546600000	-3.802374000	2.008648000	H	4.195679000	-1.338206000	4.325787000
H	4.727830000	-3.439984000	-2.277981000	H	2.220181000	-4.611481000	2.345186000
H	5.349880000	-4.647570000	-0.190571000	H	3.549438000	-3.741021000	4.265558000
C	2.948199000	1.304444000	-0.791456000	C	2.983274000	-0.721933000	-1.342677000
C	4.351870000	1.272343000	-0.813735000	C	4.339575000	-0.943719000	-1.063137000
C	2.276892000	2.438952000	-1.272612000	C	2.525519000	-0.751755000	-2.667376000
C	5.072614000	2.358132000	-1.314218000	C	5.235161000	-1.192801000	-2.103098000
C	3.002483000	3.526676000	-1.761657000	C	3.428815000	-0.995950000	-3.704279000
C	4.398454000	3.488633000	-1.786428000	C	4.779790000	-1.216201000	-3.425094000
H	4.878076000	0.399172000	-0.440801000	H	4.690356000	-0.928571000	-0.034728000
H	1.196149000	2.468925000	-1.281917000	H	1.471235000	-0.619431000	-2.887144000
H	6.158957000	2.32447000	-1.331208000	H	6.284000000	-1.372314000	-1.882005000
H	2.468037000	4.397727000	-2.130252000	H	3.068420000	-1.030142000	-4.728425000
H	4.960974000	4.333814000	-2.175279000	H	5.476615000	-1.414788000	-4.235279000
C	-0.253713000	-2.668101000	-2.341250000	C	-0.366474000	-3.362848000	-1.466945000
O	-0.934932000	-3.392316000	-2.993403000	O	-0.206815000	-4.253918000	-2.286365000
O	0.792217000	-2.011410000	-2.298278000	O	0.477097000	-2.359151000	-1.300587000
11				12			
P	2.419853000	0.181657000	0.009036000	P	-2.404922000	-0.143400000	-0.175300000
P	-2.101902000	0.648975000	0.096405000	P	2.027940000	-1.050552000	-0.195229000
Ni	0.148518000	0.346534000	0.112036000	Ni	-0.188034000	-0.570911000	-0.496686000
C	-0.730249000	-2.625823000	-0.696165000	C	1.046127000	3.313185000	-0.282339000
C	-0.019571000	-2.754299000	0.504202000	C	1.161602000	4.385207000	-1.176727000
C	-1.891356000	-3.385860000	-0.892161000	C	1.521942000	3.450334000	1.027472000
C	-0.458169000	-3.637006000	1.494451000	C	1.741601000	5.584339000	-0.765339000
C	-2.347910000	-4.243024000	0.109291000	C	2.106663000	4.648716000	1.438337000
C	-1.626914000	-4.378388000	1.301810000	C	2.216973000	5.717311000	0.543871000
H	0.891625000	-2.185414000	0.651537000	H	0.797994000	4.249640000	-2.190221000
H	0.109544000	-3.740274000	2.415446000	H	1.827839000	6.413818000	-1.462859000
H	-3.263357000	-4.809560000	-0.040548000	H	2.479607000	4.748997000	2.454630000
H	-1.975682000	-5.057120000	2.076141000	H	2.672573000	6.650896000	0.865118000
Cl	0.227278000	1.643555000	1.909184000	Cl	-0.686742000	-2.603098000	-1.192779000
H	-2.431062000	-3.277382000	-1.827219000	H	1.443462000	2.608471000	1.705926000
C	-3.123889000	-0.251162000	-1.132844000	C	2.870348000	-2.452319000	-1.015020000
C	-4.295923000	-0.939546000	-0.783981000	C	3.981278000	-2.255650000	-1.849130000
C	-2.722227000	-0.214892000	-2.477269000	C	2.388062000	-3.757656000	-0.809790000
C	-5.039666000	-1.600920000	-1.762564000	C	4.596411000	-3.344665000	-2.471571000
C	-3.462363000	-0.886496000	-3.449963000	C	3.013154000	-4.841601000	-1.425606000
C	-4.620527000	-1.583052000	-3.095499000	C	4.115584000	-4.638157000	-2.261110000
H	-4.622101000	-0.971735000	0.249386000	H	4.370548000	-1.256421000	-2.010782000
H	-1.806762000	0.294649000	-2.756510000	H	1.525462000	-3.922675000	-0.175165000
H	-5.943143000	-2.135254000	-1.480125000	H	5.455407000	-3.178183000	-3.116156000
H	-3.118702000	-0.879427000	-4.479862000	H	2.631236000	-5.845062000	-1.258601000
H	-5.192469000	-2.111273000	-3.853972000	H	4.596366000	-5.484396000	-2.744918000
C	-2.526429000	2.391864000	-0.250542000	C	2.165645000	-1.399650000	1.602923000
C	-3.865020000	2.813930000	-0.241464000	C	2.984419000	-2.416145000	2.114789000
C	-1.516227000	3.297619000	-0.597343000	C	1.412160000	-0.609524000	2.490481000
C	-4.185066000	4.134990000	-0.553796000	C	3.036814000	-2.651613000	3.491293000
C	-1.840407000	4.617260000	-0.921078000	C	1.471281000	-0.847153000	3.864504000
C	-3.171833000	5.038070000	-0.893852000	C	2.279002000	-1.871750000	4.367865000
H	-4.651513000	2.105794000	0.005100000	H	3.574334000	-3.026960000	1.439860000
H	-0.483241000	2.967727000	-0.607008000	H	0.790152000	0.188483000	2.099311000
H	-5.222469000	4.458464000	-0.539311000	H	3.671394000	-3.445540000	3.876260000
H	-1.051870000	5.314788000	-1.190567000	H	0.881645000	-0.233285000	4.540341000
H	-3.422598000	6.066135000	-1.141877000	H	2.319469000	-2.059105000	5.437746000
C	-2.828190000	0.227699000	1.712299000	C	3.107093000	0.396877000	-0.478996000
C	-2.842524000	-1.126068000	2.084389000	C	3.090165000	1.000037000	-1.746936000
C	-3.271036000	1.201869000	2.615034000	C	3.899272000	0.947487000	0.537043000

C	-3.314732000	-1.499969000	3.341742000	C	3.855158000	2.140899000	-1.989148000
C	-3.740657000	0.821588000	3.874615000	C	4.657872000	2.093494000	0.290681000
C	-3.764869000	-0.526833000	4.239587000	C	4.635929000	2.692366000	-0.970223000
H	-2.493200000	-1.885610000	1.394670000	H	2.443950000	0.608418000	-2.525833000
H	-3.238434000	2.250250000	2.338906000	H	3.910674000	0.491856000	1.521908000
H	-3.323653000	-2.551336000	3.616738000	H	3.818877000	2.612371000	-2.966933000
H	-4.081066000	1.581836000	4.572572000	H	5.256527000	2.524007000	1.088807000
H	-4.128997000	-0.817804000	5.221549000	H	5.211636000	3.595199000	-1.154109000
C	3.369686000	0.313025000	1.560960000	C	-2.941485000	-1.196818000	1.221212000
C	2.836473000	-0.255904000	2.726623000	C	-1.974208000	-1.753292000	2.069004000
C	4.643291000	0.896538000	1.589960000	C	-4.301909000	-1.408571000	1.493163000
C	3.579377000	-0.251994000	3.908056000	C	-2.360740000	-2.502680000	3.181957000
C	5.379443000	0.908138000	2.776406000	C	-4.686685000	-2.162908000	2.602570000
C	4.849913000	0.331108000	3.934072000	C	-3.716382000	-2.708687000	3.449602000
H	1.833854000	-0.671679000	2.710277000	H	-0.920024000	-1.615978000	1.852435000
H	5.052980000	1.342659000	0.688113000	H	-5.053685000	-0.987222000	0.832212000
H	3.159645000	-0.688290000	4.810306000	H	-1.599902000	-2.929408000	3.829974000
H	6.364318000	1.367152000	2.796517000	H	-5.741952000	-2.326309000	2.804878000
H	5.423460000	0.341916000	4.857240000	H	-4.018240000	-3.297565000	4.311935000
C	3.058561000	-1.347024000	-0.767851000	C	-2.775852000	1.566984000	0.376869000
C	3.750872000	-2.301225000	-0.004139000	C	-3.290718000	1.833607000	1.654283000
C	2.777366000	-1.620055000	-2.118340000	C	-2.471978000	2.642603000	-0.474860000
C	4.145543000	-3.510690000	-0.579344000	C	-3.500574000	3.151698000	2.068415000
C	3.172847000	-2.830903000	-2.685643000	C	-2.683409000	3.956278000	-0.057561000
C	3.855587000	-3.779036000	-1.918989000	C	-3.197676000	4.215034000	1.215861000
H	3.980300000	-2.102625000	1.037692000	H	-3.526190000	1.016849000	2.327816000
H	2.218717000	-0.907741000	-2.712383000	H	-2.030752000	2.455281000	-1.447233000
H	4.678736000	-4.241969000	0.022426000	H	-3.898653000	3.344191000	3.061416000
H	2.925787000	-3.035922000	-3.722903000	H	-2.426131000	4.776101000	-0.722311000
H	4.155668000	-4.724797000	-2.362494000	H	-3.353587000	5.239404000	1.543821000
C	2.997179000	1.567241000	-1.033665000	C	-3.623809000	-0.515452000	-1.494693000
C	3.994453000	1.423058000	-2.007800000	C	-4.229545000	0.492534000	-2.258640000
C	2.413461000	2.827248000	-0.817437000	C	-3.940049000	-1.860050000	-1.758215000
C	4.397905000	2.526732000	-2.764286000	C	-5.129308000	0.162299000	-3.274781000
C	2.824241000	3.926196000	-1.572042000	C	-4.842340000	-2.182949000	-2.771550000
C	3.813125000	3.777035000	-2.549709000	C	-5.436436000	-1.174388000	-3.535410000
H	4.445738000	0.451335000	-2.179897000	H	-4.015790000	1.535446000	-2.057346000
H	1.654094000	2.940145000	-0.048879000	H	-3.480167000	-2.646959000	-1.172589000
H	5.168312000	2.407190000	-3.521454000	H	-5.592747000	0.954342000	-3.857055000
H	2.370815000	4.898493000	-1.397711000	H	-5.077779000	-3.226059000	-2.964892000
H	4.127110000	4.632714000	-3.141692000	H	-6.137439000	-1.429307000	-4.325978000
C	-0.266664000	-1.733070000	-1.820371000	C	0.452474000	2.026566000	-0.771216000
O	-0.301963000	-2.135722000	-2.977274000	O	0.176169000	1.857792000	-1.965200000
O	0.149051000	-0.523868000	-1.516114000	O	0.269407000	1.123091000	0.155322000
DMI				MnCl₂			
C	0.000040000	-0.709189000	0.000016000	Mn	0.000000000	0.000000000	0.000000000
N	-1.100500000	0.114564000	0.212322000	Cl	0.000000000	0.000000000	2.200978000
C	-0.763080000	1.492708000	-0.101064000	Cl	0.000000000	0.000000000	-2.200978000
C	0.762848000	1.492861000	0.101194000				
N	1.100481000	0.114754000	-0.212301000				
O	0.000167000	-1.930813000	0.000109000				
C	-2.439062000	-0.382120000	-0.019524000				
C	2.439124000	-0.381965000	0.019336000				
H	-1.024866000	1.736165000	-1.145166000				
H	-1.278666000	2.196804000	0.561349000				
H	1.024899000	1.736329000	1.145199000				
H	1.278070000	2.197076000	-0.561394000				
H	-2.432067000	-1.461685000	0.151205000				
H	-3.143583000	0.094575000	0.672934000				
H	-2.771304000	-0.182570000	-1.052323000				
H	3.143666000	0.095469000	-0.672587000				

H	2.771096000	-0.183264000	1.052366000		
H	2.432336000	-1.461377000	-0.152351000		
Mn(O₂CPh)₂				MnPh₂	
Mn	-0.000003000	-0.020788000	-0.000181000	Mn	0.000000000
C	3.911856000	0.003164000	0.000125000	C	2.053174000
C	4.616559000	-0.835117000	-0.876716000	C	2.803112000
C	4.606910000	0.848900000	0.877501000	C	2.802793000
C	6.010449000	-0.825989000	-0.874325000	C	4.200819000
C	6.000797000	0.854603000	0.876277000	C	4.200509000
C	6.702296000	0.017993000	0.001278000	C	4.903487000
H	4.058148000	-1.480800000	-1.546293000	H	2.288106000
H	6.558270000	-1.474436000	-1.552472000	H	4.741751000
H	6.541081000	1.508782000	1.554969000	H	4.741177000
H	7.789263000	0.023702000	0.001776000	H	5.990951000
C	2.431979000	-0.005211000	0.000385000	C	-2.053174000
O	1.782152000	-0.772926000	-0.795440000	C	-2.803109000
O	1.773540000	0.754129000	0.796517000	C	-2.802796000
C	-3.911870000	0.002769000	-0.000010000	C	-4.200817000
C	-4.606124000	0.884983000	-0.841474000	C	-4.200512000
C	-4.617355000	-0.871226000	0.840468000	C	-4.903488000
C	-6.000006000	0.891274000	-0.840552000	H	-2.288114000
C	-6.011204000	-0.861536000	0.837737000	H	-4.741742000
C	-6.702273000	0.018859000	-0.001904000	H	-4.741184000
H	-4.039639000	1.551827000	-1.482919000	H	-5.990952000
H	-6.539719000	1.573733000	-1.491283000	H	2.288668000
H	-6.559602000	-1.537764000	1.487707000	H	-2.288661000
H	-7.789237000	0.025041000	-0.002705000		
C	-2.432051000	-0.006239000	0.000262000		
O	-1.773020000	0.784081000	-0.764904000		
O	-1.782640000	-0.804978000	0.765339000		
H	-4.059515000	-1.544621000	1.482672000		
H	4.040995000	1.488427000	1.546664000		
4...DMI				5...DMI	
P	-1.987598000	0.363430000	-0.136858000	P	2.384305000
P	1.054658000	-1.562970000	0.271694000	P	-2.055288000
Ni	0.249806000	0.204780000	-0.797261000	Ni	0.137829000
C	2.072928000	0.538930000	-1.257002000	C	0.169838000
C	2.796512000	1.251736000	-0.289785000	C	0.079110000
C	2.706260000	0.261465000	-2.477683000	C	0.262295000
C	4.086926000	1.727090000	-0.544839000	C	0.067297000
C	4.011523000	0.700032000	-2.725942000	C	0.247918000
C	4.704823000	1.445706000	-1.765365000	C	0.145708000
H	2.364310000	1.411466000	0.690691000	H	0.024725000
H	4.613877000	2.284696000	0.226968000	H	-0.006356000
H	4.483940000	0.469033000	-3.678681000	H	0.311813000
H	5.716404000	1.792182000	-1.964574000	H	0.134660000
Cl	-0.457287000	0.705123000	-2.922085000	Cl	0.195676000
H	2.174363000	-0.288154000	-3.246351000	H	0.319023000
C	-0.099897000	-2.432139000	1.411752000	C	-3.134938000
C	-0.732582000	-3.634701000	1.061305000	C	-4.196364000
C	-0.414752000	-1.839075000	2.645412000	C	-2.871053000
C	-1.636951000	-4.239312000	1.937634000	C	-4.957415000
C	-1.293647000	-2.458358000	3.531889000	C	-3.637474000
C	-1.909818000	-3.660590000	3.178350000	C	-4.676122000
H	-0.519394000	-4.102967000	0.107136000	H	-4.433483000
H	0.012320000	-0.878200000	2.908763000	H	-2.074717000
H	-2.123302000	-5.167170000	1.648114000	H	-5.770472000
H	-1.527432000	-1.975704000	4.474402000	H	-3.407498000
H	-2.610492000	-4.135319000	3.860208000	H	-5.265061000
C	2.678263000	-1.588973000	1.161822000	C	-2.088679000

C	2.798628000	-1.714422000	2.552405000	C	-2.823748000	-3.385137000	-0.402751000
C	3.849688000	-1.487467000	0.389100000	C	-1.284859000	-2.652226000	-2.125403000
C	4.058334000	-1.717751000	3.159929000	C	-2.739405000	-4.693080000	-0.890911000
C	5.103132000	-1.495679000	0.997021000	C	-1.206456000	-3.957535000	-2.610503000
C	5.213626000	-1.604627000	2.386072000	C	-1.927411000	-4.983280000	-1.989066000
H	1.920461000	-1.836715000	3.172974000	H	-3.453803000	-3.168293000	0.453196000
H	3.783031000	-1.390034000	-0.688161000	H	-0.722718000	-1.853614000	-2.602406000
H	4.129546000	-1.820148000	4.239807000	H	-3.308150000	-5.483985000	-0.408718000
H	5.992732000	-1.407128000	0.379622000	H	-0.580969000	-4.172166000	-3.473434000
H	6.192161000	-1.608568000	2.859548000	H	-1.859590000	-6.001862000	-2.362311000
C	1.375495000	-2.827286000	-1.030144000	C	-3.097012000	0.250232000	-1.652358000
C	0.963663000	-2.625483000	-2.353382000	C	-2.885626000	1.615570000	-1.886212000
C	2.020311000	-4.026852000	-0.683965000	C	-4.166793000	-0.403202000	-2.278779000
C	1.182664000	-3.617407000	-3.314882000	C	-3.743658000	2.319451000	-2.733631000
C	2.239417000	-5.012804000	-1.644886000	C	-5.017839000	0.301805000	-3.132678000
C	1.818629000	-4.809298000	-2.964196000	C	-4.809335000	1.665303000	-3.358557000
H	0.478485000	-1.696943000	-2.637345000	H	-2.038464000	2.107747000	-1.424418000
H	2.350371000	-4.182502000	0.339007000	H	-4.332507000	-1.461355000	-2.097893000
H	0.859858000	-3.447308000	-4.338506000	H	-3.568017000	3.375817000	-2.922027000
H	2.739407000	-5.936978000	-1.366812000	H	-5.841922000	-0.212882000	-3.619873000
H	1.991454000	-5.577121000	-3.714098000	H	-5.470614000	2.213718000	-4.024583000
C	-3.020633000	-0.874473000	-1.005965000	C	3.152213000	1.590940000	-0.765452000
C	-2.400047000	-2.031413000	-1.490420000	C	3.285559000	1.779719000	-2.151855000
C	-4.404712000	-0.717766000	-1.180714000	C	3.528091000	2.628751000	0.099563000
C	-3.144919000	-3.024932000	-2.127421000	C	3.775452000	2.984516000	-2.657245000
C	-5.151735000	-1.709291000	-1.818883000	C	4.018797000	3.832563000	-0.410120000
C	-4.522909000	-2.866086000	-2.291071000	C	4.138781000	4.017320000	-1.788969000
H	-1.329288000	-2.143947000	-1.388213000	H	2.992500000	0.990997000	-2.833468000
H	-4.890864000	0.185938000	-0.825591000	H	3.436185000	2.508997000	1.170581000
H	-2.643554000	-3.911897000	-2.506032000	H	3.867187000	3.114784000	-3.732343000
H	-6.222316000	-1.576977000	-1.952315000	H	4.304986000	4.625844000	0.275679000
H	-5.105202000	-3.634948000	-2.792515000	H	4.517401000	4.956605000	-2.184347000
C	-2.535102000	0.229429000	1.625257000	C	3.215757000	-0.258759000	1.467562000
C	-3.629841000	-0.554001000	2.015847000	C	2.888350000	0.562081000	2.560914000
C	-1.838953000	0.958284000	2.605803000	C	4.139503000	-1.297002000	1.651135000
C	-4.036269000	-0.590678000	3.351465000	C	3.504341000	0.368445000	3.796889000
C	-2.254229000	0.925954000	3.938289000	C	4.742896000	-1.496615000	2.895790000
C	-3.356592000	0.154774000	4.316470000	C	4.433391000	-0.660806000	3.969625000
H	-4.165623000	-1.146811000	1.284117000	H	2.137943000	1.335087000	2.446305000
H	-0.976361000	1.550888000	2.321085000	H	4.390998000	-1.955573000	0.827590000
H	-4.885815000	-1.206669000	3.635293000	H	3.243781000	1.014556000	4.631476000
H	-1.711604000	1.504270000	4.682435000	H	5.455087000	-2.308181000	3.021477000
H	-3.679006000	0.130533000	5.354573000	H	4.905746000	-0.815229000	4.936493000
C	-2.727529000	1.977689000	-0.642111000	C	3.082389000	-1.237161000	-1.264478000
C	-2.727582000	3.077264000	0.228450000	C	4.435269000	-1.230824000	-1.639083000
C	-3.228082000	2.141409000	-1.944289000	C	2.242109000	-2.244614000	-1.753480000
C	-3.214060000	4.315215000	-0.195489000	C	4.938045000	-2.224844000	-2.479801000
C	-3.717429000	3.379745000	-2.362828000	C	2.744497000	-3.240778000	-2.592716000
C	-3.708628000	4.471867000	-1.492032000	C	4.093131000	-3.233223000	-2.955989000
H	-2.335022000	2.978893000	1.231386000	H	5.088598000	-0.442935000	-1.275525000
H	-3.221297000	1.305874000	-2.632615000	H	1.191015000	-2.235707000	-1.493444000
H	-3.204200000	5.157144000	0.492098000	H	5.986393000	-2.211076000	-2.766416000
H	-4.097795000	3.488711000	-3.375069000	H	2.077392000	-4.014203000	-2.964852000
H	-4.086140000	5.436932000	-1.820864000	H	4.485703000	-4.005259000	-3.612901000
C	1.057441000	3.498537000	0.740697000	C	-0.497623000	3.010510000	1.039239000
N	1.150766000	4.172424000	-0.446481000	N	-1.613443000	3.197478000	1.832751000
C	2.433909000	4.854760000	-0.536068000	C	-2.712963000	3.723217000	1.036096000
C	2.811695000	5.017221000	0.948064000	C	-1.958754000	4.396644000	-0.123478000
N	2.107604000	3.897890000	1.553061000	N	-0.739312000	3.607949000	-0.180625000
O	0.207509000	2.657211000	1.046306000	O	0.531602000	2.418622000	1.366798000
C	0.495075000	3.685878000	-1.647935000	C	-1.854568000	2.390065000	3.012115000
C	2.049796000	3.742796000	2.987135000	C	0.326993000	3.947719000	-1.101072000
H	3.162539000	4.221141000	-1.063486000	H	-3.355208000	2.911264000	0.666123000

H	2.339953000	5.812841000	-1.058205000	H	-3.323847000	4.425369000	1.614125000
H	2.449412000	5.976371000	1.355849000	H	-1.734031000	5.453312000	0.098335000
H	3.891840000	4.949307000	1.118871000	H	-2.511044000	4.343345000	-1.067507000
H	-0.421918000	3.170720000	-1.365115000	H	-0.905087000	2.258210000	3.536661000
H	0.247445000	4.536349000	-2.293672000	H	-2.555092000	2.921681000	3.666560000
H	1.135027000	2.979165000	-2.188894000	H	-2.270072000	1.403759000	2.769628000
H	3.056135000	3.566999000	3.386466000	H	-0.035883000	3.847503000	-2.128596000
H	1.627981000	4.635877000	3.479472000	H	0.684107000	4.976701000	-0.931289000
H	1.417310000	2.879668000	3.210703000	H	1.147069000	3.246468000	-0.959147000
4A				4B			
P	0.522080000	-0.059013000	-0.012725000	P	-0.447500000	0.047675000	-0.015147000
Ni	-0.387763000	1.891286000	-0.121653000	Ni	0.276647000	-1.387934000	-1.400631000
C	-2.034821000	1.047527000	-0.096891000	C	1.974181000	-0.794684000	-0.956020000
C	-2.711615000	0.906681000	-1.315387000	C	2.690285000	-1.328700000	0.127923000
C	-2.627993000	0.587705000	1.084664000	C	2.630395000	0.082605000	-1.836077000
C	-3.971255000	0.300994000	-1.350409000	C	4.042642000	-1.015703000	0.309623000
C	-3.889128000	-0.020941000	1.043668000	C	3.981950000	0.389668000	-1.659438000
C	-4.559227000	-0.172450000	-0.173279000	C	4.688478000	-0.153480000	-0.581229000
H	-2.256738000	1.260150000	-2.236602000	H	2.188871000	-1.974027000	0.844511000
H	-4.489506000	0.194704000	-2.300561000	H	4.586934000	-1.437105000	1.151821000
H	-4.341814000	-0.379416000	1.965437000	H	4.479105000	1.064998000	-2.351937000
H	-5.534701000	-0.651111000	-0.203919000	H	5.735559000	0.098846000	-0.433243000
Cl	-0.486772000	4.022513000	-0.229605000	Cl	-1.156875000	-2.710421000	-2.332829000
H	-2.107460000	0.678678000	2.032894000	H	2.080121000	0.540826000	-2.655173000
C	-0.017491000	-1.382431000	-1.150698000	C	-0.222973000	-0.614827000	1.671600000
C	-1.292963000	-1.953426000	-0.993640000	C	0.027414000	0.203319000	2.781326000
C	0.809658000	-1.810194000	-2.199369000	C	-0.347413000	-2.003231000	1.842264000
C	-1.723834000	-2.943708000	-1.875560000	C	0.156771000	-0.364527000	4.051583000
C	0.366994000	-2.796969000	-3.083865000	C	-0.220043000	-2.564684000	3.112967000
C	-0.898286000	-3.365288000	-2.922686000	C	0.034620000	-1.746186000	4.218298000
H	-1.946620000	-1.624291000	-0.193110000	H	0.131665000	1.275803000	2.651097000
H	1.796521000	-1.375795000	-2.323702000	H	-0.538088000	-2.636060000	0.977902000
H	-2.711659000	-3.377622000	-1.748108000	H	0.355162000	0.273193000	4.908837000
H	1.013636000	-3.121347000	-3.894662000	H	-0.314502000	-3.639680000	3.238714000
H	-1.241314000	-4.133406000	-3.610787000	H	0.139771000	-2.185305000	5.206738000
C	2.310364000	0.159823000	-0.332093000	C	-2.250387000	0.325673000	-0.171597000
C	2.706238000	1.183855000	-1.207287000	C	-2.991743000	0.755451000	0.940331000
C	3.279138000	-0.664355000	0.260042000	C	-2.876852000	0.182844000	-1.416539000
C	4.059756000	1.374674000	-1.494244000	C	-4.350614000	1.039130000	0.804783000
C	4.630225000	-0.468743000	-0.028313000	C	-4.237082000	0.474287000	-1.547624000
C	5.020699000	0.548799000	-0.905403000	C	-4.973531000	0.900859000	-0.440008000
H	1.958289000	1.834290000	-1.656250000	H	-2.508294000	0.858728000	1.907477000
H	2.974037000	-1.448734000	0.946646000	H	-2.311622000	-0.182201000	-2.267495000
H	4.360783000	2.171851000	-2.167967000	H	-4.923151000	1.364071000	1.669384000
H	5.378720000	-1.107283000	0.433066000	H	-4.720449000	0.353422000	-2.512919000
H	6.074239000	0.701162000	-1.123840000	H	-6.033254000	1.118725000	-0.543226000
C	0.420753000	-0.780463000	1.659251000	C	0.254888000	1.739529000	0.006028000
C	0.408716000	-2.163512000	1.884718000	C	1.556519000	1.965646000	0.487512000
C	0.392655000	0.103164000	2.749606000	C	-0.493896000	2.818450000	-0.487385000
C	0.372866000	-2.657347000	3.191356000	C	2.088467000	3.253943000	0.483619000
C	0.360032000	-0.393391000	4.052689000	C	0.050619000	4.105268000	-0.501116000
C	0.349988000	-1.774531000	4.274200000	C	1.339676000	4.325743000	-0.013335000
H	0.412963000	-2.848081000	1.041880000	H	2.153088000	1.138003000	0.854573000
H	0.381131000	1.176211000	2.569667000	H	-1.500722000	2.656771000	-0.858287000
H	0.359728000	-3.730461000	3.362005000	H	3.094764000	3.416899000	0.859388000
H	0.333796000	0.295236000	4.892606000	H	-0.537318000	4.932551000	-0.889129000
H	0.318431000	-2.161093000	5.289299000	H	1.761407000	5.327358000	-0.021006000

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