

Supporting Information for

## Chemical bonding in supermolecular flowers

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Cartesian coordinates (Å)

<i>metallo_ca1</i>			H	-0.71147393	2.18969160	-1.84327386
Ca	0.00000000	0.00000000	H	1.86266293	1.35330383	-1.84327386
C	0.97764905	0.71030361	H	1.86266293	-1.35330383	-1.84327386
C	-0.37342871	1.14929539	H	-0.71147393	-2.18969160	-1.84327386
C	-1.20844069	0.00000000	<i>metallo_co6</i>			
C	-0.37342871	-1.14929539	Co	0.00000000	0.00000000	0.00000000
C	0.97764905	-0.71030361	C	0.99644969	0.72396308	1.89192956
H	1.85725788	1.34937683	C	-0.38060991	1.17139686	1.89192956
H	-0.70940938	2.18333758	C	-1.23167955	0.00000000	1.89192956
H	-2.29569699	0.00000000	C	-0.38060991	-1.17139686	1.89192956
H	-0.70940938	-2.18333758	C	0.99644969	-0.72396308	1.89192956
H	1.85725788	-1.34937683	H	1.87507074	1.36231864	1.88349384
C	-1.20844069	0.00000000	H	-0.71621329	2.20427786	1.88349384
C	-0.37342871	1.14929539	H	-2.31771490	0.00000000	1.88349384
C	0.97764905	0.71030361	H	-0.71621329	-2.20427786	1.88349384
C	0.97764905	-0.71030361	H	1.87507074	-1.36231864	1.88349384
C	-0.37342871	-1.14929539	C	-1.23167955	0.00000000	-1.89192956
H	-2.29569699	0.00000000	C	-0.38060991	1.17139686	-1.89192956
H	-0.70940938	2.18333758	C	0.99644969	0.72396308	-1.89192956
H	1.85725788	1.34937683	C	0.99644969	-0.72396308	-1.89192956
H	1.85725788	-1.34937683	C	-0.38060991	-1.17139686	-1.89192956
H	-0.70940938	-2.18333758	H	-2.31771490	0.00000000	-1.88349384
<i>metallo_co2</i>			H	-0.71621329	2.20427786	-1.88349384
Co	0.00000000	0.00000000	H	1.87507074	1.36231864	-1.88349384
C	0.98514056	0.71574651	H	1.87507074	-1.36231864	-1.88349384
C	-0.37629021	1.15810218	H	-0.71621329	-2.20427786	-1.88349384
C	-1.21770070	0.00000000	<i>metallo_cr1</i>			
C	-0.37629021	-1.15810218	Cr	0.00000000	0.00000000	0.00000000
C	0.98514056	-0.71574651	C	0.99143634	0.72032066	1.71318430
H	1.86393449	1.35422767	C	-0.37869498	1.16550332	1.71318430
H	-0.71195962	2.19118640	C	-1.22548271	0.00000000	1.71318430
H	-2.30394973	0.00000000	C	-0.37869498	-1.16550332	1.71318430
H	-0.71195962	-2.19118640	C	0.99143634	-0.72032066	1.71318430
H	1.86393449	-1.35422767	H	1.86959413	1.35833965	1.68657467
C	-1.21770070	0.00000000	H	-0.71412141	2.19783971	1.68657467
C	-0.37629021	1.15810218	H	-2.31094543	0.00000000	1.68657467
C	0.98514056	0.71574651	H	-0.71412141	-2.19783971	1.68657467
C	0.98514056	-0.71574651	H	1.86959413	-1.35833965	1.68657467
C	-0.37629021	-1.15810218	C	-1.22548271	0.00000000	-1.71318430
H	-2.30394973	0.00000000	C	-0.37869498	1.16550332	-1.71318430
H	-0.71195962	2.19118640	C	0.99143634	0.72032066	-1.71318430
H	1.86393449	1.35422767	C	0.99143634	-0.72032066	-1.71318430
H	1.86393449	-1.35422767	C	-0.37869498	-1.16550332	-1.71318430
H	-0.71195962	-2.19118640	H	-2.31094543	0.00000000	-1.68657467
<i>metallo_co4</i>			H	-0.71412141	2.19783971	-1.68657467
Co	0.00000000	0.00000000	H	1.86959413	1.35833965	-1.68657467
C	0.98388939	0.71483749	H	1.86959413	-1.35833965	-1.68657467
C	-0.37581231	1.15663135	H	-0.71412141	-2.19783971	-1.68657467
C	-1.21615417	0.00000000	<i>metallo_cr3</i>			
C	-0.37581231	-1.15663135	Cr	0.00000000	0.00000000	0.00000000
C	0.98388939	-0.71483749	C	0.98622583	0.71653501	1.78178587
H	1.86266293	1.35330383	C	-0.37670475	1.15937800	1.78178587
H	-0.71147393	2.18969160	C	-1.21904217	0.00000000	1.78178587
H	-2.30237800	0.00000000	C	-0.37670475	-1.15937800	1.78178587
H	-0.71147393	-2.18969160	C	0.98622583	-0.71653501	1.78178587
H	1.86266293	-1.35330383	H	1.86488982	1.35492177	1.76665127
C	-1.21615417	0.00000000	H	-0.71232453	2.19230947	1.76665127
C	-0.37581231	1.15663135	H	-2.30513059	0.00000000	1.76665127
C	0.98388939	0.71483749	H	-0.71232453	-2.19230947	1.76665127
C	0.98388939	-0.71483749	H	1.86488982	-1.35492177	1.76665127
C	-0.37581231	-1.15663135	C	-1.21904217	0.00000000	-1.78178587
H	-2.30237800	0.00000000				

C -0.37670475 1.15937800 -1.78178587  
 C 0.98622583 0.71653501 -1.78178587  
 C 0.98622583 -0.71653501 -1.78178587  
 C -0.37670475 -1.15937800 -1.78178587  
 H -2.30513059 0.00000000 -1.76665127  
 H -0.71232453 2.19230947 -1.76665127  
 H 1.86488982 1.35492177 -1.76665127  
 H 1.86488982 -1.35492177 -1.76665127  
 H -0.71232453 -2.19230947 -1.76665127

metallo\_cr5

Cr 0.00000000 0.00000000 0.00000000  
 C 0.98081330 0.71260258 1.99802927  
 C -0.37463735 1.15301519 1.99802927  
 C -1.21235191 0.00000000 1.99802927  
 C -0.37463735 -1.15301519 1.99802927  
 C 0.98081330 -0.71260258 1.99802927  
 H 1.86008390 1.35143006 1.99623064  
 H -0.71048883 2.18665977 1.99623064  
 H -2.29919014 0.00000000 1.99623064  
 H -0.71048883 -2.18665977 1.99623064  
 H 1.86008390 -1.35143006 1.99623064  
 C -1.21235191 0.00000000 -1.99802927  
 C -0.37463735 1.15301519 -1.99802927  
 C 0.98081330 0.71260258 -1.99802927  
 C 0.98081330 -0.71260258 -1.99802927  
 C -0.37463735 -1.15301519 -1.99802927  
 H -2.29919014 0.00000000 -1.99623064  
 H -0.71048883 2.18665977 -1.99623064  
 H 1.86008390 1.35143006 -1.99623064  
 H 1.86008390 -1.35143006 -1.99623064  
 H -0.71048883 -2.18665977 -1.99623064

metallo\_cu2

Cu 0.00000000 0.00000000 0.00000000  
 C 0.98271288 0.71398270 1.92608100  
 C -0.37536292 1.15524828 1.92608100  
 C -1.21469993 0.00000000 1.92608100  
 C -0.37536292 -1.15524828 1.92608100  
 C 0.98271288 -0.71398270 1.92608100  
 H 1.86182717 1.35269662 1.92335823  
 H -0.71115470 2.18870911 1.92335823  
 H -2.30134495 0.00000000 1.92335823  
 H -0.71115470 -2.18870911 1.92335823  
 H 1.86182717 -1.35269662 1.92335823  
 C -1.21469993 0.00000000 -1.92608100  
 C -0.37536292 1.15524828 -1.92608100  
 C 0.98271288 0.71398270 -1.92608100  
 C 0.98271288 -0.71398270 -1.92608100  
 C -0.37536292 -1.15524828 -1.92608100  
 H -2.30134495 0.00000000 -1.92335823  
 H -0.71115470 2.18870911 -1.92335823  
 H 1.86182717 1.35269662 -1.92335823  
 H 1.86182717 -1.35269662 -1.92335823  
 H -0.71115470 -2.18870911 -1.92335823

metallo\_fe1

Fe 0.00000000 0.00000000 0.00000000  
 C 0.98739999 0.71738809 1.63093414  
 C -0.37715324 1.16075831 1.63093414  
 C -1.22049351 0.00000000 1.63093414  
 C -0.37715324 -1.16075831 1.63093414  
 C 0.98739999 -0.71738809 1.63093414  
 H 1.86641677 1.35603115 1.60653358  
 H -0.71290777 2.19410450 1.60653358  
 H -2.30701800 0.00000000 1.60653358  
 H -0.71290777 -2.19410450 1.60653358  
 H 1.86641677 -1.35603115 1.60653358  
 C -1.22049351 0.00000000 -1.63093414  
 C -0.37715324 1.16075831 -1.63093414  
 C 0.98739999 0.71738809 -1.63093414  
 C 0.98739999 -0.71738809 -1.63093414  
 C -0.37715324 -1.16075831 -1.63093414  
 H -2.30701800 0.00000000 -1.60653358  
 H -0.71290777 2.19410450 -1.60653358  
 H 1.86641677 1.35603115 -1.60653358  
 H 1.86641677 -1.35603115 -1.60653358

H -0.71290777 -2.19410450 -1.60653358

metallo\_fe3

Fe 0.00000000 0.00000000 0.00000000  
 C 0.98686396 0.71699863 1.76145620  
 C -0.37694849 1.16012816 1.76145620  
 C -1.21983093 0.00000000 1.76145620  
 C -0.37694849 -1.16012816 1.76145620  
 C 0.98686396 -0.71699863 1.76145620  
 H 1.86539338 1.35528762 1.74368172  
 H -0.71251687 2.19290143 1.74368172  
 H -2.30575302 0.00000000 1.74368172  
 H -0.71251687 -2.19290143 1.74368172  
 H 1.86539338 -1.35528762 1.74368172  
 C -1.21983093 0.00000000 -1.76145620  
 C -0.37694849 1.16012816 -1.76145620  
 C 0.98686396 0.71699863 -1.76145620  
 C 0.98686396 -0.71699863 -1.76145620  
 C -0.37694849 -1.16012816 -1.76145620  
 H -2.30575302 0.00000000 -1.74368172  
 H -0.71251687 2.19290143 -1.74368172  
 H 1.86539338 1.35528762 -1.74368172  
 H 1.86539338 -1.35528762 -1.74368172  
 H -0.71251687 -2.19290143 -1.74368172

metallo\_fe5

Fe 0.00000000 0.00000000 0.00000000  
 C 0.98254653 0.71386184 1.95051754  
 C -0.37529938 1.15505272 1.95051754  
 C -1.21449430 0.00000000 1.95051754  
 C -0.37529938 -1.15505272 1.95051754  
 C 0.98254653 -0.71386184 1.95051754  
 H 1.86165418 1.35257093 1.94564965  
 H -0.71108862 2.18850574 1.94564965  
 H -2.30113111 0.00000000 1.94564965  
 H -0.71108862 -2.18850574 1.94564965  
 H 1.86165418 -1.35257093 1.94564965  
 C -1.21449430 0.00000000 -1.95051754  
 C -0.37529938 1.15505272 -1.95051754  
 C 0.98254653 0.71386184 -1.95051754  
 C 0.98254653 -0.71386184 -1.95051754  
 C -0.37529938 -1.15505272 -1.95051754  
 H -2.30113111 0.00000000 -1.94564965  
 H -0.71108862 2.18850574 -1.94564965  
 H 1.86165418 1.35257093 -1.94564965  
 H 1.86165418 -1.35257093 -1.94564965  
 H -0.71108862 -2.18850574 -1.94564965

metallo\_mg1

Mg 0.00000000 0.00000000 0.00000000  
 C 0.98020767 0.71216256 2.01582860  
 C -0.37440601 1.15230323 2.01582860  
 C -1.21160331 0.00000000 2.01582860  
 C -0.37440601 -1.15230323 2.01582860  
 C 0.98020767 -0.71216256 2.01582860  
 H 1.85953860 1.35103387 2.02860682  
 H -0.71028054 2.18601872 2.02860682  
 H -2.29851611 0.00000000 2.02860682  
 H -0.71028054 -2.18601872 2.02860682  
 H 1.85953860 -1.35103387 2.02860682  
 C -1.21160331 0.00000000 -2.01582860  
 C -0.37440601 1.15230323 -2.01582860  
 C 0.98020767 0.71216256 -2.01582860  
 C 0.98020767 -0.71216256 -2.01582860  
 C -0.37440601 -1.15230323 -2.01582860  
 H -2.29851611 0.00000000 -2.02860682  
 H -0.71028054 2.18601872 -2.02860682  
 H 1.85953860 1.35103387 -2.02860682  
 H 1.85953860 -1.35103387 -2.02860682  
 H -0.71028054 -2.18601872 -2.02860682

metallo\_mn2

Mn 0.00000000 0.00000000 0.00000000  
 C 0.98992655 0.71922374 1.67261408  
 C -0.37811830 1.16372845 1.67261408  
 C -1.22361651 0.00000000 1.67261408  
 C -0.37811830 -1.16372845 1.67261408  
 C 0.98992655 0.71922374 1.67261408  
 H 1.86823929 1.35735530 1.64864031

H -0.71360391 2.19624701 1.64864031  
 H -2.30927076 0.00000000 1.64864031  
 H -0.71360391 -2.19624701 1.64864031  
 H 1.86823929 -1.35735530 1.64864031  
 C -1.22361651 0.00000000 -1.67261408  
 C -0.37811830 1.16372845 -1.67261408  
 C 0.98992655 0.71922374 -1.67261408  
 C 0.98992655 -0.71922374 -1.67261408  
 C -0.37811830 -1.16372845 -1.67261408  
 H -2.30927076 0.00000000 -1.64864031  
 H -0.71360391 2.19624701 -1.64864031  
 H 1.86823929 1.35735530 -1.64864031  
 H 1.86823929 -1.35735530 -1.64864031  
 H -0.71360391 -2.19624701 -1.64864031

metallo\_mn4

Mn 0.00000000 0.00000000 0.00000000  
 C 0.98442858 0.71522923 1.86363947  
 C -0.37601826 1.15726521 1.86363947  
 C -1.21682065 0.00000000 1.86363947  
 C -0.37601826 -1.15726521 1.86363947  
 C 0.98442858 -0.71522923 1.86363947  
 H 1.86326981 1.35374476 1.85479206  
 H -0.71170574 2.19040503 1.85479206  
 H -2.30312815 0.00000000 1.85479206  
 H -0.71170574 -2.19040503 1.85479206  
 H 1.86326981 -1.35374476 1.85479206  
 C -1.21682065 0.00000000 -1.86363947  
 C -0.37601826 1.15726521 -1.86363947  
 C 0.98442858 0.71522923 -1.86363947  
 C -0.37601826 -1.15726521 -1.86363947  
 H -2.30312815 0.00000000 -1.85479206  
 H -0.71170574 2.19040503 -1.85479206  
 H 1.86326981 1.35374476 -1.85479206  
 H 1.86326981 -1.35374476 -1.85479206  
 H -0.71170574 -2.19040503 -1.85479206

metallo\_mn6

Mn 0.00000000 0.00000000 0.00000000  
 C 0.98105935 0.71278134 2.06325897  
 C -0.37473133 1.15330443 2.06325897  
 C -1.21265604 0.00000000 2.06325897  
 C -0.37473133 -1.15330443 2.06325897  
 C 0.98105935 -0.71278134 2.06325897  
 H 1.86050859 1.35173861 2.07045364  
 H -0.71065104 2.18715902 2.07045364  
 H -2.29971509 0.00000000 2.07045364  
 H -0.71065104 -2.18715902 2.07045364  
 H 1.86050859 -1.35173861 2.07045364  
 C -1.21265604 0.00000000 -2.06325897  
 C -0.37473133 1.15330443 -2.06325897  
 C 0.98105935 0.71278134 -2.06325897  
 C 0.98105935 -0.71278134 -2.06325897  
 C -0.37473133 -1.15330443 -2.06325897  
 H -2.29971509 0.00000000 -2.07045364  
 H -0.71065104 2.18715902 -2.07045364  
 H 1.86050859 1.35173861 -2.07045364  
 H 1.86050859 -1.35173861 -2.07045364  
 H -0.71065104 -2.18715902 -2.07045364

metallo\_ni1

Ni 0.00000000 0.00000000 0.00000000  
 C 0.98345874 0.71452460 1.81223098  
 C -0.37564781 1.15612509 1.81223098  
 C -1.21562186 0.00000000 1.81223098  
 C -0.37564781 -1.15612509 1.81223098  
 C 0.98345874 -0.71452460 1.81223098  
 H 1.86230248 1.35304195 1.80076904  
 H -0.71133625 2.18926787 1.80076904  
 H -2.30193246 0.00000000 1.80076904  
 H -0.71133625 -2.18926787 1.80076904  
 H 1.86230248 -1.35304195 1.80076904  
 C -1.21562186 0.00000000 -1.81223098  
 C -0.37564781 1.15612509 -1.81223098  
 C 0.98345874 0.71452460 -1.81223098  
 C 0.98345874 -0.71452460 -1.81223098  
 C -0.37564781 -1.15612509 -1.81223098

H -2.30193246 0.00000000 -1.80076904  
 H -0.71133625 2.18926787 -1.80076904  
 H 1.86230248 1.35304195 -1.80076904  
 H 1.86230248 -1.35304195 -1.80076904  
 H -0.71133625 -2.18926787 -1.80076904

metallo\_ni3

Ni 0.00000000 0.00000000 0.00000000  
 C 0.98299577 0.71418823 1.82098017  
 C -0.37547097 1.15558083 1.82098017  
 C -1.21504959 0.00000000 1.82098017  
 C -0.37547097 -1.15558083 1.82098017  
 C 0.98299577 -0.71418823 1.82098017  
 H 1.86180103 1.35267763 1.80644566  
 H -0.71114471 2.18867838 1.80644566  
 H -2.30131264 0.00000000 1.80644566  
 H -0.71114471 -2.18867838 1.80644566  
 H 1.86180103 -1.35267763 1.80644566  
 C -1.21504959 0.00000000 -1.82098017  
 C -0.37547097 1.15558083 -1.82098017  
 C 0.98299577 0.71418823 -1.82098017  
 C 0.98299577 -0.71418823 -1.82098017  
 C -0.37547097 -1.15558083 -1.82098017  
 H -2.30131264 0.00000000 -1.80644566  
 H -0.71114471 2.18867838 -1.80644566  
 H 1.86180103 1.35267763 -1.80644566  
 H 1.86180103 -1.35267763 -1.80644566  
 H -0.71114471 -2.18867838 -1.80644566

metallo\_cyclopentadiene

C 1.20688836 0.00000000 0.00000000  
 C 0.37294901 1.14781904 0.00000000  
 C -0.97639319 0.70939118 0.00000000  
 C -0.97639319 -0.70939118 0.00000000  
 C 0.37294901 -1.14781904 0.00000000  
 H 2.29999665 0.00000000 0.00000000  
 H 0.71073805 2.18742680 0.00000000  
 H -1.86073638 1.35190411 0.00000000  
 H -1.86073638 -1.35190411 0.00000000  
 H 0.71073805 -2.18742680 0.00000000

metallo\_sc2

Sc 0.00000000 0.00000000 0.00000000  
 C 0.98132968 0.71297774 2.13095757  
 C -0.37483458 1.15362222 2.13095757  
 C -1.21299019 0.00000000 2.13095757  
 C -0.37483458 -1.15362222 2.13095757  
 C 0.98132968 -0.71297774 2.13095757  
 H 1.86090442 1.35202621 2.15205147  
 H -0.71080224 2.18762435 2.15205147  
 H -2.30020437 0.00000000 2.15205147  
 H -0.71080224 -2.18762435 2.15205147  
 H 1.86090442 -1.35202621 2.15205147  
 C -1.21299019 0.00000000 -2.13095757  
 C -0.37483458 1.15362222 -2.13095757  
 C 0.98132968 0.71297774 -2.13095757  
 C 0.98132968 -0.71297774 -2.13095757  
 C -0.37483458 -1.15362222 -2.13095757  
 H -2.30020437 0.00000000 -2.15205147  
 H -0.71080224 2.18762435 -2.15205147  
 H 1.86090442 1.35202621 -2.15205147  
 H 1.86090442 -1.35202621 -2.15205147  
 H -0.71080224 -2.18762435 -2.15205147

metallo\_til

Ti 0.00000000 0.00000000 0.00000000  
 C 0.98501251 0.71565348 1.95797422  
 C -0.37624130 1.15795166 1.95797422  
 C -1.21754242 0.00000000 1.95797422  
 C -0.37624130 -1.15795166 1.95797422  
 C 0.98501251 -0.71565348 1.95797422  
 H 1.86422452 1.35443840 1.96021218  
 H -0.71207040 2.19152736 1.96021218  
 H -2.30430824 0.00000000 1.96021218  
 H -0.71207040 -2.19152736 1.96021218  
 H 1.86422452 -1.35443840 1.96021218  
 C -1.21754242 0.00000000 -1.95797422  
 C -0.37624130 1.15795166 -1.95797422  
 C 0.98501251 0.71565348 -1.95797422

C 0.98501251 -0.71565348 -1.95797422  
C -0.37624130 -1.15795166 -1.95797422  
H -2.30430824 0.00000000 -1.96021218  
H -0.71207040 2.19152736 -1.96021218  
H 1.86422452 1.35443840 -1.96021218  
H 1.86422452 -1.35443840 -1.96021218  
H -0.71207040 -2.19152736 -1.96021218

metallo\_ti3

Ti 0.00000000 0.00000000 0.00000000  
C 0.98343757 0.71450922 1.98006888  
C -0.37563972 1.15610020 1.98006888  
C -1.21559569 0.00000000 1.98006888  
C -0.37563972 -1.15610020 1.98006888  
C 0.98343757 -0.71450922 1.98006888  
H 1.86271284 1.35334009 1.98012159  
H -0.71149299 2.18975027 1.98012159  
H -2.30243969 0.00000000 1.98012159  
H -0.71149299 -2.18975027 1.98012159  
H 1.86271284 -1.35334009 1.98012159  
C -1.21559569 0.00000000 -1.98006888  
C -0.37563972 1.15610020 -1.98006888  
C 0.98343757 0.71450922 -1.98006888  
C 0.98343757 -0.71450922 -1.98006888  
C -0.37563972 -1.15610020 -1.98006888  
H -2.30243969 0.00000000 -1.98012159  
H -0.71149299 2.18975027 -1.98012159  
H 1.86271284 1.35334009 -1.98012159  
H 1.86271284 -1.35334009 -1.98012159  
H -0.71149299 -2.18975027 -1.98012159

metallo\_v2

V 0.00000000 0.00000000 0.00000000  
C 0.98250933 0.71383481 1.90215738  
C -0.37528517 1.15500899 1.90215738  
C -1.21444832 0.00000000 1.90215738  
C -0.37528517 -1.15500899 1.90215738  
C 0.98250933 -0.71383481 1.90215738  
H 1.86170832 1.35261027 1.90042111  
H -0.71110930 2.18856939 1.90042111  
H -2.30119804 0.00000000 1.90042111  
H -0.71110930 -2.18856939 1.90042111  
H 1.86170832 -1.35261027 1.90042111  
C -1.21444832 0.00000000 -1.90215738  
C -0.37528517 1.15500899 -1.90215738  
C 0.98250933 0.71383481 -1.90215738  
C 0.98250933 -0.71383481 -1.90215738  
C -0.37528517 -1.15500899 -1.90215738  
H -2.30119804 0.00000000 -1.90042111  
H -0.71110930 2.18856939 -1.90042111  
H 1.86170832 1.35261027 -1.90042111  
H 1.86170832 -1.35261027 -1.90042111  
H -0.71110930 -2.18856939 -1.90042111

metallo\_v4

V 0.00000000 0.00000000 0.00000000  
C 0.98158008 0.71315967 1.91934013  
C -0.37493023 1.15391659 1.91934013  
C -1.21329970 0.00000000 1.91934013  
C -0.37493023 -1.15391659 1.91934013  
C 0.98158008 -0.71315967 1.91934013  
H 1.86066909 1.35185522 1.91338982  
H -0.71071235 2.18734770 1.91338982  
H -2.29991348 0.00000000 1.91338982  
H -0.71071235 -2.18734770 1.91338982  
H 1.86066909 -1.35185522 1.91338982  
C -1.21329970 0.00000000 -1.91934013  
C -0.37493023 1.15391659 -1.91934013  
C 0.98158008 0.71315967 -1.91934013  
C 0.98158008 -0.71315967 -1.91934013  
C -0.37493023 -1.15391659 -1.91934013  
H -2.29991348 0.00000000 -1.91338982  
H -0.71071235 2.18734770 -1.91338982  
H 1.86066909 1.35185522 -1.91338982  
H 1.86066909 -1.35185522 -1.91338982  
H -0.71071235 -2.18734770 -1.91338982

metallo\_zn1

Zn 0.00000000 0.00000000 0.00000000

C 0.98365555 0.71466759 1.97166220  
C -0.37572299 1.15635645 1.97166220  
C -1.21586512 0.00000000 1.97166220  
C -0.37572299 -1.15635645 1.97166220  
C 0.98365555 -0.71466759 1.97166220  
H 1.86279379 1.35339891 1.97322920  
H -0.71152391 2.18984543 1.97322920  
H -2.30253975 0.00000000 1.97322920  
H -0.71152391 -2.18984543 1.97322920  
H 1.86279379 -1.35339891 1.97322920  
C -1.21586512 0.00000000 -1.97166220  
C -0.37572299 1.15635645 -1.97166220  
C 0.98365555 0.71466759 -1.97166220  
C 0.98365555 -0.71466759 -1.97166220  
C -0.37572299 -1.15635645 -1.97166220  
H -2.30253975 0.00000000 -1.97322920  
H -0.71152391 2.18984543 -1.97322920  
H 1.86279379 1.35339891 -1.97322920  
H 1.86279379 -1.35339891 -1.97322920  
H -0.71152391 -2.18984543 -1.97322920

super[5]phane\_ca1

Ca	0-00000000	0-00000000	0-00000000
C	0-37710000	1-16060000	-1-97620000
C	-0-98730000	0-71730000	-1-97620000
C	-0-98730000	-0-71730000	-1-97620000
C	0-82460000	2-53770000	-1-54520000
C	-2-15870000	1-56840000	-1-54520000
C	-2-15870000	-1-56840000	-1-54520000
C	1-00340000	3-08800000	0-00000000
H	1-80780000	2-72220000	-2-00100000
H	0-13750000	3-26490000	-2-00100000
C	-2-62680000	1-90850000	0-00000000
H	-2-03030000	2-56060000	-2-00100000
H	-3-06260000	1-13970000	-2-00100000
H	-2-03030000	-2-56060000	-2-00100000
C	-2-62680000	-1-90850000	0-00000000
C	-0-98730000	-0-71730000	1-97620000
C	1-22040000	0-00000000	-1-97620000
C	-0-98730000	0-71730000	1-97620000
C	0-37710000	-1-16060000	1-97620000
C	0-37710000	-1-16060000	-1-97620000
C	0-37710000	1-16060000	1-97620000
C	1-22040000	0-00000000	1-97620000
H	-3-06260000	-1-13970000	-2-00100000
C	-2-15870000	-1-56840000	1-54520000
C	2-66830000	0-00000000	-1-54520000
C	-2-15870000	1-56840000	1-54520000
C	0-82460000	-2-53770000	1-54520000
C	0-82460000	-2-53770000	-1-54520000
C	0-82460000	2-53770000	1-54520000
C	2-66830000	0-00000000	1-54520000
H	0-13750000	3-26490000	2-00100000
H	-3-06260000	-1-13970000	2-00100000
H	-2-03030000	-2-56060000	2-00100000
C	3-24690000	0-00000000	0-00000000
H	3-14760000	0-87810000	-2-00100000
H	3-14760000	-0-87810000	-2-00100000
H	3-14760000	-0-87810000	2-00100000
H	-3-06260000	1-13970000	2-00100000
H	-2-03030000	2-56060000	2-00100000
H	3-14760000	0-87810000	2-00100000
H	0-13750000	-3-26490000	2-00100000
H	1-80780000	-2-72220000	2-00100000
C	1-00340000	-3-08800000	0-00000000
H	1-80780000	-2-72220000	-2-00100000
H	0-13750000	-3-26490000	-2-00100000
H	1-80780000	2-72220000	2-00100000
H	0-38170000	3-99220000	0-00000000
H	2-03780000	3-45410000	0-00000000
H	3-91480000	0-87070000	0-00000000
H	3-91480000	-0-87070000	0-00000000
H	0-38170000	-3-99220000	0-00000000
H	2-03780000	-3-45410000	0-00000000
H	-2-65530000	-3-00540000	0-00000000
H	-3-67890000	-1-59670000	0-00000000
H	-3-67890000	1-59670000	0-00000000
H	-2-65530000	3-00540000	0-00000000

super[5]phane\_co2

Co	0-00000000	0-00000000	0-00000000
C	0-38160000	1-17450000	-1-55990000
C	-0-99910000	0-72590000	-1-55990000
C	-0-99910000	-0-72590000	-1-55990000
C	0-84390000	2-59720000	-1-41700000
C	-2-20930000	1-60520000	-1-41700000
C	-2-20930000	-1-60520000	-1-41700000
C	1-06600000	3-28070000	0-00000000
H	1-79660000	2-68830000	-1-96300000
H	0-12660000	3-23090000	-1-96300000
C	-2-79070000	2-02760000	0-00000000
H	-2-00150000	2-53940000	-1-96300000
H	-3-03360000	1-11880000	-1-96300000
H	-2-00150000	-2-53940000	-1-96300000
C	-2-79070000	-2-02760000	0-00000000
C	-0-99910000	-0-72590000	1-55990000
C	1-23500000	0-00000000	-1-55990000

C	-0-99910000	0-72590000	1-55990000
C	0-38160000	-1-17450000	1-55990000
C	0-38160000	-1-17450000	-1-55990000
C	0-38160000	1-17450000	1-55990000
C	1-23500000	0-00000000	1-55990000
H	-3-03360000	-1-11880000	-1-96300000
C	-2-20930000	-1-60520000	1-41700000
C	2-73090000	0-00000000	-1-41700000
C	-2-20930000	1-60520000	1-41700000
C	0-84390000	-2-59720000	1-41700000
C	0-84390000	-2-59720000	-1-41700000
C	0-84390000	2-59720000	1-41700000
C	2-73090000	0-00000000	1-41700000
H	0-12660000	3-23090000	1-96300000
H	-3-03360000	-1-11880000	1-96300000
H	-2-00150000	-2-53940000	1-96300000
C	3-44950000	0-00000000	0-00000000
H	3-11190000	0-87800000	-1-96300000
H	3-11190000	-0-87800000	-1-96300000
H	3-11190000	-0-87800000	1-96300000
H	-3-03360000	1-11880000	1-96300000
H	-2-00150000	-2-53940000	1-96300000
H	3-11190000	0-87800000	1-96300000
H	0-12660000	-3-23090000	1-96300000
H	1-79660000	-2-68830000	1-96300000
C	1-06600000	-3-28070000	0-00000000
H	1-79660000	-2-68830000	-1-96300000
H	0-12660000	-3-23090000	-1-96300000
H	1-79660000	2-68830000	1-96300000
H	0-44460000	4-18810000	0-00000000
H	2-10200000	3-64960000	0-00000000
H	4-12050000	0-87140000	0-00000000
H	4-12050000	-0-87140000	0-00000000
H	0-44460000	-4-18810000	0-00000000
H	2-10200000	-3-64960000	0-00000000
H	-2-82140000	-3-12690000	0-00000000
H	-3-84570000	-1-71700000	0-00000000
H	-3-84570000	1-71700000	0-00000000
H	-2-82140000	3-12690000	0-00000000

super[5]phane\_co4

Co	0-00000000	0-00000000	0-00000000
C	0-38170000	1-17460000	-1-63800000
C	-0-99920000	0-72590000	-1-63800000
C	-0-99920000	-0-72590000	-1-63800000
C	0-84280000	2-59380000	-1-43740000
C	-2-20640000	1-60310000	-1-43740000
C	-2-20640000	-1-60310000	-1-43740000
C	1-05760000	3-25480000	0-00000000
H	1-80070000	2-70210000	-1-97050000
H	0-13140000	3-24440000	-1-97050000
C	-2-76870000	2-01160000	0-00000000
H	-2-01340000	2-54750000	-1-97050000
H	-3-04500000	1-12760000	-1-97050000
H	-2-01340000	-2-54750000	-1-97050000
C	-2-76870000	-2-01160000	0-00000000
C	-0-99920000	-0-72590000	1-63800000
C	1-23510000	0-00000000	-1-63800000
C	-0-99920000	0-72590000	1-63800000
C	0-38170000	-1-17460000	1-63800000
C	0-38170000	-1-17460000	-1-63800000
C	0-38170000	1-17460000	1-63800000
C	1-23510000	0-00000000	1-63800000
H	-3-04500000	-1-12760000	-1-97050000
C	-2-20640000	-1-60310000	1-43740000
C	2-72730000	0-00000000	-1-43740000
C	-2-20640000	1-60310000	1-43740000
C	0-84280000	-2-59380000	1-43740000
C	0-84280000	-2-59380000	-1-43740000
C	0-84280000	2-59380000	1-43740000
C	2-72730000	0-00000000	1-43740000
H	0-13140000	3-24440000	1-97050000
H	-3-04500000	-1-12760000	1-97050000
H	-2-01340000	-2-54750000	1-97050000
C	3-42230000	0-00000000	0-00000000
H	3-12630000	0-87760000	-1-97050000

H	3.12630000	-0.87760000	-1.97050000	H	-3.79660000	-1.66820000	0.00000000
H	3.12630000	-0.87760000	-1.97050000	H	-3.79660000	1.66820000	0.00000000
H	-3.04500000	1.12760000	1.97050000	H	-2.75980000	3.09530000	0.00000000
H	-2.01340000	2.54750000	1.97050000	super[5]phane_cr1			
H	3.12630000	0.87760000	1.97050000	Cr	0.00000000	0.00000000	0.00000000
H	0.13140000	-3.24440000	1.97050000	C	-0.38430000	-1.18270000	-1.57830000
H	1.80070000	-2.70210000	1.97050000	C	1.00610000	-0.73100000	-1.57830000
C	1.05760000	-3.25480000	0.00000000	C	1.00610000	0.73100000	-1.57830000
H	1.80070000	-2.70210000	-1.97050000	C	-0.84670000	-2.60600000	-1.41580000
H	0.13140000	-3.24440000	-1.97050000	C	2.21680000	-1.61060000	-1.41580000
H	1.80070000	2.70210000	1.97050000	C	2.21680000	1.61060000	-1.41580000
H	0.43690000	4.16240000	0.00000000	C	-1.06930000	-3.29100000	0.00000000
H	2.09320000	3.62430000	0.00000000	H	-1.79900000	-2.69690000	-1.96210000
H	4.09370000	0.87080000	0.00000000	H	-0.12980000	-3.23930000	-1.96210000
H	4.09370000	-0.87080000	0.00000000	C	2.79950000	-2.03390000	0.00000000
H	0.43690000	-4.16240000	0.00000000	H	2.00900000	-2.54430000	-1.96210000
H	2.09320000	-3.62430000	0.00000000	H	3.04060000	-1.12450000	-1.96210000
H	-2.80000000	-3.11070000	0.00000000	H	2.00900000	2.54430000	-1.96210000
H	-3.82370000	-1.70170000	0.00000000	C	2.79950000	2.03390000	0.00000000
H	-3.82370000	1.70170000	0.00000000	C	1.00610000	0.73100000	1.57830000
H	-2.80000000	3.11070000	0.00000000	C	-1.24360000	0.00000000	-1.57830000
super[5]phane_co6				C	1.00610000	-0.73100000	1.57830000
Co	0.00000000	0.00000000	0.00000000	C	-0.38430000	1.18270000	1.57830000
C	0.38050000	1.17110000	-1.63860000	C	-0.38430000	1.18270000	-1.57830000
C	-0.99620000	0.72380000	-1.63860000	C	-0.38430000	-1.18270000	1.57830000
C	-0.99620000	-0.72380000	-1.63860000	C	-1.24360000	0.00000000	1.57830000
C	0.83750000	2.57740000	-1.43490000	H	3.04060000	1.12450000	-1.96210000
C	-2.19250000	1.59290000	-1.43490000	C	2.21680000	1.61060000	1.41580000
C	-2.19250000	-1.59290000	-1.43490000	C	-2.74010000	0.00000000	-1.41580000
C	1.04820000	3.22590000	0.00000000	C	2.21680000	-1.61060000	1.41580000
H	1.80100000	2.67660000	-1.96340000	C	-0.84670000	2.60600000	1.41580000
H	0.11620000	3.22400000	-1.96340000	C	-0.84670000	2.60600000	-1.41580000
C	-2.74410000	1.99370000	0.00000000	C	-0.84670000	-2.60600000	1.41580000
H	-1.98910000	2.54000000	-1.96340000	C	-2.74010000	0.00000000	1.41580000
H	-3.03030000	1.10680000	-1.96340000	H	-0.12980000	-3.23930000	1.96210000
H	-1.98910000	-2.54000000	-1.96340000	H	3.04060000	1.12450000	1.96210000
C	-2.74410000	-1.99370000	0.00000000	H	2.00900000	2.54430000	1.96210000
C	-0.99620000	0.72380000	1.63860000	C	-3.46030000	0.00000000	0.00000000
C	1.23130000	0.00000000	-1.63860000	H	-3.12080000	-0.87750000	-1.96210000
C	-0.99620000	0.72380000	1.63860000	H	-3.12080000	0.87750000	-1.96210000
C	0.38050000	-1.17110000	1.63860000	H	-3.12080000	0.87750000	1.96210000
C	0.38050000	-1.17110000	-1.63860000	H	3.04060000	-1.12450000	1.96210000
C	0.38050000	1.17110000	1.63860000	H	2.00900000	-2.54430000	1.96210000
C	1.23130000	0.00000000	1.63860000	H	-3.12080000	-0.87750000	1.96210000
H	-3.03030000	-1.10680000	-1.96340000	H	-0.12980000	3.23930000	1.96210000
C	-2.19250000	-1.59290000	1.43490000	H	-1.79900000	2.69690000	1.96210000
C	2.71010000	0.00000000	-1.43490000	C	-1.06930000	3.29100000	0.00000000
C	-2.19250000	1.59290000	1.43490000	H	-1.79900000	2.69690000	-1.96210000
C	0.83750000	-2.57740000	1.43490000	H	-0.12980000	3.23930000	-1.96210000
C	0.83750000	-2.57740000	-1.43490000	H	-1.79900000	-2.69690000	1.96210000
C	0.83750000	2.57740000	1.43490000	H	-0.44790000	-4.19880000	0.00000000
C	2.71010000	0.00000000	1.43490000	H	-2.10560000	-3.66020000	0.00000000
H	0.11620000	3.22400000	1.96340000	H	-4.13170000	-0.87150000	0.00000000
H	-3.03030000	-1.10680000	1.96340000	H	-4.13170000	0.87150000	0.00000000
H	-1.98910000	-2.54000000	1.96340000	H	-0.44790000	4.19880000	0.00000000
C	3.39190000	0.00000000	0.00000000	H	-2.10560000	3.66020000	0.00000000
H	3.10210000	0.88570000	-1.96340000	H	2.83040000	3.13360000	0.00000000
H	3.10210000	-0.88570000	-1.96340000	H	3.85480000	1.72350000	0.00000000
H	3.10210000	-0.88570000	1.96340000	H	3.85480000	-1.72350000	0.00000000
H	-3.03030000	1.10680000	1.96340000	H	2.83040000	-3.13360000	0.00000000
H	-1.98910000	2.54000000	1.96340000	super[5]phane_cr3			
H	3.10210000	0.88570000	1.96340000	Cr	0.00000000	0.00000000	0.00000000
H	0.11620000	-3.22400000	1.96340000	C	-0.38250000	-1.17720000	-1.61400000
H	1.80100000	-2.67660000	1.96340000	C	1.00140000	-0.72760000	-1.61400000
C	1.04820000	-3.22590000	0.00000000	C	1.00140000	0.72760000	-1.61400000
H	1.80100000	-2.67660000	-1.96340000	C	-0.84420000	-2.59800000	-1.42970000
H	0.11620000	-3.22400000	-1.96340000	C	2.21000000	-1.60570000	-1.42970000
H	1.80100000	2.67660000	1.96340000	C	2.21000000	1.60570000	-1.42970000
H	0.41340000	4.12630000	0.00000000	C	-1.06210000	-3.26880000	0.00000000
H	2.09100000	3.58120000	0.00000000	H	-1.79970000	-2.69980000	-1.96810000
H	4.05210000	0.88200000	0.00000000	H	-0.13090000	-3.24200000	-1.96810000
H	4.05210000	-0.88200000	0.00000000	C	2.78060000	-2.02020000	0.00000000
H	0.41340000	-4.12630000	0.00000000	H	2.01150000	-2.54590000	-1.96810000
H	2.09100000	-3.58120000	0.00000000	H	3.04290000	-1.12630000	-1.96810000
H	-2.75980000	-3.09530000	0.00000000	H	2.01150000	2.54590000	-1.96810000

C	2.78060000	2.02020000	0.00000000	H	1.97120000	2.53170000	1.95840000
C	1.00140000	0.72760000	1.61400000	C	-3.39010000	0.00000000	0.00000000
C	-1.23780000	0.00000000	-1.61400000	H	-3.08290000	-0.88950000	-1.95840000
C	1.00140000	-0.72760000	1.61400000	H	-3.08290000	0.88950000	-1.95840000
C	-0.38250000	1.17720000	1.61400000	H	-3.08290000	0.88950000	1.95840000
C	-0.38250000	1.17720000	-1.61400000	H	3.01690000	-1.09240000	1.95840000
C	-0.38250000	-1.17720000	1.61400000	H	1.97120000	-2.53170000	1.95840000
C	-1.23780000	0.00000000	1.61400000	H	-3.08290000	-0.88950000	1.95840000
H	3.04290000	1.12630000	-1.96810000	H	-0.10670000	3.20690000	1.95840000
C	2.21000000	1.60570000	1.42970000	H	-1.79870000	2.65710000	1.95840000
C	-2.73170000	0.00000000	-1.42970000	C	-1.04760000	3.22420000	0.00000000
C	2.21000000	-1.60570000	1.42970000	H	-1.79870000	2.65710000	-1.95840000
C	-0.84420000	2.59800000	1.42970000	H	-0.10670000	3.20690000	-1.95840000
C	-0.84420000	2.59800000	-1.42970000	H	-1.79870000	-2.65710000	1.95840000
C	-0.84420000	-2.59800000	1.42970000	H	-0.40750000	-4.11960000	0.00000000
C	-2.73170000	0.00000000	1.42970000	H	-2.09180000	-3.57240000	0.00000000
H	-0.13090000	-3.24200000	1.96810000	H	-4.04390000	-0.88550000	0.00000000
H	3.04290000	1.12630000	1.96810000	H	-4.04390000	0.88550000	0.00000000
H	2.01150000	2.54590000	1.96810000	H	-0.40750000	4.11960000	0.00000000
C	-3.43700000	0.00000000	0.00000000	H	-2.09180000	3.57240000	0.00000000
H	-3.12380000	-0.87730000	-1.96810000	H	2.75110000	3.09340000	0.00000000
H	-3.12380000	0.87730000	-1.96810000	H	3.79210000	1.66060000	0.00000000
H	-3.12380000	0.87730000	1.96810000	H	3.79210000	-1.66060000	0.00000000
H	3.04290000	-1.12630000	1.96810000	H	2.75110000	-3.09340000	0.00000000
H	2.01150000	-2.54590000	1.96810000				
H	-3.12380000	-0.87730000	1.96810000	super[5]phane_cu2			
H	-0.13090000	3.24200000	1.96810000	Cu	0.00000000	0.00000000	0.00000000
H	-1.79970000	2.69980000	1.96810000	C	0.38090000	1.17240000	-1.66190000
C	-1.06210000	3.26880000	0.00000000	C	-0.99730000	0.72460000	-1.66190000
H	-1.79970000	2.69980000	-1.96810000	C	-0.99730000	-0.72460000	-1.66190000
H	-0.13090000	3.24200000	-1.96810000	C	0.84120000	2.58910000	-1.44680000
H	-1.79970000	-2.69980000	1.96810000	C	-2.20240000	1.60010000	-1.44680000
H	-0.44110000	-4.17650000	0.00000000	C	-2.20240000	-1.60010000	-1.44680000
H	-2.09810000	-3.63810000	0.00000000	C	1.05280000	3.24020000	0.00000000
H	-4.10840000	-0.87110000	0.00000000	H	1.80170000	2.70480000	-1.97360000
H	-4.10840000	0.87110000	0.00000000	H	0.13230000	3.24720000	-1.97360000
H	-0.44110000	4.17650000	0.00000000	C	-2.75620000	2.00250000	0.00000000
H	-2.09810000	3.63810000	0.00000000	H	-2.01570000	2.54930000	-1.97360000
H	3.83580000	1.71010000	0.00000000	H	-3.04740000	1.12920000	-1.97360000
H	3.83580000	-1.71010000	0.00000000	H	-2.01570000	-2.54930000	-1.97360000
H	2.81170000	-3.11960000	0.00000000	C	-2.75620000	-2.00250000	0.00000000
				C	-0.99730000	-0.72460000	1.66190000
super[5]phane_cr5				C	1.23280000	0.00000000	-1.66190000
Cr	0.00000000	0.00000000	0.00000000	C	-0.99730000	0.72460000	1.66190000
C	-0.37860000	-1.16510000	-1.62130000	C	0.38090000	-1.17240000	1.66190000
C	0.99110000	-0.72010000	-1.62130000	C	0.38090000	-1.17240000	-1.66190000
C	0.99110000	0.72010000	-1.62130000	C	0.38090000	1.17240000	1.66190000
C	-0.83550000	-2.57150000	-1.42840000	C	1.23280000	0.00000000	1.66190000
C	2.18740000	-1.58920000	-1.42840000	H	-3.04740000	-1.12920000	-1.97360000
C	2.18740000	1.58920000	-1.42840000	C	-2.20240000	-1.60010000	1.44680000
C	-1.04760000	-3.22420000	0.00000000	C	2.72230000	0.00000000	-1.44680000
H	-1.79870000	-2.65710000	-1.95840000	C	-2.20240000	1.60010000	1.44680000
H	-0.10670000	-3.20690000	-1.95840000	C	0.84120000	-2.58910000	1.44680000
C	2.74260000	-1.99260000	0.00000000	C	0.84120000	-2.58910000	-1.44680000
H	1.97120000	-2.53170000	-1.95840000	C	0.84120000	2.58910000	1.44680000
H	3.01690000	-1.09240000	-1.95840000	C	2.72230000	0.00000000	1.44680000
H	1.97120000	2.53170000	-1.95840000	H	0.13230000	3.24720000	1.97360000
C	2.74260000	1.99260000	0.00000000	H	-3.04740000	-1.12920000	1.97360000
C	0.99110000	0.72010000	1.62130000	H	-2.01570000	-2.54930000	1.97360000
C	-1.22510000	0.00000000	-1.62130000	C	3.40690000	0.00000000	0.00000000
C	0.99110000	-0.72010000	1.62130000	H	3.12910000	0.87770000	-1.97360000
C	-0.37860000	1.16510000	1.62130000	H	3.12910000	-0.87770000	-1.97360000
C	-0.37860000	1.16510000	-1.62130000	H	3.12910000	-0.87770000	1.97360000
C	-0.37860000	-1.16510000	1.62130000	H	-3.04740000	1.12920000	1.97360000
C	-1.22510000	0.00000000	1.62130000	H	-2.01570000	2.54930000	1.97360000
H	3.01690000	1.09240000	-1.95840000	H	3.12910000	0.87770000	1.97360000
C	2.18740000	1.58920000	1.42840000	H	0.13230000	-3.24720000	1.97360000
C	-2.70380000	0.00000000	-1.42840000	H	1.80170000	-2.70480000	1.97360000
C	2.18740000	-1.58920000	1.42840000	C	1.05280000	-3.24020000	0.00000000
C	-0.83550000	2.57150000	1.42840000	H	1.80170000	-2.70480000	-1.97360000
C	-0.83550000	2.57150000	-1.42840000	H	0.13230000	-3.24720000	-1.97360000
C	-0.83550000	-2.57150000	1.42840000	H	1.80170000	2.70480000	1.97360000
C	-2.70380000	0.00000000	1.42840000	H	0.43220000	4.14750000	0.00000000
H	-0.10670000	-3.20690000	1.95840000	H	2.08820000	3.60940000	0.00000000
H	3.01690000	1.09240000	1.95840000	H	4.07810000	0.87060000	0.00000000
				H	4.07810000	-0.87060000	0.00000000



H	0.43220000	-4.14750000	0.00000000	H	-2.00790000	2.54380000	-1.96480000
H	2.08820000	-3.60940000	0.00000000	H	-3.03980000	1.12350000	-1.96480000
H	-2.78750000	-3.10140000	0.00000000	H	-2.00790000	-2.54380000	-1.96480000
H	-3.81100000	-1.69270000	0.00000000	C	-2.78810000	-2.02570000	0.00000000
H	-3.81100000	1.69270000	0.00000000	C	-1.00200000	-0.72800000	1.58670000
H	-2.78750000	3.10140000	0.00000000	C	1.23850000	0.00000000	-1.58670000
super[5]phane_fe1				C	-1.00200000	0.72800000	1.58670000
Fe	0.00000000	0.00000000	0.00000000	C	0.38270000	-1.17790000	1.58670000
C	0.38200000	1.17580000	-1.51810000	C	0.38270000	-1.17790000	-1.58670000
C	-1.00020000	0.72670000	-1.51810000	C	0.38270000	1.17790000	1.58670000
C	-1.00020000	-0.72670000	-1.51810000	C	1.23850000	0.00000000	1.58670000
C	0.84520000	2.60130000	-1.40390000	H	-3.03980000	-1.12350000	-1.96480000
C	-2.21280000	1.60770000	-1.40390000	C	-2.21130000	-1.60660000	1.42250000
C	-2.21280000	-1.60770000	-1.40390000	C	2.73330000	0.00000000	-1.42250000
C	1.07170000	3.29840000	0.00000000	C	-2.21130000	1.60660000	1.42250000
H	1.79410000	2.68120000	-1.95820000	C	0.84460000	-2.59950000	1.42250000
H	0.12450000	3.22370000	-1.95820000	C	0.84460000	-2.59950000	-1.42250000
C	-2.80580000	2.03850000	0.00000000	C	0.84460000	2.59950000	1.42250000
H	-1.99560000	2.53480000	-1.95820000	C	2.73330000	0.00000000	1.42250000
H	-3.02740000	1.11460000	-1.95820000	H	0.12920000	3.23820000	1.96480000
H	-1.99560000	-2.53480000	-1.95820000	H	-3.03980000	-1.12350000	1.96480000
C	-2.80580000	-2.03850000	0.00000000	H	-2.00790000	-2.54380000	1.96480000
C	-1.00020000	0.72670000	1.51810000	C	3.44630000	0.00000000	0.00000000
C	1.23630000	0.00000000	-1.51810000	H	3.11960000	0.87780000	-1.96480000
C	-1.00020000	0.72670000	1.51810000	H	3.11960000	-0.87780000	-1.96480000
C	0.38200000	-1.17580000	1.51810000	H	3.11960000	-0.87780000	1.96480000
C	0.38200000	-1.17580000	-1.51810000	H	-3.03980000	1.12350000	1.96480000
C	0.38200000	1.17580000	1.51810000	H	-2.00790000	2.54380000	1.96480000
C	1.23630000	0.00000000	1.51810000	H	3.11960000	0.87780000	1.96480000
H	-3.02740000	-1.11460000	-1.95820000	H	0.12920000	-3.23820000	1.96480000
C	-2.21280000	-1.60770000	1.40390000	H	1.79890000	-2.69570000	1.96480000
C	2.73510000	0.00000000	-1.40390000	C	1.06500000	-3.27770000	0.00000000
C	-2.21280000	1.60770000	1.40390000	H	1.79890000	-2.69570000	-1.96480000
C	0.84520000	-2.60130000	1.40390000	H	0.12920000	-3.23820000	-1.96480000
C	0.84520000	-2.60130000	-1.40390000	H	1.79890000	2.69570000	1.96480000
C	0.84520000	2.60130000	1.40390000	H	0.44370000	4.18520000	0.00000000
C	2.73510000	0.00000000	1.40390000	H	2.10100000	3.64670000	0.00000000
H	0.12450000	3.22370000	1.95820000	H	4.11750000	0.87130000	0.00000000
H	-3.02740000	-1.11460000	1.95820000	H	4.11750000	-0.87130000	0.00000000
H	-1.99560000	-2.53480000	1.95820000	H	0.44370000	-4.18520000	0.00000000
C	3.46820000	0.00000000	0.00000000	H	2.10100000	-3.64670000	0.00000000
H	3.10440000	0.87780000	-1.95820000	H	-2.81900000	-3.12510000	0.00000000
H	3.10440000	-0.87780000	-1.95820000	H	-3.84320000	-1.71530000	0.00000000
H	3.10440000	-0.87780000	1.95820000	H	-3.84320000	1.71530000	0.00000000
H	-3.02740000	1.11460000	1.95820000	H	-2.81900000	3.12510000	0.00000000
H	-1.99560000	2.53480000	1.95820000	super[5]phane_fe5			
H	3.10440000	0.87780000	1.95820000	Fe	0.00000000	0.00000000	0.00000000
H	0.12450000	-3.22370000	1.95820000	C	0.38130000	1.17350000	-1.68910000
H	1.79410000	-2.68120000	1.95820000	C	-0.99820000	0.72530000	-1.68910000
C	1.07170000	-3.29840000	0.00000000	C	-0.99820000	-0.72530000	-1.68910000
H	1.79410000	-2.68120000	-1.95820000	C	0.84140000	2.58960000	-1.45300000
H	0.12450000	-3.22370000	-1.95820000	C	-2.20290000	1.60050000	-1.45300000
H	1.79410000	2.68120000	1.95820000	C	-2.20290000	-1.60050000	-1.45300000
H	0.45010000	4.20570000	0.00000000	C	1.05110000	3.23500000	0.00000000
H	2.10800000	3.66710000	0.00000000	H	1.80310000	2.70970000	-1.97620000
H	4.13900000	0.87160000	0.00000000	H	0.13400000	3.25200000	-1.97620000
H	4.13900000	-0.87160000	0.00000000	C	-2.75180000	1.99930000	0.00000000
H	0.45010000	-4.20570000	0.00000000	H	-2.01990000	2.55220000	-1.97620000
H	2.10800000	-3.66710000	0.00000000	H	-3.05140000	1.13240000	-1.97620000
H	-2.83620000	-3.13800000	0.00000000	H	-2.01990000	-2.55220000	-1.97620000
H	-3.86080000	-1.72770000	0.00000000	C	-2.75180000	-1.99930000	0.00000000
H	-3.86080000	1.72770000	0.00000000	C	-0.99820000	-0.72530000	1.68910000
H	-2.83620000	3.13800000	0.00000000	C	1.23390000	0.00000000	-1.68910000
super[5]phane_fe3				C	-0.99820000	0.72530000	1.68910000
Fe	0.00000000	0.00000000	0.00000000	C	0.38130000	-1.17350000	1.68910000
C	0.38270000	1.17790000	-1.58670000	C	0.38130000	-1.17350000	-1.68910000
C	-1.00200000	0.72800000	-1.58670000	C	0.38130000	1.17350000	1.68910000
C	-1.00200000	-0.72800000	-1.58670000	C	1.23390000	0.00000000	1.68910000
C	0.84460000	2.59950000	-1.42250000	H	-3.05140000	-1.13240000	-1.97620000
C	-2.21130000	1.60660000	-1.42250000	C	-2.20290000	-1.60050000	1.45300000
C	-2.21130000	-1.60660000	-1.42250000	C	2.72290000	0.00000000	-1.45300000
C	1.06500000	3.27770000	0.00000000	C	-2.20290000	1.60050000	1.45300000
H	1.79890000	2.69570000	-1.96480000	C	0.84140000	-2.58960000	1.45300000
H	0.12920000	3.23820000	-1.96480000	C	0.84140000	-2.58960000	-1.45300000
C	-2.78810000	2.02570000	0.00000000	C	0.84140000	2.58960000	1.45300000



C	2.72290000	0.00000000	1.45300000	H	-2.10720000	-3.66480000	0.00000000
H	0.13400000	3.25200000	1.97620000	H	-4.13660000	-0.87160000	0.00000000
H	-3.05140000	-1.13240000	1.97620000	H	-4.13660000	0.87160000	0.00000000
H	-2.01990000	-2.55220000	1.97620000	H	-0.44940000	4.20350000	0.00000000
C	3.40150000	0.00000000	0.00000000	H	-2.10720000	3.66480000	0.00000000
H	3.13430000	0.87750000	-1.97620000	H	2.83430000	3.13660000	0.00000000
H	3.13430000	-0.87750000	-1.97620000	H	3.85890000	1.72630000	0.00000000
H	3.13430000	-0.87750000	1.97620000	H	3.85890000	-1.72630000	0.00000000
H	-3.05140000	1.13240000	1.97620000	H	2.83430000	-3.13660000	0.00000000
H	-2.01990000	2.55220000	1.97620000	super[5]phane_mn4			
H	3.13430000	0.87750000	1.97620000	Mn	0.00000000	0.00000000	0.00000000
H	0.13400000	-3.25200000	1.97620000	C	-0.38200000	-1.17570000	-1.64820000
H	1.80310000	-2.70970000	1.97620000	C	1.00020000	-0.72670000	-1.64820000
C	1.05110000	-3.23500000	0.00000000	C	1.00020000	0.72670000	-1.64820000
H	1.80310000	-2.70970000	-1.97620000	C	-0.84290000	-2.59420000	-1.44060000
H	0.13400000	-3.25200000	-1.97620000	C	2.20680000	-1.60330000	-1.44060000
H	1.80310000	2.70970000	1.97620000	C	2.20680000	1.60330000	-1.44060000
H	0.43050000	4.14240000	0.00000000	C	-1.05720000	-3.25370000	0.00000000
H	2.08660000	3.60430000	0.00000000	H	-1.80150000	-2.70460000	-1.97180000
H	4.07270000	0.87070000	0.00000000	H	-0.13220000	-3.24700000	-1.97180000
H	4.07270000	-0.87070000	0.00000000	C	2.76770000	-2.01090000	0.00000000
H	0.43050000	-4.14240000	0.00000000	H	2.01550000	-2.54910000	-1.97180000
H	2.08660000	-3.60430000	0.00000000	H	3.04720000	-1.12920000	-1.97180000
H	-2.78310000	-3.09830000	0.00000000	H	2.01550000	2.54910000	-1.97180000
H	-3.80670000	-1.68950000	0.00000000	C	2.76770000	2.01090000	0.00000000
H	-3.80670000	1.68950000	0.00000000	C	1.00020000	0.72670000	1.64820000
H	-2.78310000	3.09830000	0.00000000	C	-1.23630000	0.00000000	-1.64820000
super[5]phane_mn2				C	1.00020000	-0.72670000	1.64820000
Mn	0.00000000	0.00000000	0.00000000	C	-0.38200000	1.17570000	1.64820000
C	-0.38350000	-1.18020000	-1.54620000	C	-0.38200000	1.17570000	-1.64820000
C	1.00400000	-0.72940000	-1.54620000	C	-0.38200000	-1.17570000	1.64820000
C	1.00400000	0.72940000	-1.54620000	C	-1.23630000	0.00000000	1.64820000
C	-0.84630000	-2.60460000	-1.40980000	H	3.04720000	1.12920000	-1.97180000
C	2.21560000	-1.60970000	-1.40980000	C	2.20680000	1.60330000	1.44060000
C	2.21560000	1.60970000	-1.40980000	C	-2.72770000	0.00000000	-1.44060000
C	-1.07090000	-3.29590000	0.00000000	C	2.20680000	-1.60330000	1.44060000
H	-1.79670000	-2.69020000	-1.96030000	C	-0.84290000	2.59420000	1.44060000
H	-0.12770000	-3.23250000	-1.96030000	C	-0.84290000	-2.59420000	-1.44060000
C	2.80370000	-2.03700000	0.00000000	C	-2.72770000	0.00000000	1.44060000
H	2.00330000	-2.54010000	-1.96030000	H	-0.13220000	-3.24700000	1.97180000
H	3.03480000	-1.12030000	-1.96030000	H	3.04720000	1.12920000	1.97180000
H	2.00330000	2.54010000	-1.96030000	H	2.01550000	2.54910000	1.97180000
C	2.80370000	2.03700000	0.00000000	C	-3.42110000	0.00000000	0.00000000
C	1.00400000	0.72940000	1.54620000	H	-3.12900000	-0.87760000	-1.97180000
C	-1.24100000	0.00000000	-1.54620000	H	-3.12900000	0.87760000	-1.97180000
C	1.00400000	-0.72940000	1.54620000	H	-3.12900000	0.87760000	1.97180000
C	-0.38350000	1.18020000	1.54620000	H	3.04720000	-1.12920000	1.97180000
C	-0.38350000	-1.18020000	-1.54620000	H	2.01550000	-2.54910000	1.97180000
C	-0.38350000	-1.18020000	1.54620000	H	-3.12900000	-0.87760000	1.97180000
C	-1.24100000	0.00000000	1.54620000	H	-0.13220000	3.24700000	1.97180000
H	3.03480000	1.12030000	-1.96030000	H	-1.80150000	2.70460000	1.97180000
C	2.21560000	1.60970000	1.40980000	H	-0.43630000	-4.16130000	0.00000000
C	-2.73860000	0.00000000	-1.40980000	H	-2.09300000	-3.62300000	0.00000000
C	2.21560000	-1.60970000	1.40980000	H	-4.09240000	-0.87100000	0.00000000
C	-0.84630000	2.60460000	1.40980000	H	-4.09240000	0.87100000	0.00000000
C	-0.84630000	2.60460000	-1.40980000	H	-0.43630000	4.16130000	0.00000000
C	-0.84630000	-2.60460000	1.40980000	H	-2.09300000	3.62300000	0.00000000
C	-2.73860000	0.00000000	1.40980000	H	2.79890000	3.11010000	0.00000000
H	-0.12770000	-3.23250000	1.96030000	H	3.82280000	1.70080000	0.00000000
H	3.03480000	1.12030000	1.96030000	H	3.82280000	-1.70080000	0.00000000
H	2.00330000	2.54010000	1.96030000	H	2.79890000	-3.11010000	0.00000000
C	-3.46550000	0.00000000	0.00000000	super[5]phane_mn6			
H	-3.11370000	-0.87750000	-1.96030000	Mn	0.00000000	0.00000000	0.00000000
H	-3.11370000	0.87750000	-1.96030000	C	-0.38040000	-1.17070000	-1.75660000
H	-3.11370000	0.87750000	1.96030000	C	0.99590000	-0.72350000	-1.75660000
H	3.03480000	-1.12030000	1.96030000	C	0.99590000	0.72350000	-1.75660000
H	2.00330000	-2.54010000	1.96030000	C	-0.83890000	-2.58170000	-1.47370000
H	-0.12770000	-3.23250000	-1.96030000	C	2.19610000	-1.59560000	-1.47370000
H	-1.79670000	-2.69020000	-1.96030000	C	2.19610000	1.59560000	-1.47370000
H	-0.44940000	-4.20350000	0.00000000	C	-1.04160000	-3.20580000	0.00000000

H	-1.80550000	-2.71720000	-1.98320000	C	0.84250000	-2.59310000	1.43120000
H	-0.13650000	-3.25950000	-1.98320000	C	0.84250000	-2.59310000	-1.43120000
C	2.72700000	-1.98130000	0.00000000	C	0.84250000	2.59310000	1.43120000
H	2.02630000	-2.55680000	-1.98320000	C	2.72650000	0.00000000	1.43120000
H	3.05780000	-1.13700000	-1.98320000	H	0.12910000	3.23870000	1.96800000
H	2.02630000	2.55680000	-1.98320000	H	-3.04030000	-1.12350000	1.96800000
C	2.72700000	1.98130000	0.00000000	H	-2.00800000	-2.54430000	1.96800000
C	0.99590000	0.72350000	1.75660000	C	3.42960000	0.00000000	1.96800000
C	-1.23100000	0.00000000	-1.75660000	H	3.12000000	0.87810000	-1.96800000
C	0.99590000	-0.72350000	1.75660000	H	3.12000000	-0.87810000	-1.96800000
C	-0.38040000	1.17070000	1.75660000	H	3.12000000	-0.87810000	1.96800000
C	-0.38040000	1.17070000	-1.75660000	H	-3.04030000	1.12350000	1.96800000
C	-0.38040000	-1.17070000	1.75660000	H	-2.00800000	2.54430000	1.96800000
C	-1.23100000	0.00000000	1.75660000	H	3.12000000	0.87810000	1.96800000
H	3.05780000	1.13700000	-1.98320000	H	0.12910000	-3.23870000	1.96800000
C	2.19610000	1.59560000	1.47370000	H	1.79920000	-2.69600000	1.96800000
C	-2.71460000	0.00000000	-1.47370000	C	1.05980000	-3.26180000	0.00000000
C	2.19610000	-1.59560000	1.47370000	H	1.79920000	-2.69600000	-1.96800000
C	-0.83890000	2.58170000	1.47370000	H	0.12910000	-3.23870000	-1.96800000
C	-0.83890000	2.58170000	-1.47370000	H	1.79920000	2.69600000	1.96800000
C	-0.83890000	-2.58170000	1.47370000	H	0.43870000	4.16910000	0.00000000
C	-2.71460000	0.00000000	1.47370000	H	2.09560000	3.63080000	0.00000000
H	-0.13650000	-3.25950000	1.98320000	H	4.10060000	0.87110000	0.00000000
H	3.05780000	1.13700000	1.98320000	H	4.10060000	-0.87110000	0.00000000
H	2.02630000	2.55680000	1.98320000	H	0.43870000	-4.16910000	0.00000000
C	-3.37080000	0.00000000	0.00000000	H	2.09560000	-3.63080000	0.00000000
H	-3.14210000	-0.87740000	-1.98320000	H	-2.80550000	-3.11500000	0.00000000
H	-3.14210000	0.87740000	-1.98320000	H	-3.82950000	-1.70560000	0.00000000
H	-3.14210000	0.87740000	1.98320000	H	-3.82950000	1.70560000	0.00000000
H	3.05780000	-1.13700000	1.98320000	H	-2.80550000	3.11500000	0.00000000
H	2.02630000	-2.55680000	1.98320000				
H	-3.14210000	-0.87740000	1.98320000				
H	-0.13650000	3.25950000	1.98320000				
H	-1.80550000	2.71720000	1.98320000				
C	-1.04160000	3.20580000	0.00000000				
H	-1.80550000	2.71720000	-1.98320000				
H	-0.13650000	3.25950000	-1.98320000				
H	-1.80550000	-2.71720000	1.98320000				
H	-0.42100000	-4.11280000	0.00000000				
H	-2.07690000	-3.57470000	0.00000000				
H	-4.04160000	-0.87060000	0.00000000				
H	-4.04160000	0.87060000	0.00000000				
H	-0.42100000	4.11280000	0.00000000				
H	-2.07690000	3.57470000	0.00000000				
H	2.75800000	3.07990000	0.00000000				
H	3.78140000	1.67130000	0.00000000				
H	3.78140000	-1.67130000	0.00000000				
H	2.75800000	-3.07990000	0.00000000				
super[5]phane_ni1							
Ni	0.00000000	0.00000000	0.00000000				
C	0.38130000	1.17350000	-1.60700000				
C	-0.99820000	0.72520000	-1.60700000				
C	-0.99820000	-0.72520000	-1.60700000				
C	0.84250000	2.59310000	-1.43120000				
C	-2.20580000	1.60260000	-1.43120000				
C	-2.20580000	-1.60260000	-1.43120000				
C	1.05980000	3.26180000	0.00000000				
H	1.79920000	2.69600000	-1.96800000				
H	0.12910000	3.23870000	-1.96800000				
C	-2.77460000	2.01590000	0.00000000				
H	-2.00800000	2.54430000	-1.96800000				
H	-3.04030000	1.12350000	-1.96800000				
H	-2.00800000	-2.54430000	-1.96800000				
C	-2.77460000	-2.01590000	0.00000000				
C	-0.99820000	-0.72520000	1.60700000				
C	1.23390000	0.00000000	-1.60700000				
C	-0.99820000	0.72520000	1.60700000				
C	0.38130000	-1.17350000	1.60700000				
C	0.38130000	-1.17350000	-1.60700000				
C	0.38130000	1.17350000	1.60700000				
C	1.23390000	0.00000000	1.60700000				
H	-3.04030000	-1.12350000	-1.96800000				
C	-2.20580000	-1.60260000	1.43120000				
C	2.72650000	0.00000000	-1.43120000				
C	-2.20580000	1.60260000	1.43120000				
super[5]phane_ni3							
Ni	0.00000000	0.00000000	0.00000000				
C	0.38110000	1.17280000	-1.61170000				
C	-0.99760000	0.72480000	-1.61170000				
C	-0.99760000	-0.72480000	-1.61170000				
C	0.84250000	2.59290000	-1.43210000				
C	-2.20570000	1.60250000	-1.43210000				
C	-2.20570000	-1.60250000	-1.43210000				
C	1.05910000	3.25960000	0.00000000				
H	1.79910000	2.69660000	-1.96870000				
H	0.12950000	3.23910000	-1.96870000				
C	-2.77280000	2.01450000	0.00000000				
H	-2.00870000	2.54430000	-1.96870000				
H	-3.04050000	1.12410000	-1.96870000				
H	-2.00870000	-2.54430000	-1.96870000				
C	-2.77280000	-2.01450000	0.00000000				
C	-0.99760000	-0.72480000	1.61170000				
C	1.23310000	0.00000000	-1.61170000				
C	-0.99760000	0.72480000	1.61170000				
C	0.38110000	-1.17280000	1.61170000				
C	0.38110000	-1.17280000	-1.61170000				
C	0.38110000	1.17280000	1.61170000				
C	1.23310000	0.00000000	1.61170000				
H	-3.04050000	-1.12410000	-1.96870000				
C	-2.20570000	-1.60250000	1.43210000				
C	2.72640000	0.00000000	-1.43210000				
C	-2.20570000	1.60250000	1.43210000				
C	0.84250000	-2.59290000	-1.43210000				
C	0.84250000	2.59290000	1.43210000				
C	2.72640000	0.00000000	1.43210000				
H	0.12950000	3.23910000	1.96870000				
H	-3.04050000	-1.12410000	-1.96870000				
H	-2.00870000	-2.54430000	1.96870000				
C	3.42730000	0.00000000	0.00000000				
H	3.12050000	0.87770000	-1.96870000				
H	3.12050000	-0.87770000	-1.96870000				
H	3.12050000	-0.87770000	1.96870000				
H	-3.04050000	1.12410000	1.96870000				
H	-2.00870000	2.54430000	1.96870000				
H	3.12050000	0.87770000	1.96870000				
H	0.12950000	-3.23910000	1.96870000				
H	1.79910000	-2.69660000	1.96870000				
C	1.05910000	-3.25960000	0.00000000				

H	1.79910000	-2.69660000	-1.96870000	C	-2.18380000	1.58660000	-1.49920000
H	0.12950000	-3.23910000	-1.96870000	C	-2.18380000	-1.58660000	-1.49920000
H	1.79910000	2.69660000	1.96870000	C	1.02980000	3.16930000	0.00000000
H	0.43820000	4.16700000	0.00000000	H	1.80720000	2.72200000	-1.98930000
H	2.09480000	3.62880000	0.00000000	H	0.13790000	3.26440000	-1.98930000
H	4.09850000	0.87090000	0.00000000	C	-2.69600000	1.95870000	0.00000000
H	4.09850000	-0.87090000	0.00000000	H	-2.03030000	2.55990000	-1.98930000
H	0.43820000	-4.16700000	0.00000000	H	-3.06200000	1.13990000	-1.98930000
H	2.09480000	-3.62880000	0.00000000	H	-2.03030000	-2.55990000	-1.98930000
H	-2.80380000	-3.11360000	0.00000000	C	-2.69600000	-1.95870000	0.00000000
H	-3.82770000	-1.70440000	0.00000000	C	-0.99470000	-0.72270000	1.84810000
H	-3.82770000	1.70440000	0.00000000	C	1.22960000	0.00000000	-1.84810000
H	-2.80380000	3.11360000	0.00000000	C	-0.99470000	0.72270000	1.84810000
super[5]phane_nometal				C	0.38000000	-1.16940000	1.84810000
C	0.37340000	1.14910000	-1.49060000	C	0.38000000	-1.16940000	-1.84810000
C	-0.97750000	0.71020000	-1.49060000	C	0.38000000	1.16940000	1.84810000
C	-0.97750000	-0.71020000	-1.49060000	C	1.22960000	0.00000000	1.84810000
C	0.83510000	2.57030000	-1.40330000	H	-3.06200000	-1.13990000	-1.98930000
C	-2.18640000	1.58850000	-1.40330000	C	-2.18380000	-1.58660000	1.49920000
C	-2.18640000	-1.58850000	-1.40330000	C	2.69930000	0.00000000	-1.49920000
C	1.06630000	3.28180000	0.00000000	C	-2.18380000	1.58660000	1.49920000
H	1.79380000	2.66450000	-1.95370000	C	0.83410000	-2.56720000	1.49920000
H	0.11490000	3.21000000	-1.95370000	C	0.83410000	-2.56720000	-1.49920000
C	-2.79170000	2.02830000	0.00000000	C	0.83410000	2.56720000	1.49920000
H	-1.97980000	2.52940000	-1.95370000	C	2.69930000	0.00000000	1.49920000
H	-3.01740000	1.10120000	-1.95370000	H	0.13790000	3.26440000	1.98930000
H	-1.97980000	-2.52940000	-1.95370000	H	-3.06200000	-1.13990000	1.98930000
C	-2.79170000	-2.02830000	0.00000000	H	-2.03030000	-2.55990000	1.98930000
C	-0.97750000	-0.71020000	1.49060000	C	3.33240000	0.00000000	0.00000000
C	1.20820000	0.00000000	-1.49060000	H	3.14720000	0.87760000	-1.98930000
C	-0.97750000	0.71020000	1.49060000	H	3.14720000	-0.87760000	-1.98930000
C	0.37340000	-1.14910000	1.49060000	H	3.14720000	-0.87760000	1.98930000
C	0.37340000	-1.14910000	-1.49060000	H	-3.06200000	1.13990000	1.98930000
C	0.37340000	1.14910000	1.49060000	H	-2.03030000	2.55990000	1.98930000
C	1.20820000	0.00000000	1.49060000	H	3.14720000	0.87760000	1.98930000
H	-3.01740000	-1.10120000	-1.95370000	H	0.13790000	-3.26440000	1.98930000
C	-2.18640000	-1.58850000	1.40330000	H	1.80720000	-2.72200000	1.98930000
C	2.70260000	0.00000000	-1.40330000	C	1.02980000	-3.16930000	0.00000000
C	-2.18640000	1.58850000	1.40330000	H	1.80720000	-2.72200000	-1.98930000
C	0.83510000	-2.57030000	1.40330000	H	0.13790000	-3.26440000	-1.98930000
C	0.83510000	-2.57030000	-1.40330000	H	1.80720000	2.72200000	1.98930000
C	0.83510000	2.57030000	1.40330000	H	0.40880000	4.07580000	0.00000000
C	2.70260000	0.00000000	1.40330000	H	2.06500000	3.53770000	0.00000000
H	0.11490000	3.21000000	1.95370000	H	4.00270000	0.87070000	0.00000000
H	-3.01740000	-1.10120000	1.95370000	H	4.00270000	-0.87070000	0.00000000
H	-1.97980000	-2.52940000	1.95370000	H	0.40880000	-4.07580000	0.00000000
C	3.45070000	0.00000000	0.00000000	H	2.06500000	-3.53770000	0.00000000
H	3.08840000	0.88260000	-1.95370000	H	-2.72640000	-3.05710000	0.00000000
H	3.08840000	-0.88260000	-1.95370000	H	-3.75000000	-1.64830000	0.00000000
H	3.08840000	-0.88260000	1.95370000	H	-3.75000000	1.64830000	0.00000000
H	-3.01740000	1.10120000	1.95370000	H	-2.72640000	3.05710000	0.00000000
H	-1.97980000	2.52940000	1.95370000	super[5]phane_til			
H	3.08840000	0.88260000	1.95370000	Ti	0.00000000	0.00000000	0.00000000
H	0.11490000	-3.21000000	1.95370000	C	0.38190000	1.17540000	-1.74210000
H	1.79380000	-2.66450000	1.95370000	C	-0.99990000	0.72650000	-1.74210000
C	1.06630000	-3.28180000	0.00000000	C	-0.99990000	-0.72650000	-1.74210000
H	1.79380000	-2.66450000	-1.95370000	C	0.84020000	2.58600000	-1.46440000
H	0.11490000	-3.21000000	-1.95370000	C	-2.19980000	1.59820000	-1.46440000
H	1.79380000	2.66450000	1.95370000	C	-2.19980000	-1.59820000	-1.46440000
H	0.43990000	4.19460000	0.00000000	C	1.04730000	3.22330000	0.00000000
H	2.10960000	3.65210000	0.00000000	H	1.80490000	2.71590000	-1.97910000
H	4.12520000	0.87780000	0.00000000	H	0.13620000	3.25810000	-1.97910000
H	4.12520000	-0.87780000	0.00000000	C	-2.74190000	1.99210000	0.00000000
H	0.43990000	-4.19460000	0.00000000	H	-2.02520000	2.55580000	-1.97910000
H	2.10960000	-3.65210000	0.00000000	H	-3.05660000	1.13630000	-1.97910000
H	-2.82140000	-3.13490000	0.00000000	H	-2.02520000	-2.55580000	-1.97910000
H	-3.85340000	-1.71460000	0.00000000	C	-2.74190000	-1.99210000	0.00000000
H	-3.85340000	1.71460000	0.00000000	C	-0.99990000	-0.72650000	1.74210000
H	-2.82140000	3.13490000	0.00000000	C	1.23590000	0.00000000	-1.74210000
super[5]phane_sc2				C	-0.99990000	0.72650000	1.74210000
Sc	0.00000000	0.00000000	0.00000000	C	0.38190000	-1.17540000	1.74210000
C	0.38000000	1.16940000	-1.84810000	C	0.38190000	-1.17540000	-1.74210000
C	-0.99470000	0.72270000	-1.84810000	C	0.38190000	1.17540000	1.74210000
C	-0.99470000	-0.72270000	-1.84810000	C	1.23590000	0.00000000	1.74210000
C	0.83410000	2.56720000	-1.49920000	H	-3.05660000	-1.13630000	-1.97910000

C	-2.19980000	-1.59820000	1.46440000	H	1.80470000	-2.71580000	1.97990000
C	2.71900000	0.00000000	-1.46440000	C	1.04550000	-3.21770000	0.00000000
C	-2.19980000	1.59820000	1.46440000	H	1.80470000	-2.71580000	-1.97990000
C	0.84020000	-2.58600000	1.46440000	H	0.13630000	-3.25790000	-1.97990000
C	0.84020000	-2.58600000	-1.46440000	H	1.80470000	2.71580000	1.97990000
C	0.84020000	2.58600000	1.46440000	H	0.42500000	4.12520000	0.00000000
C	2.71900000	0.00000000	1.46440000	H	2.08090000	3.58720000	0.00000000
H	0.13620000	3.25810000	1.97910000	H	4.05460000	0.87060000	0.00000000
H	-3.05660000	-1.13630000	1.97910000	H	4.05460000	-0.87060000	0.00000000
H	-2.02520000	-2.55580000	1.97910000	H	0.42500000	-4.12520000	0.00000000
C	3.38920000	0.00000000	0.00000000	H	2.08090000	-3.58720000	0.00000000
H	3.14070000	0.87730000	-1.97910000	H	-2.76860000	-3.08760000	0.00000000
H	3.14070000	-0.87730000	-1.97910000	H	-3.79200000	-1.67900000	0.00000000
H	3.14070000	-0.87730000	1.97910000	H	-3.79200000	1.67900000	0.00000000
H	-3.05660000	1.13630000	1.97910000	H	-2.76860000	3.08760000	0.00000000
H	-2.02520000	2.55580000	1.97910000	super[5]phane_v2			
H	3.14070000	0.87730000	1.97910000	V	0.00000000	0.00000000	0.00000000
H	0.13620000	-3.25810000	1.97910000	C	0.38310000	1.17910000	-1.65700000
H	1.80490000	-2.71590000	1.97910000	C	-1.00300000	0.72870000	-1.65700000
C	1.04730000	-3.22330000	0.00000000	C	-1.00300000	-0.72870000	-1.65700000
H	1.80490000	-2.71590000	-1.97910000	C	0.84400000	2.59750000	-1.43860000
H	0.13620000	-3.25810000	-1.97910000	C	-2.20950000	1.60530000	-1.43860000
H	1.80490000	2.71590000	1.97910000	C	-2.20950000	-1.60530000	-1.43860000
H	0.42660000	4.13080000	0.00000000	C	1.05930000	3.26010000	0.00000000
H	2.08290000	3.59260000	0.00000000	H	1.80200000	2.70730000	-1.97060000
H	4.06050000	0.87080000	0.00000000	H	0.13350000	3.24950000	-1.97060000
H	4.06050000	-0.87080000	0.00000000	C	-2.77320000	2.01480000	0.00000000
H	0.42660000	-4.13080000	0.00000000	H	-2.01800000	2.55040000	-1.97060000
H	2.08290000	-3.59260000	0.00000000	H	-3.04920000	1.13110000	-1.97060000
H	-2.77320000	-3.09110000	0.00000000	H	-2.01800000	-2.55040000	-1.97060000
H	-3.79680000	-1.68220000	0.00000000	C	-2.77320000	-2.01480000	0.00000000
H	-3.79680000	1.68220000	0.00000000	C	-1.00300000	-0.72870000	1.65700000
H	-2.77320000	3.09110000	0.00000000	C	1.23980000	0.00000000	-1.65700000
super[5]phane_ti3				C	-1.00300000	0.72870000	1.65700000
Ti	0.00000000	0.00000000	0.00000000	C	0.38310000	-1.17910000	1.65700000
C	0.38140000	1.17380000	-1.74960000	C	0.38310000	-1.17910000	-1.65700000
C	-0.99850000	0.72540000	-1.74960000	C	0.38310000	1.17910000	1.65700000
C	-0.99850000	-0.72540000	-1.74960000	C	1.23980000	0.00000000	1.65700000
C	0.83960000	2.58410000	-1.46680000	H	-3.04920000	-1.13110000	-1.97060000
C	-2.19810000	1.59700000	-1.46680000	C	-2.20950000	-1.60530000	1.43860000
C	-2.19810000	-1.59700000	-1.46680000	C	2.73110000	0.00000000	-1.43860000
C	1.04550000	3.21770000	0.00000000	C	-2.20950000	1.60530000	1.43860000
H	1.80470000	2.71580000	-1.97990000	C	0.84400000	-2.59750000	1.43860000
H	0.13630000	3.25790000	-1.97990000	C	0.84400000	-2.59750000	-1.43860000
C	-2.73710000	1.98860000	0.00000000	C	0.84400000	2.59750000	1.43860000
H	-2.02520000	2.55560000	-1.97990000	C	2.73110000	0.00000000	1.43860000
H	-3.05640000	1.13640000	-1.97990000	H	0.13350000	3.24950000	1.97060000
H	-2.02520000	-2.55560000	-1.97990000	H	-3.04920000	-1.13110000	1.97060000
C	-2.73710000	-1.98860000	0.00000000	H	-2.01800000	-2.55040000	1.97060000
C	-0.99850000	-0.72540000	1.74960000	C	3.42780000	0.00000000	0.00000000
C	1.23420000	0.00000000	-1.74960000	H	3.13170000	0.87720000	-1.97060000
C	-0.99850000	0.72540000	1.74960000	H	3.13170000	-0.87720000	-1.97060000
C	0.38140000	-1.17380000	1.74960000	H	3.13170000	-0.87720000	1.97060000
C	0.38140000	-1.17380000	-1.74960000	H	-3.04920000	1.13110000	1.97060000
C	0.38140000	1.17380000	1.74960000	H	-2.01800000	2.55040000	1.97060000
C	1.23420000	0.00000000	1.74960000	H	3.13170000	0.87720000	1.97060000
H	-3.05640000	-1.13640000	-1.97990000	H	0.13350000	-3.24950000	1.97060000
C	-2.19810000	-1.59700000	1.46680000	H	1.80200000	-2.70730000	1.97060000
C	2.71700000	0.00000000	-1.46680000	C	1.05930000	-3.26010000	0.00000000
C	-2.19810000	1.59700000	1.46680000	H	1.80200000	-2.70730000	-1.97060000
C	0.83960000	-2.58410000	1.46680000	H	0.13350000	-3.24950000	-1.97060000
C	0.83960000	-2.58410000	-1.46680000	H	1.80200000	2.70730000	1.97060000
C	0.83960000	2.58410000	1.46680000	H	0.43860000	4.16810000	0.00000000
C	2.71700000	0.00000000	1.46680000	H	2.09510000	3.62980000	0.00000000
H	0.13630000	3.25790000	1.97990000	H	4.09960000	0.87090000	0.00000000
H	-3.05640000	-1.13640000	1.97990000	H	4.09960000	-0.87090000	0.00000000
H	-2.02520000	-2.55560000	1.97990000	H	0.43860000	-4.16810000	0.00000000
C	3.38330000	0.00000000	0.00000000	H	2.09510000	-3.62980000	0.00000000
H	3.14060000	0.87720000	-1.97990000	H	-2.80470000	-3.11430000	0.00000000
H	3.14060000	-0.87720000	-1.97990000	H	-3.82850000	-1.70510000	0.00000000
H	3.14060000	-0.87720000	1.97990000	H	-3.82850000	1.70510000	0.00000000
H	-3.05640000	1.13640000	1.97990000	H	-2.80470000	3.11430000	0.00000000
H	-2.02520000	2.55560000	1.97990000	super[5]phane_v4			
H	3.14060000	0.87720000	1.97990000	V	0.00000000	0.00000000	0.00000000
H	0.13630000	-3.25790000	1.97990000	C	0.38090000	1.17240000	-1.69560000

C	-0.99730000	0.72460000	-1.69560000	C	-0.38130000	-1.17360000	1.70220000
C	-0.99730000	-0.72460000	-1.69560000	C	-1.23400000	0.00000000	1.70220000
C	0.84110000	2.58850000	-1.45440000	H	3.05570000	1.13640000	-1.97990000
C	-2.20190000	1.59980000	-1.45440000	C	2.20410000	1.60140000	1.45890000
C	-2.20190000	-1.59980000	-1.45440000	C	-2.72440000	0.00000000	-1.45890000
C	1.05040000	3.23290000	0.00000000	C	2.20410000	-1.60140000	1.45890000
H	1.80290000	2.70920000	-1.97730000	C	-0.84190000	2.59110000	1.45890000
H	0.13390000	3.25150000	-1.97730000	C	-0.84190000	2.59110000	-1.45890000
C	-2.75010000	1.99800000	0.00000000	C	-0.84190000	-2.59110000	1.45890000
H	-2.01950000	2.55180000	-1.97730000	C	-2.72440000	0.00000000	1.45890000
H	-3.05100000	1.13210000	-1.97730000	H	-0.13650000	-3.25730000	1.97990000
H	-2.01950000	-2.55180000	-1.97730000	H	3.05570000	1.13640000	1.97990000
C	-2.75010000	-1.99800000	0.00000000	H	2.02500000	2.55500000	1.97990000
C	-0.99730000	-0.72460000	1.69560000	C	-3.39450000	0.00000000	0.00000000
C	1.23270000	0.00000000	-1.69560000	H	-3.14000000	-0.87670000	-1.97990000
C	-0.99730000	0.72460000	1.69560000	H	-3.14000000	0.87670000	-1.97990000
C	0.38090000	-1.17240000	1.69560000	H	-3.14000000	0.87670000	1.97990000
C	0.38090000	-1.17240000	-1.69560000	H	3.05570000	-1.13640000	1.97990000
C	0.38090000	1.17240000	1.69560000	H	2.02500000	-2.55500000	1.97990000
C	1.23270000	0.00000000	1.69560000	H	-3.14000000	-0.87670000	1.97990000
H	-3.05100000	-1.13210000	-1.97730000	H	-0.13650000	3.25730000	1.97990000
C	-2.20190000	-1.59980000	1.45440000	H	-1.80420000	2.71540000	1.97990000
C	2.72170000	0.00000000	-1.45440000	C	-1.04900000	3.22840000	0.00000000
C	-2.20190000	1.59980000	1.45440000	H	-1.80420000	2.71540000	-1.97990000
C	0.84110000	-2.58850000	1.45440000	H	-0.13650000	3.25730000	-1.97990000
C	0.84110000	-2.58850000	-1.45440000	H	-1.80420000	-2.71540000	1.97990000
C	0.84110000	2.58850000	1.45440000	H	-0.42860000	-4.13560000	0.00000000
C	2.72170000	0.00000000	1.45440000	H	-2.08410000	-3.59770000	0.00000000
H	0.13390000	3.25150000	1.97730000	H	-4.06570000	-0.87040000	0.00000000
H	-3.05100000	-1.13210000	1.97730000	H	-4.06570000	0.87040000	0.00000000
H	-2.01950000	-2.55180000	1.97730000	H	-0.42860000	4.13560000	0.00000000
C	3.39930000	0.00000000	0.00000000	H	-2.08410000	3.59770000	0.00000000
H	3.13370000	0.87740000	-1.97730000	H	2.77760000	3.09390000	0.00000000
H	3.13370000	-0.87740000	-1.97730000	H	3.80080000	1.68560000	0.00000000
H	3.13370000	-0.87740000	1.97730000	H	3.80080000	-1.68560000	0.00000000
H	-3.05100000	1.13210000	1.97730000	H	2.77760000	-3.09390000	0.00000000
H	-2.01950000	2.55180000	1.97730000				
H	3.13370000	0.87740000	1.97730000				
H	0.13390000	-3.25150000	1.97730000				
H	1.80290000	-2.70920000	1.97730000				
C	1.05040000	-3.23290000	0.00000000				
H	1.80290000	-2.70920000	-1.97730000				
H	0.13390000	-3.25150000	-1.97730000				
H	1.80290000	2.70920000	1.97730000				
H	0.42990000	4.14060000	0.00000000				
H	2.08600000	3.60250000	0.00000000				
H	4.07080000	0.87070000	0.00000000				
H	4.07080000	-0.87070000	0.00000000				
H	0.42990000	-4.14060000	0.00000000				
H	2.08600000	-3.60250000	0.00000000				
H	-2.78150000	-3.09710000	0.00000000				
H	-3.80510000	-1.68830000	0.00000000				
H	-3.80510000	1.68830000	0.00000000				
H	-2.78150000	3.09710000	0.00000000				
super[5]phane_zn1							
Zn	0.00000000	0.00000000	0.00000000				
C	-0.38130000	-1.17360000	-1.70220000				
C	0.99830000	-0.72530000	-1.70220000				
C	0.99830000	0.72530000	-1.70220000				
C	-0.84190000	-2.59110000	-1.45890000				
C	2.20410000	-1.60140000	-1.45890000				
C	2.20410000	1.60140000	-1.45890000				
C	-1.04900000	-3.22840000	0.00000000				
H	-1.80420000	-2.71540000	-1.97990000				
H	-0.13650000	-3.25730000	-1.97990000				
C	2.74620000	-1.99520000	0.00000000				
H	2.02500000	-2.55500000	-1.97990000				
H	3.05570000	-1.13640000	-1.97990000				
H	2.02500000	2.55500000	-1.97990000				
C	2.74620000	1.99520000	0.00000000				
C	0.99830000	0.72530000	1.70220000				
C	-1.23400000	0.00000000	-1.70220000				
C	0.99830000	-0.72530000	1.70220000				
C	-0.38130000	1.17360000	1.70220000				
C	-0.38130000	1.17360000	-1.70220000				

super[6]phane\_cationic\_ca1

Ca	0.00000000	0.00000000	0.00000000
C	-0.71840000	1.24440000	1.88970000
C	-1.43690000	0.00000000	1.88970000
C	-0.71840000	-1.24440000	1.88970000
C	0.71840000	-1.24440000	1.88970000
C	1.43690000	0.00000000	1.88970000
C	0.71840000	1.24440000	1.88970000
H	-0.93570000	-3.35470000	1.99410000
C	-1.75540000	-3.04040000	0.00000000
H	2.43740000	-2.48770000	1.99410000
H	3.37310000	-0.86700000	1.99410000
H	0.93570000	3.35470000	1.99410000
H	-0.93570000	3.35470000	1.99410000
C	-0.71840000	1.24440000	-1.88970000
C	-1.43690000	0.00000000	-1.88970000
C	-0.71840000	-1.24440000	-1.88970000
C	0.71840000	-1.24440000	-1.88970000
C	1.43690000	0.00000000	-1.88970000
C	0.71840000	1.24440000	-1.88970000
C	-1.75540000	3.04040000	0.00000000
H	-2.43740000	-2.48770000	-1.99410000
H	0.93570000	-3.35470000	-1.99410000
C	3.51070000	0.00000000	0.00000000
H	-2.43740000	-2.48770000	1.99410000
C	-2.90990000	0.00000000	1.51290000
C	-1.45490000	2.52000000	-1.51290000
H	-0.93570000	3.35470000	-1.99410000
H	-2.43740000	2.48770000	-1.99410000
C	1.45490000	2.52000000	-1.51290000
H	2.43740000	2.48770000	-1.99410000
H	0.93570000	3.35470000	-1.99410000
C	2.90990000	0.00000000	-1.51290000
H	3.37310000	-0.86700000	-1.99410000
H	3.37310000	0.86700000	-1.99410000
C	1.45490000	-2.52000000	-1.51290000
H	2.43740000	-2.48770000	-1.99410000
C	1.75540000	3.04040000	0.00000000
C	-1.45490000	-2.52000000	-1.51290000
H	-0.93570000	-3.35470000	-1.99410000
C	1.75540000	-3.04040000	0.00000000
C	-2.90990000	0.00000000	-1.51290000
H	-3.37310000	0.86700000	-1.99410000
H	-3.37310000	-0.86700000	-1.99410000
C	-1.45490000	2.52000000	1.51290000
H	-3.37310000	-0.86700000	1.99410000
H	-2.43740000	2.48770000	1.99410000
C	1.45490000	2.52000000	1.51290000
H	2.43740000	2.48770000	1.99410000
C	-3.51070000	0.00000000	0.00000000
C	2.90990000	0.00000000	1.51290000
H	-3.37310000	0.86700000	1.99410000
H	3.37310000	0.86700000	1.99410000
C	1.45490000	-2.52000000	1.51290000
H	0.93570000	-3.35470000	1.99410000
C	-1.45490000	-2.52000000	1.51290000
H	1.33420000	-4.05160000	0.00000000
H	2.84170000	-3.18130000	0.00000000
H	4.17590000	-0.87030000	0.00000000
H	4.17590000	0.87030000	0.00000000
H	2.84170000	3.18130000	0.00000000
H	1.33420000	4.05160000	0.00000000
H	-1.33420000	4.05160000	0.00000000
H	-2.84170000	3.18130000	0.00000000
H	-2.84170000	-3.18130000	0.00000000
H	-1.33420000	-4.05160000	0.00000000
H	-4.17590000	0.87030000	0.00000000
H	-4.17590000	-0.87030000	0.00000000

super[6]phane\_cationic\_co2

Co	0.00000000	0.00000000	0.00000000
C	-1.25080000	-0.72210000	1.50830000
C	0.00000000	-1.44430000	1.50830000
C	1.25080000	-0.72210000	1.50830000
C	1.25080000	0.72210000	1.50830000
C	0.00000000	1.44430000	1.50830000

C	-1.25080000	0.72210000	1.50830000
H	3.31070000	-0.91030000	1.95450000
C	3.18850000	-1.84090000	0.00000000
H	2.44370000	2.41210000	1.95450000
H	0.86710000	3.32230000	1.95450000
H	-3.31070000	0.91030000	1.95450000
H	-3.31070000	-0.91030000	1.95450000
C	-1.25080000	-0.72210000	-1.50830000
C	0.00000000	-1.44430000	-1.50830000
C	1.25080000	-0.72210000	-1.50830000
C	1.25080000	0.72210000	-1.50830000
C	0.00000000	1.44430000	-1.50830000
C	-1.25080000	0.72210000	-1.50830000
C	-3.18850000	-1.84090000	0.00000000
H	2.44370000	-2.41210000	-1.95450000
H	3.31070000	0.91030000	-1.95450000
C	0.00000000	3.68180000	0.00000000
H	2.44370000	-2.41210000	1.95450000
C	0.00000000	-2.94970000	1.39830000
C	-2.55450000	-1.47490000	-1.39830000
H	-3.31070000	-0.91030000	-1.95450000
H	-2.44370000	-2.41210000	-1.95450000
C	-2.55450000	1.47490000	-1.39830000
H	-2.44370000	2.41210000	-1.95450000
H	-3.31070000	0.91030000	-1.95450000
C	0.00000000	2.94970000	-1.39830000
H	0.86710000	3.32230000	-1.95450000
H	-0.86710000	3.32230000	-1.95450000
C	2.55450000	1.47490000	-1.39830000
H	2.44370000	2.41210000	-1.95450000
C	-3.18850000	1.84090000	0.00000000
C	2.55450000	-1.47490000	-1.39830000
H	3.31070000	-0.91030000	-1.95450000
C	3.18850000	1.84090000	0.00000000
C	0.00000000	-2.94970000	-1.39830000
H	-0.86710000	-3.32230000	-1.95450000
H	0.86710000	-3.32230000	-1.95450000
C	-2.55450000	-1.47490000	-1.39830000
H	0.86710000	-3.32230000	-1.95450000
C	-2.55450000	1.47490000	-1.39830000
H	-2.44370000	-2.41210000	1.95450000
C	-2.55450000	1.47490000	1.39830000
H	-2.44370000	2.41210000	1.95450000
C	0.00000000	-3.68180000	0.00000000
C	0.00000000	2.94970000	1.39830000
H	-0.86710000	-3.32230000	1.95450000
H	-0.86710000	3.32230000	1.95450000
C	2.55450000	1.47490000	1.39830000
H	3.31070000	0.91030000	1.95450000
C	-2.55450000	-1.47490000	-1.39830000
H	4.20110000	1.41980000	0.00000000
H	3.33020000	2.92840000	0.00000000
H	0.87090000	4.34820000	0.00000000
H	-0.87090000	4.34820000	0.00000000
H	-3.33020000	2.92840000	0.00000000
H	-4.20110000	1.41980000	0.00000000
H	-4.20110000	-1.41980000	0.00000000
H	-3.33020000	-2.92840000	0.00000000
H	3.33020000	-2.92840000	0.00000000
H	4.20110000	-1.41980000	0.00000000
H	-0.87090000	-4.34820000	0.00000000
H	0.87090000	-4.34820000	0.00000000

super[6]phane\_cationic\_co4

Co	0.00000000	0.00000000	0.00000000
C	-1.25410000	-0.72410000	1.55430000
C	0.00000000	-1.44810000	1.55430000
C	1.25410000	-0.72410000	1.55430000
C	1.25410000	0.72410000	1.55430000
C	0.00000000	1.44810000	1.55430000
C	-1.25410000	0.72410000	1.55430000
H	3.32330000	-0.91750000	1.96220000
C	3.17570000	-1.83350000	0.00000000
H	2.45620000	2.41930000	1.96220000
H	0.86700000	3.33680000	1.96220000
H	-3.32330000	0.91750000	1.96220000
H	-3.32330000	-0.91750000	1.96220000





H	-2.45530000	-2.41700000	-1.96490000	C	2.56010000	1.47810000	-1.40400000
C	-2.55570000	1.47550000	-1.41460000	H	2.45260000	2.41630000	-1.95880000
H	-2.45530000	2.41700000	-1.96490000	C	-3.18700000	1.84000000	0.00000000
H	-3.32090000	0.91790000	-1.96490000	C	2.56010000	-1.47810000	-1.40400000
C	0.00000000	2.95110000	-1.41460000	H	3.31890000	-0.91590000	-1.95880000
H	0.86550000	3.33490000	-1.96490000	C	3.18700000	1.84000000	0.00000000
H	-0.86550000	3.33490000	-1.96490000	C	0.00000000	-2.95610000	-1.40400000
C	2.55570000	1.47550000	-1.41460000	H	-0.86630000	-3.33210000	-1.95880000
H	2.45530000	2.41700000	-1.96490000	H	0.86630000	-3.33210000	-1.95880000
C	-3.17230000	1.83150000	0.00000000	C	-2.56010000	-1.47810000	1.40400000
C	2.55570000	-1.47550000	-1.41460000	H	0.86630000	-3.33210000	1.95880000
H	3.32090000	-0.91790000	-1.96490000	H	-2.45260000	-2.41630000	1.95880000
C	3.17230000	1.83150000	0.00000000	C	-2.56010000	1.47810000	1.40400000
C	0.00000000	-2.95110000	-1.41460000	H	-2.45260000	2.41630000	1.95880000
H	-0.86550000	-3.33490000	-1.96490000	C	0.00000000	-3.68010000	0.00000000
H	0.86550000	-3.33490000	-1.96490000	C	0.00000000	2.95610000	1.40400000
C	-2.55570000	-1.47550000	1.41460000	H	-0.86630000	-3.33210000	1.95880000
H	0.86550000	-3.33490000	1.96490000	H	-0.86630000	3.33210000	1.95880000
H	-2.45530000	-2.41700000	1.96490000	C	2.56010000	1.47810000	1.40400000
C	-2.55570000	1.47550000	1.41460000	H	3.31890000	0.91590000	1.95880000
H	-2.45530000	2.41700000	1.96490000	C	2.56010000	-1.47810000	1.40400000
C	0.00000000	-3.66310000	0.00000000	H	4.19980000	1.41850000	0.00000000
C	0.00000000	2.95110000	1.41460000	H	3.32840000	2.92790000	0.00000000
H	-0.86550000	-3.33490000	1.96490000	H	0.87140000	4.34640000	0.00000000
H	-0.86550000	3.33490000	1.96490000	H	-0.87140000	4.34640000	0.00000000
C	2.55570000	1.47550000	1.41460000	H	-3.32840000	2.92790000	0.00000000
H	3.32090000	0.91790000	1.96490000	H	-4.19980000	1.41850000	0.00000000
C	2.55570000	-1.47550000	1.41460000	H	-4.19980000	-1.41850000	0.00000000
H	4.18480000	1.40870000	0.00000000	H	-3.32840000	-2.92790000	0.00000000
H	3.31240000	2.91980000	0.00000000	H	3.32840000	-2.92790000	0.00000000
H	0.87240000	4.32850000	0.00000000	H	4.19980000	-1.41850000	0.00000000
H	-0.87240000	4.32850000	0.00000000	H	-0.87140000	-4.34640000	0.00000000
H	-3.31240000	2.91980000	0.00000000	H	0.87140000	-4.34640000	0.00000000
H	-4.18480000	1.40870000	0.00000000	super[6]phane_cationic_cr5			
H	-4.18480000	-1.40870000	0.00000000	Cr	0.00000000	0.00000000	0.00000000
H	-3.31240000	-2.91980000	0.00000000	C	-1.25400000	-0.72400000	1.62650000
H	3.31240000	-2.91980000	0.00000000	C	0.00000000	-1.44800000	1.62650000
H	4.18480000	-1.40870000	0.00000000	C	1.25400000	-0.72400000	1.62650000
H	-0.87240000	-4.32850000	0.00000000	C	1.25400000	0.72400000	1.62650000
H	0.87240000	-4.32850000	0.00000000	C	0.00000000	1.44800000	1.62650000
super[6]phane_cationic_cr3				C	-1.25400000	0.72400000	1.62650000
Cr	0.00000000	0.00000000	0.00000000	H	3.33560000	-0.92510000	1.97220000
C	-1.25570000	-0.72500000	1.52800000	C	3.14920000	-1.81820000	0.00000000
C	0.00000000	-1.45000000	1.52800000	H	2.46900000	2.42620000	1.97220000
C	1.25570000	-0.72500000	1.52800000	H	0.86660000	3.35130000	1.97220000
C	1.25570000	0.72500000	1.52800000	H	-3.33560000	0.92510000	1.97220000
C	0.00000000	1.45000000	1.52800000	H	-3.33560000	-0.92510000	1.97220000
C	-1.25570000	0.72500000	1.52800000	C	-1.25400000	-0.72400000	-1.62650000
H	3.31890000	-0.91590000	1.95880000	C	0.00000000	-1.44800000	-1.62650000
C	3.18700000	-1.84000000	0.00000000	C	1.25400000	-0.72400000	-1.62650000
H	2.45260000	2.41630000	1.95880000	C	1.25400000	0.72400000	-1.62650000
H	0.86630000	3.33210000	1.95880000	C	0.00000000	1.44800000	-1.62650000
H	-3.31890000	0.91590000	1.95880000	C	-1.25400000	0.72400000	-1.62650000
H	-3.31890000	-0.91590000	1.95880000	C	-3.14920000	-1.81820000	0.00000000
C	-1.25570000	-0.72500000	-1.52800000	H	2.46900000	-2.42620000	-1.97220000
C	0.00000000	-1.45000000	-1.52800000	H	3.33560000	0.92510000	-1.97220000
C	1.25570000	-0.72500000	-1.52800000	C	0.00000000	3.63630000	0.00000000
C	1.25570000	0.72500000	-1.52800000	H	2.46900000	-2.42620000	1.97220000
C	0.00000000	1.45000000	-1.52800000	C	0.00000000	-2.94880000	1.43720000
C	-1.25570000	0.72500000	-1.52800000	C	-2.55370000	-1.47440000	-1.43720000
C	-3.18700000	-1.84000000	0.00000000	H	-3.33560000	-0.92510000	-1.97220000
H	2.45260000	-2.41630000	-1.95880000	H	-2.46900000	-2.42620000	-1.97220000
H	3.31890000	0.91590000	-1.95880000	C	-2.55370000	1.47440000	-1.43720000
C	0.00000000	3.68010000	0.00000000	H	-2.46900000	2.42620000	-1.97220000
H	2.45260000	-2.41630000	1.95880000	H	-3.33560000	0.92510000	-1.97220000
C	0.00000000	-2.95610000	1.40400000	C	0.00000000	2.94880000	-1.43720000
C	-2.56010000	-1.47810000	-1.40400000	H	0.86660000	3.35130000	-1.97220000
H	-3.31890000	-0.91590000	-1.95880000	H	-0.86660000	3.35130000	-1.97220000
H	-2.45260000	-2.41630000	-1.95880000	C	2.55370000	1.47440000	-1.43720000
C	-2.56010000	1.47810000	-1.40400000	H	2.46900000	2.42620000	-1.97220000
H	-2.45260000	2.41630000	-1.95880000	C	-3.14920000	1.81820000	0.00000000
H	-3.31890000	0.91590000	-1.95880000	C	2.55370000	-1.47440000	-1.43720000
C	0.00000000	2.95610000	-1.40400000	H	3.33560000	-0.92510000	-1.97220000
H	0.86630000	3.33210000	-1.95880000	C	3.14920000	1.81820000	0.00000000
H	-0.86630000	3.33210000	-1.95880000	C	0.00000000	-2.94880000	-1.43720000

H	-0.86660000	-3.35130000	-1.97220000	C	0.00000000	-3.64700000	0.00000000
H	0.86660000	-3.35130000	-1.97220000	C	0.00000000	2.94650000	1.42650000
C	-2.55370000	-1.47440000	1.43720000	H	-0.86720000	-3.34180000	1.96650000
H	0.86660000	-3.35130000	1.97220000	H	-0.86720000	3.34180000	1.96650000
H	-2.46900000	-2.42620000	1.97220000	C	2.55180000	1.47330000	1.42650000
C	-2.55370000	1.47440000	1.43720000	H	3.32770000	0.91990000	1.96650000
H	-2.46900000	2.42620000	1.97220000	C	2.55180000	-1.47330000	1.42650000
C	0.00000000	-3.63630000	0.00000000	H	4.17080000	1.40280000	0.00000000
C	0.00000000	2.94880000	1.43720000	H	3.30030000	2.91070000	0.00000000
H	-0.86660000	-3.35130000	1.97220000	H	0.87060000	4.31340000	0.00000000
H	-0.86660000	3.35130000	1.97220000	H	-0.87060000	4.31340000	0.00000000
C	2.55370000	1.47440000	1.43720000	H	-3.30030000	2.91070000	0.00000000
H	3.33560000	0.92510000	1.97220000	H	-4.17080000	1.40280000	0.00000000
C	2.55370000	-1.47440000	1.43720000	H	-4.17080000	-1.40280000	0.00000000
H	4.16170000	1.39700000	0.00000000	H	-3.30030000	-2.91070000	0.00000000
H	3.29060000	2.90560000	0.00000000	H	3.30030000	-2.91070000	0.00000000
H	0.87100000	4.30260000	0.00000000	H	4.17080000	-1.40280000	0.00000000
H	-0.87100000	4.30260000	0.00000000	H	-0.87060000	-4.31340000	0.00000000
H	-3.29060000	2.90560000	0.00000000	H	0.87060000	-4.31340000	0.00000000
H	-4.16170000	1.39700000	0.00000000	super[6]phane_cationic_fe1			
H	-4.16170000	-1.39700000	0.00000000	Fe	0.00000000	0.00000000	0.00000000
H	-3.29060000	-2.90560000	0.00000000	C	-0.72150000	1.24960000	1.47490000
H	3.29060000	-2.90560000	0.00000000	C	-1.44290000	0.00000000	1.47490000
H	4.16170000	-1.39700000	0.00000000	C	-0.72150000	-1.24960000	1.47490000
H	-0.87100000	-4.30260000	0.00000000	C	0.72150000	-1.24960000	1.47490000
H	0.87100000	-4.30260000	0.00000000	C	1.44290000	0.00000000	1.47490000
super[6]phane_cationic_cu2				C	0.72150000	1.24960000	1.47490000
Cu	0.00000000	0.00000000	0.00000000	H	-0.90570000	-3.30220000	1.94870000
C	-1.25180000	-0.72270000	1.59060000	C	-1.84800000	-3.20080000	0.00000000
C	0.00000000	-1.44550000	1.59060000	H	2.40690000	-2.43540000	1.94870000
C	1.25180000	-0.72270000	1.59060000	H	3.31260000	-0.86670000	1.94870000
C	1.25180000	0.72270000	1.59060000	H	0.90570000	3.30220000	1.94870000
C	0.00000000	1.44550000	1.59060000	H	-0.90570000	3.30220000	1.94870000
C	-1.25180000	0.72270000	1.59060000	C	-0.72150000	1.24960000	-1.47490000
H	3.32770000	-0.91990000	1.96650000	C	-1.44290000	0.00000000	-1.47490000
C	3.15840000	-1.82350000	0.00000000	C	-0.72150000	-1.24960000	-1.47490000
H	2.46050000	2.42190000	1.96650000	C	0.72150000	-1.24960000	-1.47490000
H	0.86720000	3.34180000	1.96650000	C	1.44290000	0.00000000	-1.47490000
H	-3.32770000	0.91990000	1.96650000	C	0.72150000	1.24960000	-1.47490000
H	-3.32770000	-0.91990000	1.96650000	C	-1.84800000	3.20080000	0.00000000
C	-1.25180000	-0.72270000	-1.59060000	H	-2.40690000	-2.43540000	-1.94870000
C	0.00000000	-1.44550000	-1.59060000	H	0.90570000	-3.30220000	-1.94870000
C	1.25180000	-0.72270000	-1.59060000	C	3.69590000	0.00000000	0.00000000
C	1.25180000	0.72270000	-1.59060000	H	-2.40690000	-2.43540000	1.94870000
C	0.00000000	1.44550000	-1.59060000	C	-2.95030000	0.00000000	1.38530000
C	-1.25180000	0.72270000	-1.59060000	C	-1.47520000	2.55500000	-1.38530000
C	-3.15840000	-1.82350000	0.00000000	H	-0.90570000	3.30220000	-1.94870000
H	2.46050000	-2.42190000	-1.96650000	H	-2.40690000	2.43540000	-1.94870000
H	3.32770000	0.91990000	-1.96650000	C	1.47520000	2.55500000	-1.38530000
C	0.00000000	3.64700000	0.00000000	H	2.40690000	2.43540000	-1.94870000
H	2.46050000	-2.42190000	1.96650000	H	0.90570000	3.30220000	-1.94870000
C	0.00000000	-2.94650000	1.42650000	C	2.95030000	0.00000000	-1.38530000
C	-2.55180000	-1.47330000	-1.42650000	H	3.31260000	-0.86670000	-1.94870000
H	-3.32770000	-0.91990000	-1.96650000	H	3.31260000	0.86670000	-1.94870000
H	-2.46050000	-2.42190000	-1.96650000	C	1.47520000	-2.55500000	-1.38530000
C	-2.55180000	1.47330000	-1.42650000	H	2.40690000	-2.43540000	-1.94870000
H	-2.46050000	2.42190000	-1.96650000	C	1.84800000	3.20080000	0.00000000
H	-3.32770000	0.91990000	-1.96650000	C	-1.47520000	-2.55500000	-1.38530000
C	0.00000000	2.94650000	-1.42650000	H	-0.90570000	-3.30220000	-1.94870000
H	0.86720000	3.34180000	-1.96650000	C	1.84800000	-3.20080000	0.00000000
H	-0.86720000	3.34180000	-1.96650000	C	-2.95030000	0.00000000	-1.38530000
C	2.55180000	1.47330000	-1.42650000	H	-3.31260000	0.86670000	-1.94870000
H	2.46050000	2.42190000	-1.96650000	H	-3.31260000	-0.86670000	-1.94870000
C	-3.15840000	1.82350000	0.00000000	C	-1.47520000	2.55500000	1.38530000
C	2.55180000	-1.47330000	-1.42650000	H	-3.31260000	-0.86670000	1.94870000
H	3.32770000	-0.91990000	-1.96650000	H	-2.40690000	2.43540000	1.94870000
C	3.15840000	1.82350000	0.00000000	C	1.47520000	2.55500000	1.38530000
C	0.00000000	-2.94650000	-1.42650000	H	2.40690000	2.43540000	1.94870000
H	-0.86720000	-3.34180000	-1.96650000	C	-3.69590000	0.00000000	0.00000000
H	0.86720000	-3.34180000	-1.96650000	C	2.95030000	0.00000000	1.38530000
C	-2.55180000	-1.47330000	1.42650000	H	-3.31260000	0.86670000	1.94870000
H	0.86720000	-3.34180000	1.96650000	H	3.31260000	0.86670000	1.94870000
H	-2.46050000	-2.42190000	1.96650000	C	1.47520000	-2.55500000	1.38530000
C	-2.55180000	1.47330000	1.42650000	H	0.90570000	-3.30220000	1.94870000
H	-2.46050000	2.42190000	1.96650000	C	-1.47520000	-2.55500000	1.38530000

H	1.42670000	-4.21340000	0.00000000	H	-3.33340000	-2.93040000	0.00000000
H	2.93560000	-3.34220000	0.00000000	H	3.33340000	-2.93040000	0.00000000
H	4.36220000	-0.87110000	0.00000000	H	4.20450000	-1.42170000	0.00000000
H	4.36220000	0.87110000	0.00000000	H	-0.87110000	-4.35200000	0.00000000
H	2.93560000	3.34220000	0.00000000	H	0.87110000	-4.35200000	0.00000000
H	1.42670000	4.21340000	0.00000000	super[6]phane_cationic_fe5			
H	-1.42670000	4.21340000	0.00000000	Fe	0.00000000	0.00000000	0.00000000
H	-2.93560000	3.34220000	0.00000000	C	-1.25470000	-0.72440000	1.59170000
H	-2.93560000	-3.34220000	0.00000000	C	0.00000000	-1.44880000	1.59170000
H	-1.42670000	-4.21340000	0.00000000	C	1.25470000	-0.72440000	1.59170000
H	-4.36220000	0.87110000	0.00000000	C	1.25470000	0.72440000	1.59170000
H	-4.36220000	-0.87110000	0.00000000	C	0.00000000	1.44880000	1.59170000
super[6]phane_cationic_fe3				C	-1.25470000	0.72440000	1.59170000
Fe	0.00000000	0.00000000	0.00000000	H	3.33120000	-0.92290000	1.96900000
C	-1.25520000	-0.72470000	1.51470000	C	3.16100000	-1.82500000	0.00000000
C	0.00000000	-1.44940000	1.51470000	H	2.46480000	2.42350000	1.96900000
C	1.25520000	-0.72470000	1.51470000	H	0.86640000	3.34630000	1.96900000
C	1.25520000	0.72470000	1.51470000	H	-3.33120000	0.92290000	1.96900000
C	0.00000000	1.44940000	1.51470000	H	-3.33120000	-0.92290000	1.96900000
C	-1.25520000	0.72470000	1.51470000	C	-1.25470000	-0.72440000	-1.59170000
H	3.31600000	-0.91320000	1.95570000	C	0.00000000	-1.44880000	-1.59170000
C	3.19180000	-1.84280000	0.00000000	C	1.25470000	-0.72440000	-1.59170000
H	2.44890000	2.41510000	1.95570000	C	1.25470000	0.72440000	-1.59170000
H	0.86710000	3.32840000	1.95570000	C	0.00000000	1.44880000	-1.59170000
H	-3.31600000	0.91320000	1.95570000	C	-1.25470000	0.72440000	-1.59170000
H	-3.31600000	-0.91320000	1.95570000	C	-3.16100000	-1.82500000	0.00000000
C	-1.25520000	-0.72470000	-1.51470000	H	2.46480000	-2.42350000	-1.96900000
C	0.00000000	-1.44940000	-1.51470000	H	3.33120000	0.92290000	-1.96900000
C	1.25520000	-0.72470000	-1.51470000	C	0.00000000	3.65000000	0.00000000
C	1.25520000	0.72470000	-1.51470000	H	2.46480000	-2.42350000	1.96900000
C	0.00000000	1.44940000	-1.51470000	C	0.00000000	-2.95220000	1.42700000
C	-1.25520000	0.72470000	-1.51470000	C	-2.55670000	-1.47610000	-1.42700000
C	-3.19180000	-1.84280000	0.00000000	H	-3.33120000	-0.92290000	-1.96900000
H	2.44890000	-2.41510000	-1.95570000	H	-2.46480000	-2.42350000	-1.96900000
H	3.31600000	0.91320000	-1.95570000	C	-2.55670000	1.47610000	-1.42700000
C	0.00000000	3.68560000	0.00000000	H	-2.46480000	2.42350000	-1.96900000
H	2.44890000	-2.41510000	1.95570000	H	-3.33120000	0.92290000	-1.96900000
C	0.00000000	-2.95570000	1.39950000	C	0.00000000	2.95220000	-1.42700000
C	-2.55970000	-1.47790000	-1.39950000	H	0.86640000	3.34630000	-1.96900000
H	-3.31600000	-0.91320000	-1.95570000	H	-0.86640000	3.34630000	-1.96900000
H	-2.44890000	-2.41510000	-1.95570000	C	2.55670000	1.47610000	-1.42700000
C	-2.55970000	1.47790000	-1.39950000	H	2.46480000	2.42350000	-1.96900000
H	-2.44890000	2.41510000	-1.95570000	C	-3.16100000	1.82500000	0.00000000
H	-3.31600000	0.91320000	-1.95570000	C	2.55670000	-1.47610000	-1.42700000
C	0.00000000	2.95570000	-1.39950000	H	3.33120000	-0.92290000	-1.96900000
H	0.86710000	3.32840000	-1.95570000	C	3.16100000	1.82500000	0.00000000
H	-0.86710000	3.32840000	-1.95570000	C	0.00000000	-2.95220000	-1.42700000
C	2.55970000	1.47790000	-1.39950000	H	-0.86640000	-3.34630000	-1.96900000
H	2.44890000	2.41510000	-1.95570000	H	0.86640000	-3.34630000	-1.96900000
C	-3.19180000	1.84280000	0.00000000	C	-2.55670000	-1.47610000	1.42700000
C	2.55970000	-1.47790000	-1.39950000	H	0.86640000	-3.34630000	1.96900000
H	3.31600000	-0.91320000	-1.95570000	H	-2.46480000	-2.42350000	1.96900000
C	3.19180000	1.84280000	0.00000000	C	-2.55670000	1.47610000	1.42700000
C	0.00000000	-2.95570000	-1.39950000	H	-2.46480000	2.42350000	1.96900000
H	-0.86710000	-3.32840000	-1.95570000	C	0.00000000	-3.65000000	0.00000000
H	0.86710000	-3.32840000	-1.95570000	C	0.00000000	2.95220000	1.42700000
C	-2.55970000	-1.47790000	1.39950000	H	-0.86640000	-3.34630000	1.96900000
H	0.86710000	-3.32840000	1.95570000	H	-0.86640000	3.34630000	1.96900000
H	-2.44890000	-2.41510000	1.95570000	C	2.55670000	1.47610000	1.42700000
C	-2.55970000	1.47790000	1.39950000	H	3.33120000	0.92290000	1.96900000
H	-2.44890000	2.41510000	1.95570000	C	2.55670000	-1.47610000	1.42700000
C	0.00000000	-3.68560000	0.00000000	H	4.17360000	1.40370000	0.00000000
C	0.00000000	2.95570000	1.39950000	H	3.30240000	2.91260000	0.00000000
H	-0.86710000	-3.32840000	1.95570000	H	0.87120000	4.31630000	0.00000000
H	-0.86710000	3.32840000	1.95570000	H	-0.87120000	4.31630000	0.00000000
C	2.55970000	1.47790000	1.39950000	H	-3.30240000	2.91260000	0.00000000
H	3.31600000	0.91320000	1.95570000	H	-4.17360000	1.40370000	0.00000000
C	2.55970000	-1.47790000	1.39950000	H	-4.17360000	-1.40370000	0.00000000
H	4.20450000	1.42170000	0.00000000	H	-3.30240000	-2.91260000	0.00000000
H	3.33340000	2.93040000	0.00000000	H	3.30240000	-2.91260000	0.00000000
H	0.87110000	4.35200000	0.00000000	H	4.17360000	-1.40370000	0.00000000
H	-0.87110000	4.35200000	0.00000000	H	-0.87120000	-4.31630000	0.00000000
H	-3.33340000	2.93040000	0.00000000	H	0.87120000	-4.31630000	0.00000000
H	-4.20450000	1.42170000	0.00000000	super[6]phane_cationic_mn2			
H	-4.20450000	-1.42170000	0.00000000				

Mn	0.00000000	0.00000000	0.00000000	H	3.32560000	-0.91930000	1.96350000
C	-1.25490000	-0.72450000	1.48180000	C	3.17540000	-1.83330000	0.00000000
C	0.00000000	-1.44900000	1.48180000	H	2.45900000	2.42040000	1.96350000
C	1.25490000	-0.72450000	1.48180000	H	0.86660000	3.33970000	1.96350000
C	1.25490000	0.72450000	1.48180000	H	-3.32560000	0.91930000	1.96350000
C	0.00000000	1.44900000	1.48180000	H	-3.32560000	-0.91930000	1.96350000
C	-1.25490000	0.72450000	1.48180000	C	-1.25590000	-0.72510000	-1.55870000
H	3.30850000	-0.90930000	1.95020000	C	0.00000000	-1.45020000	-1.55870000
C	3.20440000	-1.85010000	0.00000000	C	1.25590000	-0.72510000	-1.55870000
H	2.44170000	2.41060000	1.95020000	C	1.25590000	0.72510000	-1.55870000
H	0.86670000	3.31990000	1.95020000	C	0.00000000	1.45020000	-1.55870000
H	-3.30850000	0.90930000	1.95020000	C	-1.25590000	0.72510000	-1.55870000
H	-3.30850000	-0.90930000	1.95020000	C	-3.17540000	-1.83330000	0.00000000
C	-1.25490000	-0.72450000	-1.48180000	H	2.45900000	-2.42040000	-1.96350000
C	0.00000000	-1.44900000	-1.48180000	H	3.32560000	0.91930000	-1.96350000
C	1.25490000	-0.72450000	-1.48180000	C	0.00000000	3.66660000	0.00000000
C	1.25490000	0.72450000	-1.48180000	H	2.45900000	-2.42040000	1.96350000
C	0.00000000	1.44900000	-1.48180000	C	0.00000000	-2.95450000	1.41550000
C	-1.25490000	0.72450000	-1.48180000	C	-2.55870000	-1.47730000	-1.41550000
C	-3.20440000	-1.85010000	0.00000000	H	-3.32560000	-0.91930000	-1.96350000
H	2.44170000	-2.41060000	-1.95020000	H	-2.45900000	-2.42040000	-1.96350000
H	3.30850000	0.90930000	-1.95020000	C	-2.55870000	1.47730000	-1.41550000
C	0.00000000	3.70010000	0.00000000	H	-2.45900000	2.42040000	-1.96350000
H	2.44170000	-2.41060000	1.95020000	H	-3.32560000	0.91930000	-1.96350000
C	0.00000000	-2.95720000	1.38700000	C	0.00000000	2.95450000	-1.41550000
C	-2.56100000	-1.47860000	-1.38700000	H	0.86660000	3.33970000	-1.96350000
H	-3.30850000	-0.90930000	-1.95020000	H	-0.86660000	3.33970000	-1.96350000
H	-2.44170000	-2.41060000	-1.95020000	C	2.55870000	1.47730000	-1.41550000
C	-2.56100000	1.47860000	-1.38700000	H	2.45900000	2.42040000	-1.96350000
H	-2.44170000	2.41060000	-1.95020000	C	-3.17540000	1.83330000	0.00000000
H	-3.30850000	0.90930000	-1.95020000	C	2.55870000	-1.47730000	-1.41550000
C	0.00000000	2.95720000	-1.38700000	H	3.32560000	-0.91930000	-1.96350000
H	0.86670000	3.31990000	-1.95020000	C	3.17540000	1.83330000	0.00000000
H	-0.86670000	3.31990000	-1.95020000	C	0.00000000	-2.95450000	-1.41550000
C	2.56100000	1.47860000	-1.38700000	H	-0.86660000	-3.33970000	-1.96350000
H	2.44170000	2.41060000	-1.95020000	H	0.86660000	-3.33970000	-1.96350000
C	-3.20440000	1.85010000	0.00000000	C	-2.55870000	-1.47730000	1.41550000
C	2.56100000	-1.47860000	-1.38700000	H	0.86660000	-3.33970000	1.96350000
H	3.30850000	-0.90930000	-1.95020000	H	-2.45900000	-2.42040000	1.96350000
C	3.20440000	1.85010000	0.00000000	C	-2.55870000	1.47730000	1.41550000
C	0.00000000	-2.95720000	-1.38700000	H	-2.45900000	2.42040000	1.96350000
H	-0.86670000	-3.31990000	-1.95020000	C	0.00000000	-3.66660000	0.00000000
H	0.86670000	-3.31990000	-1.95020000	C	0.00000000	2.95450000	1.41550000
C	-2.56100000	-1.47860000	1.38700000	H	-0.86660000	-3.33970000	1.96350000
H	0.86670000	-3.31990000	1.95020000	H	-0.86660000	3.33970000	1.96350000
H	-2.44170000	-2.41060000	1.95020000	C	2.55870000	1.47730000	1.41550000
C	-2.56100000	1.47860000	1.38700000	H	3.32560000	0.91930000	1.96350000
H	-2.44170000	2.41060000	1.95020000	C	2.55870000	-1.47730000	1.41550000
C	0.00000000	-3.70010000	0.00000000	H	4.18800000	1.41180000	0.00000000
C	0.00000000	2.95720000	1.38700000	H	3.31670000	2.92100000	0.00000000
H	-0.86670000	-3.31990000	1.95020000	H	0.87130000	4.33280000	0.00000000
H	-0.86670000	3.31990000	1.95020000	H	-0.87130000	4.33280000	0.00000000
C	2.56100000	1.47860000	1.38700000	H	-3.31670000	2.92100000	0.00000000
H	3.30850000	0.90930000	1.95020000	H	-4.18800000	1.41180000	0.00000000
C	2.56100000	-1.47860000	1.38700000	H	-4.18800000	-1.41180000	0.00000000
H	4.21710000	1.42870000	0.00000000	H	-3.31670000	-2.92100000	0.00000000
H	3.34580000	2.93780000	0.00000000	H	3.31670000	-2.92100000	0.00000000
H	0.87130000	4.36650000	0.00000000	H	4.18800000	-1.41180000	0.00000000
H	-0.87130000	4.36650000	0.00000000	H	-0.87130000	-4.33280000	0.00000000
H	-3.34580000	2.93780000	0.00000000	H	0.87130000	-4.33280000	0.00000000
H	-4.21710000	1.42870000	0.00000000	super[6]phane_cationic_mn6			
H	-4.21710000	-1.42870000	0.00000000	Mn	0.00000000	0.00000000	0.00000000
H	-3.34580000	-2.93780000	0.00000000	C	-1.25340000	-0.72370000	1.65950000
H	3.34580000	-2.93780000	0.00000000	C	0.00000000	-1.44730000	1.65950000
H	4.21710000	-1.42870000	0.00000000	C	1.25340000	-0.72370000	1.65950000
H	-0.87130000	-4.36650000	0.00000000	C	1.25340000	0.72370000	1.65950000
H	0.87130000	-4.36650000	0.00000000	C	0.00000000	1.44730000	1.65950000
super[6]phane_cationic_mn4				C	-1.25340000	0.72370000	1.65950000
Mn	0.00000000	0.00000000	0.00000000	H	3.34100000	-0.92830000	1.97690000
C	-1.25590000	-0.72510000	1.55870000	C	3.13600000	-1.81060000	0.00000000
C	0.00000000	-1.45020000	1.55870000	H	2.47450000	2.42920000	1.97690000
C	1.25590000	-0.72510000	1.55870000	H	0.86660000	3.35760000	1.97690000
C	1.25590000	0.72510000	1.55870000	H	-3.34100000	0.92830000	1.97690000
C	0.00000000	1.45020000	1.55870000	H	-3.34100000	-0.92830000	1.97690000
C	-1.25590000	0.72510000	1.55870000	C	-1.25340000	-0.72370000	-1.65950000

C	0.00000000	-1.44730000	-1.65950000	H	3.31940000	0.91490000	-1.96000000
C	1.25340000	-0.72370000	-1.65950000	C	0.00000000	3.66690000	0.00000000
C	1.25340000	0.72370000	-1.65950000	H	2.45200000	-2.41720000	1.96000000
C	0.00000000	1.44730000	-1.65950000	C	0.00000000	-2.94880000	1.41150000
C	-1.25340000	0.72370000	-1.65950000	C	-2.55370000	-1.47440000	-1.41150000
C	-3.13600000	-1.81060000	0.00000000	H	-3.31940000	-0.91490000	-1.96000000
H	2.47450000	-2.42920000	-1.97690000	H	-2.45200000	-2.41720000	-1.96000000
H	3.34100000	0.92830000	-1.97690000	C	-2.55370000	1.47440000	-1.41150000
C	0.00000000	3.62120000	0.00000000	H	-2.45200000	2.41720000	-1.96000000
H	2.47450000	-2.42920000	1.97690000	H	-3.31940000	0.91490000	-1.96000000
C	0.00000000	-2.94670000	1.44820000	C	0.00000000	2.94880000	-1.41150000
C	-2.55190000	-1.47330000	-1.44820000	H	0.86730000	3.33210000	-1.96000000
H	-3.34100000	-0.92830000	-1.97690000	H	-0.86730000	3.33210000	-1.96000000
H	-2.47450000	-2.42920000	-1.97690000	C	2.55370000	1.47440000	-1.41150000
C	-2.55190000	1.47330000	-1.44820000	H	2.45200000	2.41720000	-1.96000000
H	-2.47450000	2.42920000	-1.97690000	C	-3.17560000	1.83350000	0.00000000
H	-3.34100000	0.92830000	-1.97690000	C	2.55370000	-1.47440000	-1.41150000
C	0.00000000	2.94670000	-1.44820000	H	3.31940000	-0.91490000	-1.96000000
H	0.86660000	3.35760000	-1.97690000	C	3.17560000	1.83350000	0.00000000
H	-0.86660000	3.35760000	-1.97690000	C	0.00000000	-2.94880000	-1.41150000
C	2.55190000	1.47330000	-1.44820000	H	-0.86730000	-3.33210000	-1.96000000
H	2.47450000	2.42920000	-1.97690000	H	0.86730000	-3.33210000	-1.96000000
C	-3.13600000	1.81060000	0.00000000	C	-2.55370000	-1.47440000	-1.41150000
C	2.55190000	-1.47330000	-1.44820000	H	0.86730000	-3.33210000	-1.96000000
H	3.34100000	-0.92830000	-1.97690000	H	-2.45200000	-2.41720000	1.96000000
C	3.13600000	1.81060000	0.00000000	C	-2.55370000	1.47440000	1.41150000
C	0.00000000	-2.94670000	-1.44820000	H	-2.45200000	2.41720000	1.96000000
H	-0.86660000	-3.35760000	-1.97690000	C	0.00000000	-3.66690000	0.00000000
H	0.86660000	-3.35760000	-1.97690000	C	0.00000000	2.94880000	1.41150000
C	-2.55190000	-1.47330000	1.44820000	H	-0.86730000	-3.33210000	1.96000000
H	0.86660000	-3.35760000	1.97690000	H	-0.86730000	3.33210000	1.96000000
H	-2.47450000	-2.42920000	1.97690000	C	2.55370000	1.47440000	1.41150000
C	-2.55190000	1.47330000	1.44820000	H	3.31940000	0.91490000	1.96000000
H	-2.47450000	2.42920000	1.97690000	C	2.55370000	-1.47440000	1.41150000
C	0.00000000	-3.62120000	0.00000000	H	4.18820000	1.41260000	0.00000000
C	0.00000000	2.94670000	1.44820000	H	3.31740000	2.92080000	0.00000000
H	-0.86660000	-3.35760000	1.97690000	H	0.87080000	4.33330000	0.00000000
H	-0.86660000	3.35760000	1.97690000	H	-0.87080000	4.33330000	0.00000000
C	2.55190000	1.47330000	1.44820000	H	-3.31740000	2.92080000	0.00000000
H	3.34100000	0.92830000	1.97690000	H	-4.18820000	1.41260000	0.00000000
C	2.55190000	-1.47330000	1.44820000	H	-4.18820000	-1.41260000	0.00000000
H	4.14840000	1.38930000	0.00000000	H	-3.31740000	-2.92080000	0.00000000
H	3.27740000	2.89790000	0.00000000	H	3.31740000	-2.92080000	0.00000000
H	0.87100000	4.28730000	0.00000000	H	4.18820000	-1.41260000	0.00000000
H	-0.87100000	4.28730000	0.00000000	H	-0.87080000	-4.33330000	0.00000000
H	-3.27740000	2.89790000	0.00000000	H	0.87080000	-4.33330000	0.00000000
H	-4.14840000	1.38930000	0.00000000				
H	-4.14840000	-1.38930000	0.00000000				
H	-3.27740000	-2.89790000	0.00000000				
H	3.27740000	-2.89790000	0.00000000				
H	4.14840000	-1.38930000	0.00000000				
H	-0.87100000	-4.28730000	0.00000000				
H	0.87100000	-4.28730000	0.00000000				
	super[6]phane_cationic_ni1						
Ni	0.00000000	0.00000000	0.00000000				
C	-1.25170000	-0.72270000	1.54440000				
C	0.00000000	-1.44540000	1.54440000				
C	1.25170000	-0.72270000	1.54440000				
C	1.25170000	0.72270000	1.54440000				
C	0.00000000	1.44540000	1.54440000				
C	-1.25170000	0.72270000	1.54440000				
H	3.31940000	-0.91490000	1.96000000				
C	3.17560000	-1.83350000	0.00000000				
H	2.45200000	2.41720000	1.96000000				
H	0.86730000	3.33210000	1.96000000				
H	-3.31940000	0.91490000	1.96000000				
H	-3.31940000	-0.91490000	1.96000000				
C	-1.25170000	-0.72270000	-1.54440000				
C	0.00000000	-1.44540000	-1.54440000				
C	1.25170000	-0.72270000	-1.54440000				
C	1.25170000	0.72270000	-1.54440000				
C	0.00000000	1.44540000	-1.54440000				
C	-1.25170000	0.72270000	-1.54440000				
C	-3.17560000	-1.83350000	0.00000000				
H	2.45200000	-2.41720000	-1.96000000				
H	0.86730000	-3.33210000	-1.96000000				
H	-3.31940000	0.91490000	-1.96000000				
H	-3.31940000	-0.91490000	-1.96000000				
C	-1.25170000	-0.72270000	1.54440000				
C	0.00000000	-1.44540000	1.54440000				
C	1.25170000	-0.72270000	1.54440000				
C	1.25170000	0.72270000	1.54440000				
C	0.00000000	1.44540000	1.54440000				
C	-1.25170000	0.72270000	1.54440000				
C	-3.17560000	-1.83350000	0.00000000				
H	2.45200000	-2.41720000	-1.96000000				
H	0.86730000	-3.33210000	-1.96000000				
H	-3.31940000	0.91490000	-1.96000000				
H	-3.31940000	-0.91490000	-1.96000000				
C	-1.25170000	-0.72270000	-1.54440000				
C	0.00000000	-1.44540000	-1.54440000				
C	1.25170000	-0.72270000	-1.54440000				
C	1.25170000	0.72270000	-1.54440000				
C	0.00000000	1.44540000	-1.54440000				
C	-1.25170000	0.72270000	-1.54440000				
C	-3.17560000	-1.83350000	0.00000000				
H	2.45200000	-2.41720000	-1.96000000				
H	0.86730000	-3.33210000	-1.96000000				
H	-3.31940000	0.91490000	-1.96000000				
H	-3.31940000	-0.91490000	-1.96000000				
C	-1.25170000	-0.72270000	1.54440000				
C	0.00000000	-1.44540000	1.54440000				
C	1.25170000	-0.72270000	1.54440000				
C	1.25170000	0.72270000	1.54440000				
C	0.00000000	1.44540000	1.54440000				
C	-1.25170000	0.72270000	1.54440000				
C	-3.17560000	-1.83350000	0.00000000				
H	2.45200000	-2.41720000	-1.96000000				
H	0.86730000	-3.33210000	-1.96000000				
H	-3.31940000	0.91490000	-1.96000000				
H	-3.31940000	-0.91490000	-1.96000000				
C	-1.25170000	-0.72270000	-1.54440000				
C	0.00000000	-1.44540000	-1.54440000				
C	1.25170000	-0.72270000	-1.54440000				
C	1.25170000	0.72270000	-1.54440000				
C	0.00000000	1.44540000	-1.54440000				
C	-1.25170000	0.72270000	-1.54440000				
C	-3.17560000	-1.83350000	0.00000000				
H	2.45200000	-2.41720000	-1.96000000				
H	0.86730000	-3.33210000	-1.96000000				
H	-3.31940000	0.91490000	-1.96000000				
H	-3.31940000	-0.91490000	-1.96000000				
C	-1.25170000	-0.72270000	1.54440000				
C	0.00000000	-1.44540000	1.54440000				
C	1.25170000	-0.72270000	1.54440000				
C	1.25170000	0.72270000	1.54440000				
C	0.00000000	1.44540000	1.54440000				
C	-1.25170000	0.72270000	1.54440000				
C	-3.17560000	-1.83350000	0.00000000				
H	2.45200000	-2.41720000	-1.96000000				
H	0.86730000	-3.33210000	-1.96000000				
H	-3.31940000	0.91490000	-1.96000000				
H	-3.31940000	-0.91490000	-1.96000000				
C	-1.25170000	-0.72270000	-1.54440000				
C	0.00000000	-1.44540000	-1.54440000				
C	1.25170000	-0.72270000	-1.54440000				
C	1.25170000	0.72270000	-1.54440000				
C	0.00000000	1.44540000	-1.54440000				
C	-1.25170000	0.72270000	-1.54440000				
C	-3.17560000	-1.83350000	0.00000000				
H	2.45200000	-2.41720000	-1.96000000				
H	0.86730000	-3.33210000	-1.96000000				
H	-3.31940000	0.91490000	-1.96000000				
H	-3.31940000	-0.91490000	-1.96000000				
C	-1.25170000	-0.72270000	1.54440000				
C	0.00000000	-1.44540000	1.54440000				
C	1.25170000	-0.72270000	1.54440000				
C	1.25170000	0.72270000	1.54440000				
C	0.00000000	1.44540000	1.54440000				
C	-1.25170000	0.72270000	1.54440000				
C	-3.17560000	-1.83350000	0.00000000				
H	2.45200000						

C	-2.55350000	1.47430000	-1.41260000	C	1.83250000	3.17390000	0.00000000
H	-2.45240000	2.41700000	-1.96110000	C	-1.46390000	-2.53560000	-1.39320000
H	-3.31940000	0.91530000	-1.96110000	H	-0.90130000	-3.29410000	-1.95080000
C	0.00000000	2.94850000	-1.41260000	C	1.83250000	-3.17390000	0.00000000
H	0.86700000	3.33240000	-1.96110000	C	-2.92780000	0.00000000	-1.39320000
H	-0.86700000	3.33240000	-1.96110000	H	-3.30340000	0.86650000	-1.95080000
C	2.55350000	1.47430000	-1.41260000	H	-3.30340000	-0.86650000	-1.95080000
H	2.45240000	2.41700000	-1.96110000	C	-1.46390000	2.53560000	1.39320000
C	-3.17330000	1.83210000	0.00000000	H	-3.30340000	-0.86650000	1.95080000
C	2.55350000	-1.47430000	-1.41260000	H	-2.40210000	2.42760000	1.95080000
H	3.31940000	-0.91530000	-1.96110000	C	1.46390000	2.53560000	1.39320000
C	3.17330000	1.83210000	0.00000000	H	2.40210000	2.42760000	1.95080000
C	0.00000000	-2.94850000	-1.41260000	C	-3.66490000	0.00000000	0.00000000
H	-0.86700000	-3.33240000	-1.96110000	C	2.92780000	0.00000000	1.39320000
H	0.86700000	-3.33240000	-1.96110000	H	-3.30340000	0.86650000	1.95080000
C	-2.55350000	-1.47430000	1.41260000	H	3.30340000	0.86650000	1.95080000
H	0.86700000	-3.33240000	1.96110000	C	1.46390000	-2.53560000	1.39320000
H	-2.45240000	2.41700000	1.96110000	H	-0.90130000	-3.29410000	1.95080000
C	-2.55350000	1.47430000	1.41260000	C	-1.46390000	-2.53560000	1.39320000
H	-2.45240000	2.41700000	1.96110000	H	1.41030000	-4.18910000	0.00000000
C	0.00000000	-3.66420000	0.00000000	H	2.92270000	-3.31590000	0.00000000
C	0.00000000	2.94850000	1.41260000	H	4.33300000	-0.87320000	0.00000000
H	-0.86700000	-3.33240000	1.96110000	H	4.33300000	0.87320000	0.00000000
H	-0.86700000	3.33240000	1.96110000	H	2.92270000	3.31590000	0.00000000
C	2.55350000	1.47430000	1.41260000	H	1.41030000	4.18910000	0.00000000
H	3.31940000	0.91530000	1.96110000	H	-1.41030000	4.18910000	0.00000000
C	2.55350000	-1.47430000	1.41260000	H	-2.92270000	3.31590000	0.00000000
H	4.18580000	1.41130000	0.00000000	H	-2.92270000	-3.31590000	0.00000000
H	3.31510000	2.91940000	0.00000000	H	-1.41030000	-4.18910000	0.00000000
H	0.87070000	4.33070000	0.00000000	H	-4.33300000	0.87320000	0.00000000
H	-0.87070000	4.33070000	0.00000000	H	-4.33300000	-0.87320000	0.00000000
H	-3.31510000	2.91940000	0.00000000				
H	-4.18580000	1.41130000	0.00000000	super[6]phane_cationic_sc2			
H	-4.18580000	-1.41130000	0.00000000	Sc	0.00000000	0.00000000	0.00000000
H	-3.31510000	-2.91940000	0.00000000	C	-1.25430000	-0.72410000	1.74220000
H	3.31510000	-2.91940000	0.00000000	C	0.00000000	-1.44830000	1.74220000
H	4.18580000	-1.41130000	0.00000000	C	1.25430000	-0.72410000	1.74220000
H	-0.87070000	-4.33070000	0.00000000	C	0.00000000	1.44830000	1.74220000
H	0.87070000	-4.33070000	0.00000000	C	-1.25430000	0.72410000	1.74220000
				H	3.35050000	-0.93350000	1.98230000
super[6]phane_cationic_nometal				C	3.11290000	-1.79720000	0.00000000
C	-0.70620000	1.22320000	1.45820000	H	2.48360000	2.43490000	1.98230000
C	-1.41240000	0.00000000	1.45820000	H	0.86690000	3.36830000	1.98230000
C	-0.70620000	-1.22320000	1.45820000	H	-3.35050000	0.93350000	1.98230000
C	0.70620000	-1.22320000	1.45820000	H	-3.35050000	-0.93350000	1.98230000
C	1.41240000	0.00000000	1.45820000	C	-1.25430000	-0.72410000	-1.74220000
C	0.70620000	1.22320000	1.45820000	C	0.00000000	-1.44830000	-1.74220000
H	-0.90130000	-3.29410000	1.95080000	C	1.25430000	-0.72410000	-1.74220000
C	-1.83250000	-3.17390000	0.00000000	C	1.25430000	0.72410000	-1.74220000
H	2.40210000	-2.42760000	1.95080000	C	0.00000000	1.44830000	-1.74220000
H	3.30340000	-0.86650000	1.95080000	C	-1.25430000	0.72410000	-1.74220000
H	0.90130000	3.29410000	1.95080000	C	-3.11290000	-1.79720000	0.00000000
H	-0.90130000	3.29410000	1.95080000	H	2.48360000	-2.43490000	-1.98230000
C	-0.70620000	1.22320000	-1.45820000	H	3.35050000	0.93350000	-1.98230000
C	-1.41240000	0.00000000	-1.45820000	C	0.00000000	3.59450000	0.00000000
C	-0.70620000	-1.22320000	-1.45820000	H	2.48360000	-2.43490000	1.98230000
C	0.70620000	-1.22320000	-1.45820000	C	0.00000000	-2.94020000	1.46830000
C	1.41240000	0.00000000	-1.45820000	C	-2.54630000	-1.47010000	-1.46830000
C	0.70620000	1.22320000	-1.45820000	H	-3.35050000	-0.93350000	-1.98230000
C	-1.83250000	3.17390000	0.00000000	H	-2.48360000	-2.43490000	-1.98230000
H	-2.40210000	-2.42760000	-1.95080000	C	-2.54630000	1.47010000	-1.46830000
H	0.90130000	-3.29410000	-1.95080000	H	-2.48360000	2.43490000	-1.98230000
C	3.66490000	0.00000000	0.00000000	H	-3.35050000	0.93350000	-1.98230000
H	-2.40210000	-2.42760000	1.95080000	C	0.00000000	2.94020000	-1.46830000
C	-2.92780000	0.00000000	1.39320000	H	0.86690000	3.36830000	-1.98230000
C	-1.46390000	2.53560000	-1.39320000	H	-0.86690000	3.36830000	-1.98230000
H	-0.90130000	3.29410000	-1.95080000	C	2.54630000	1.47010000	-1.46830000
H	-2.40210000	2.42760000	-1.95080000	H	2.48360000	2.43490000	-1.98230000
C	1.46390000	2.53560000	-1.39320000	C	-3.11290000	1.79720000	0.00000000
H	2.40210000	2.42760000	-1.95080000	C	2.54630000	-1.47010000	-1.46830000
H	0.90130000	3.29410000	-1.95080000	H	3.35050000	-0.93350000	-1.98230000
C	2.92780000	0.00000000	-1.39320000	C	3.11290000	1.79720000	0.00000000
H	3.30340000	-0.86650000	-1.95080000	C	0.00000000	-2.94020000	-1.46830000
H	3.30340000	0.86650000	-1.95080000	H	-0.86690000	-3.36830000	-1.98230000
C	1.46390000	-2.53560000	-1.39320000	H	0.86690000	-3.36830000	-1.98230000
H	2.40210000	-2.42760000	-1.95080000				

C	-2.54630000	-1.47010000	1.46830000	H	-0.86640000	-3.35570000	1.97080000
H	0.86690000	-3.36830000	1.98230000	H	-0.86640000	3.35570000	1.97080000
H	-2.48360000	-2.43490000	1.98230000	C	2.56090000	1.47850000	1.43250000
C	-2.54630000	1.47010000	1.46830000	H	3.33930000	0.92750000	1.97080000
H	-2.48360000	2.43490000	1.98230000	C	2.56090000	-1.47850000	1.43250000
C	0.00000000	-3.59450000	0.00000000	H	4.17390000	1.40370000	0.00000000
C	0.00000000	2.94020000	1.46830000	H	3.30260000	2.91290000	0.00000000
H	-0.86690000	-3.36830000	1.98230000	H	0.87130000	4.31660000	0.00000000
H	-0.86690000	3.36830000	1.98230000	H	-0.87130000	4.31660000	0.00000000
C	2.54630000	1.47010000	1.46830000	H	-3.30260000	2.91290000	0.00000000
H	3.35050000	0.93350000	1.98230000	H	-4.17390000	1.40370000	0.00000000
C	2.54630000	-1.47010000	1.46830000	H	-4.17390000	-1.40370000	0.00000000
H	4.12510000	1.37620000	0.00000000	H	-3.30260000	-2.91290000	0.00000000
H	3.25430000	2.88440000	0.00000000	H	3.30260000	-2.91290000	0.00000000
H	0.87080000	4.26050000	0.00000000	H	4.17390000	-1.40370000	0.00000000
H	-0.87080000	4.26050000	0.00000000	H	-0.87130000	-4.31660000	0.00000000
H	-3.25430000	2.88440000	0.00000000	H	0.87130000	-4.31660000	0.00000000
H	-4.12510000	1.37620000	0.00000000	super[6]phane_cationic_ti3			
H	-4.12510000	-1.37620000	0.00000000	Ti	0.00000000	0.00000000	0.00000000
H	-3.25430000	-2.88440000	0.00000000	C	-1.25830000	-0.72650000	1.63140000
H	3.25430000	-2.88440000	0.00000000	C	0.00000000	-1.45300000	1.63140000
H	4.12510000	-1.37620000	0.00000000	C	1.25830000	-0.72650000	1.63140000
H	-0.87080000	-4.26050000	0.00000000	C	1.25830000	0.72650000	1.63140000
H	0.87080000	-4.26050000	0.00000000	C	0.00000000	1.45300000	1.63140000
super[6]phane_cationic_ti1			C	-1.25830000	0.72650000	1.63140000	
Ti	0.00000000	0.00000000	0.00000000	H	3.33920000	-0.92740000	1.97130000
C	-1.26000000	-0.72750000	1.62120000	C	3.15690000	-1.82270000	0.00000000
C	0.00000000	-1.45490000	1.62120000	H	2.47270000	2.42810000	1.97130000
C	1.26000000	-0.72750000	1.62120000	H	0.86650000	3.35550000	1.97130000
C	1.26000000	0.72750000	1.62120000	H	-3.33920000	0.92740000	1.97130000
C	0.00000000	1.45490000	1.62120000	H	-3.33920000	-0.92740000	1.97130000
C	-1.26000000	0.72750000	1.62120000	C	-1.25830000	-0.72650000	-1.63140000
H	3.33930000	-0.92750000	1.97080000	C	0.00000000	-1.45300000	-1.63140000
C	3.16120000	-1.82510000	0.00000000	C	1.25830000	-0.72650000	-1.63140000
H	2.47290000	2.42820000	1.97080000	C	1.25830000	0.72650000	-1.63140000
H	0.86640000	3.35570000	1.97080000	C	0.00000000	1.45300000	-1.63140000
H	-3.33930000	0.92750000	1.97080000	C	-1.25830000	0.72650000	-1.63140000
H	-3.33930000	-0.92750000	1.97080000	C	-3.15690000	-1.82270000	0.00000000
C	-1.26000000	-0.72750000	-1.62120000	H	2.47270000	-2.42810000	-1.97130000
C	0.00000000	-1.45490000	-1.62120000	H	3.33920000	0.92740000	-1.97130000
C	1.26000000	-0.72750000	-1.62120000	C	0.00000000	3.64530000	0.00000000
C	1.26000000	0.72750000	-1.62120000	H	2.47270000	-2.42810000	1.97130000
C	0.00000000	1.45490000	-1.62120000	C	0.00000000	-2.95490000	1.43460000
C	-1.26000000	0.72750000	-1.62120000	C	-2.55910000	-1.47750000	-1.43460000
C	-3.16120000	-1.82510000	0.00000000	H	-3.33920000	-0.92740000	-1.97130000
H	2.47290000	-2.42820000	-1.97080000	H	-2.47270000	-2.42810000	-1.97130000
H	3.33930000	0.92750000	-1.97080000	C	-2.55910000	1.47750000	-1.43460000
C	0.00000000	3.65020000	0.00000000	H	-2.47270000	2.42810000	-1.97130000
H	2.47290000	-2.42820000	1.97080000	H	-3.33920000	0.92740000	-1.97130000
C	0.00000000	-2.95700000	1.43250000	C	0.00000000	2.95490000	-1.43460000
C	-2.56090000	-1.47850000	-1.43250000	H	0.86650000	3.35550000	-1.97130000
H	-3.33930000	-0.92750000	-1.97080000	H	-0.86650000	3.35550000	-1.97130000
H	-2.47290000	-2.42820000	-1.97080000	C	2.55910000	1.47750000	-1.43460000
C	-2.56090000	1.47850000	-1.43250000	H	2.47270000	2.42810000	-1.97130000
H	-2.47290000	2.42820000	-1.97080000	C	-3.15690000	1.82270000	0.00000000
H	-3.33930000	0.92750000	-1.97080000	C	2.55910000	-1.47750000	-1.43460000
C	0.00000000	2.95700000	-1.43250000	H	3.33920000	-0.92740000	-1.97130000
H	0.86640000	3.35570000	-1.97080000	C	3.15690000	1.82270000	0.00000000
H	-0.86640000	3.35570000	-1.97080000	C	0.00000000	-2.95490000	-1.43460000
C	2.56090000	1.47850000	-1.43250000	H	-0.86650000	-3.35550000	-1.97130000
H	2.47290000	2.42820000	-1.97080000	H	0.86650000	-3.35550000	-1.97130000
C	-3.16120000	1.82510000	0.00000000	C	-2.55910000	-1.47750000	1.43460000
C	2.56090000	-1.47850000	-1.43250000	H	0.86650000	-3.35550000	1.97130000
H	3.33930000	-0.92750000	-1.97080000	H	-2.47270000	-2.42810000	1.97130000
C	3.16120000	1.82510000	0.00000000	C	-2.55910000	1.47750000	1.43460000
C	0.00000000	-2.95700000	-1.43250000	H	-2.47270000	2.42810000	1.97130000
H	-0.86640000	-3.35570000	-1.97080000	C	0.00000000	-3.64530000	0.00000000
H	0.86640000	-3.35570000	-1.97080000	C	0.00000000	2.95490000	1.43460000
C	-2.56090000	-1.47850000	-1.43250000	H	-0.86650000	-3.35550000	1.97130000
H	0.86640000	-3.35570000	1.97080000	H	-0.86650000	3.35550000	1.97130000
H	-2.47290000	-2.42820000	1.97080000	C	2.55910000	1.47750000	1.43460000
C	-2.56090000	1.47850000	1.43250000	H	3.33920000	0.92740000	1.97130000
H	-2.47290000	2.42820000	1.97080000	C	2.55910000	-1.47750000	1.43460000
C	0.00000000	-3.65020000	0.00000000	H	4.16980000	1.40190000	0.00000000
C	0.00000000	2.95700000	1.43250000	H	3.29900000	2.91020000	0.00000000



H 0.87080000 4.31210000 0.00000000  
 H -0.87080000 4.31210000 0.00000000  
 H -3.29900000 2.91020000 0.00000000  
 H -4.16980000 1.40190000 0.00000000  
 H -4.16980000 -1.40190000 0.00000000  
 H -3.29900000 -2.91020000 0.00000000  
 H 3.29900000 -2.91020000 0.00000000  
 H 4.16980000 -1.40190000 0.00000000  
 H -0.87080000 -4.31210000 0.00000000  
 H 0.87080000 -4.31210000 0.00000000  
 super[6]phane\_cationic\_v2  
 V 0.00000000 0.00000000 0.00000000  
 C -1.26090000 -0.72800000 1.54030000  
 C 0.00000000 -1.45600000 1.54030000  
 C 1.26090000 -0.72800000 1.54030000  
 C 1.26090000 0.72800000 1.54030000  
 C 0.00000000 1.45600000 1.54030000  
 C -1.26090000 0.72800000 1.54030000  
 H 3.32640000 -0.92010000 1.96080000  
 C 3.18980000 -1.84160000 0.00000000  
 H 2.46000000 2.42070000 1.96080000  
 H 0.86640000 3.34080000 1.96080000  
 H -3.32640000 0.92010000 1.96080000  
 H -3.32640000 -0.92010000 1.96080000  
 C -1.26090000 -0.72800000 -1.54030000  
 C 0.00000000 -1.45600000 -1.54030000  
 C 1.26090000 -0.72800000 -1.54030000  
 C 1.26090000 0.72800000 -1.54030000  
 C 0.00000000 1.45600000 -1.54030000  
 C -1.26090000 0.72800000 -1.54030000  
 C -3.18980000 -1.84160000 0.00000000  
 H 2.46000000 -2.42070000 -1.96080000  
 H 3.32640000 0.92010000 -1.96080000  
 C 0.00000000 3.68320000 0.00000000  
 H 2.46000000 -2.42070000 1.96080000  
 C 0.00000000 -2.96350000 1.40710000  
 C -2.56650000 -1.48170000 -1.40710000  
 H -3.32640000 -0.92010000 -1.96080000  
 H -2.46000000 -2.42070000 -1.96080000  
 C -2.56650000 1.48170000 -1.40710000  
 H -2.46000000 2.42070000 -1.96080000  
 H -3.32640000 0.92010000 -1.96080000  
 C 0.00000000 2.96350000 -1.40710000  
 H 0.86640000 3.34080000 -1.96080000  
 H -0.86640000 3.34080000 -1.96080000  
 C 2.56650000 1.48170000 -1.40710000  
 H 2.46000000 2.42070000 -1.96080000  
 C -3.18980000 1.84160000 0.00000000  
 C 2.56650000 -1.48170000 -1.40710000  
 H 3.32640000 -0.92010000 -1.96080000  
 C 3.18980000 1.84160000 0.00000000  
 C 0.00000000 -2.96350000 -1.40710000  
 H -0.86640000 -3.34080000 -1.96080000  
 H 0.86640000 -3.34080000 -1.96080000  
 C -2.56650000 -1.48170000 1.40710000  
 H 0.86640000 -3.34080000 1.96080000  
 H -2.46000000 -2.42070000 1.96080000  
 C -2.56650000 1.48170000 1.40710000  
 H -2.46000000 2.42070000 1.96080000  
 C 0.00000000 -3.68320000 0.00000000  
 C 0.00000000 2.96350000 1.40710000  
 H -0.86640000 -3.34080000 1.96080000  
 H 0.86640000 3.34080000 1.96080000  
 C 2.56650000 1.48170000 1.40710000  
 H 3.32640000 0.92010000 1.96080000  
 C 2.56650000 -1.48170000 1.40710000  
 H 4.20270000 1.42000000 0.00000000  
 H 3.33100000 2.92960000 0.00000000  
 H 0.87160000 4.34960000 0.00000000  
 H -0.87160000 4.34960000 0.00000000  
 H -3.33100000 2.92960000 0.00000000  
 H -4.20270000 1.42000000 0.00000000  
 H -4.20270000 -1.42000000 0.00000000  
 H -3.33100000 -2.92960000 0.00000000  
 H 3.33100000 -2.92960000 0.00000000

H 4.20270000 -1.42000000 0.00000000  
 H -0.87160000 -4.34960000 0.00000000  
 H 0.87160000 -4.34960000 0.00000000  
 super[6]phane\_cationic\_v4  
 V 0.00000000 0.00000000 0.00000000  
 C -1.25450000 -0.72430000 1.59820000  
 C 0.00000000 -1.44860000 1.59820000  
 C 1.25450000 -0.72430000 1.59820000  
 C 1.25450000 0.72430000 1.59820000  
 C 0.00000000 1.44860000 1.59820000  
 C -1.25450000 0.72430000 1.59820000  
 H 3.33100000 -0.92280000 1.96870000  
 C 3.16100000 -1.82500000 0.00000000  
 H 2.46470000 2.42330000 1.96870000  
 H 0.86630000 3.34610000 1.96870000  
 H -3.33100000 0.92280000 1.96870000  
 H -3.33100000 -0.92280000 1.96870000  
 C -1.25450000 -0.72430000 -1.59820000  
 C 0.00000000 -1.44860000 -1.59820000  
 C 1.25450000 -0.72430000 -1.59820000  
 C 1.25450000 0.72430000 -1.59820000  
 C 0.00000000 1.44860000 -1.59820000  
 C -1.25450000 0.72430000 -1.59820000  
 C -3.16100000 -1.82500000 0.00000000  
 H 2.46470000 -2.42330000 -1.96870000  
 H 3.33100000 0.92280000 -1.96870000  
 C 0.00000000 3.65000000 0.00000000  
 H 2.46470000 -2.42330000 1.96870000  
 C 0.00000000 -2.95160000 1.42740000  
 C -2.55610000 -1.47580000 -1.42740000  
 H -3.33100000 -0.92280000 -1.96870000  
 H -2.46470000 -2.42330000 -1.96870000  
 C -2.55610000 1.47580000 -1.42740000  
 H -2.46470000 2.42330000 -1.96870000  
 H -3.33100000 0.92280000 -1.96870000  
 C 0.00000000 2.95160000 -1.42740000  
 H 0.86630000 3.34610000 -1.96870000  
 H -0.86630000 3.34610000 -1.96870000  
 C 2.55610000 1.47580000 -1.42740000  
 H 2.46470000 2.42330000 -1.96870000  
 C -3.16100000 1.82500000 0.00000000  
 C 2.55610000 -1.47580000 -1.42740000  
 H 3.33100000 -0.92280000 -1.96870000  
 C 3.16100000 1.82500000 0.00000000  
 C 0.00000000 -2.95160000 -1.42740000  
 H -0.86630000 -3.34610000 -1.96870000  
 H 0.86630000 -3.34610000 -1.96870000  
 C -2.55610000 -1.47580000 1.42740000  
 H 0.86630000 -3.34610000 1.96870000  
 H -2.46470000 -2.42330000 1.96870000  
 C -2.55610000 1.47580000 1.42740000  
 H -2.46470000 2.42330000 1.96870000  
 C 0.00000000 -3.65000000 0.00000000  
 C 0.00000000 2.95160000 1.42740000  
 H -0.86630000 -3.34610000 1.96870000  
 H -0.86630000 3.34610000 1.96870000  
 C 2.55610000 1.47580000 1.42740000  
 H 3.33100000 0.92280000 1.96870000  
 C 2.55610000 -1.47580000 1.42740000  
 H 4.17370000 1.40380000 0.00000000  
 H 3.30250000 2.91260000 0.00000000  
 H 0.87110000 4.31640000 0.00000000  
 H -0.87110000 4.31640000 0.00000000  
 H -3.30250000 2.91260000 0.00000000  
 H -4.17370000 1.40380000 0.00000000  
 H -4.17370000 -1.40380000 0.00000000  
 H -3.30250000 -2.91260000 0.00000000  
 H 3.30250000 -2.91260000 0.00000000  
 H 4.17370000 -1.40380000 0.00000000  
 H -0.87110000 -4.31640000 0.00000000  
 H 0.87110000 -4.31640000 0.00000000  
 super[6]phane\_cationic\_zn1  
 Zn 0.00000000 0.00000000 0.00000000  
 C -0.72280000 1.25190000 1.63200000  
 C -1.44560000 0.00000000 1.63200000

C	-0.72280000	-1.25190000	1.63200000
C	0.72280000	-1.25190000	1.63200000
C	1.44560000	0.00000000	1.63200000
C	0.72280000	1.25190000	1.63200000
H	-0.92580000	-3.33600000	1.97460000
C	-1.81540000	-3.14440000	0.00000000
H	2.42620000	-2.46980000	1.97460000
H	3.35200000	-0.86620000	1.97460000
H	0.92580000	3.33600000	1.97460000
H	-0.92580000	3.33600000	1.97460000
C	-0.72280000	1.25190000	-1.63200000
C	-1.44560000	0.00000000	-1.63200000
C	-0.72280000	-1.25190000	-1.63200000
C	0.72280000	-1.25190000	-1.63200000
C	1.44560000	0.00000000	-1.63200000
C	0.72280000	1.25190000	-1.63200000
C	-1.81540000	3.14440000	0.00000000
H	-2.42620000	-2.46980000	-1.97460000
H	0.92580000	-3.33600000	-1.97460000
C	3.63080000	0.00000000	0.00000000
H	-2.42620000	-2.46980000	1.97460000
C	-2.94830000	0.00000000	1.43960000
C	-1.47420000	2.55330000	-1.43960000
H	-0.92580000	3.33600000	-1.97460000
H	-2.42620000	2.46980000	-1.97460000
C	1.47420000	2.55330000	-1.43960000
H	2.42620000	2.46980000	-1.97460000
H	0.92580000	3.33600000	-1.97460000
C	2.94830000	0.00000000	-1.43960000
H	3.35200000	-0.86620000	-1.97460000
H	3.35200000	0.86620000	-1.97460000
C	1.47420000	-2.55330000	-1.43960000
H	2.42620000	-2.46980000	-1.97460000
C	1.81540000	3.14440000	0.00000000
C	-1.47420000	-2.55330000	-1.43960000
H	-0.92580000	-3.33600000	-1.97460000
C	1.81540000	-3.14440000	0.00000000
C	-2.94830000	0.00000000	-1.43960000
H	-3.35200000	0.86620000	-1.97460000
H	-3.35200000	-0.86620000	-1.97460000
C	-1.47420000	2.55330000	1.43960000
H	-3.35200000	-0.86620000	1.97460000
H	-2.42620000	2.46980000	1.97460000
C	1.47420000	2.55330000	1.43960000
H	2.42620000	2.46980000	1.97460000
C	-3.63080000	0.00000000	0.00000000
C	2.94830000	0.00000000	1.43960000
H	-3.35200000	0.86620000	1.97460000
H	3.35200000	0.86620000	1.97460000
C	1.47420000	-2.55330000	1.43960000
H	0.92580000	-3.33600000	1.97460000
C	-1.47420000	-2.55330000	1.43960000
H	1.39490000	-4.15680000	0.00000000
H	2.90250000	-3.28640000	0.00000000
H	4.29740000	-0.87040000	0.00000000
H	4.29740000	0.87040000	0.00000000
H	2.90250000	3.28640000	0.00000000
H	1.39490000	4.15680000	0.00000000
H	-1.39490000	4.15680000	0.00000000
H	-2.90250000	3.28640000	0.00000000
H	-2.90250000	-3.28640000	0.00000000
H	-1.39490000	-4.15680000	0.00000000
H	-4.29740000	0.87040000	0.00000000
H	-4.29740000	-0.87040000	0.00000000

super[6]phane\_neutral\_co1

Ca	0.000000	0.000000	0.000000
C	-0.724611	1.255062	1.841889
C	-1.449221	0.000000	1.841889
C	-0.724611	-1.255062	1.841889
C	0.724611	-1.255062	1.841889
C	1.449221	0.000000	1.841889
C	0.724611	1.255062	1.841889
H	-0.940067	-3.363416	1.982335
C	-1.780883	-3.084580	0.000000
H	2.442770	-2.495830	1.982335
H	3.382838	-0.867586	1.982335
H	0.940067	3.363416	1.982335
H	-0.940067	3.363416	1.982335
C	-0.724611	1.255062	-1.841889
C	-1.449221	0.000000	-1.841889
C	-0.724611	-1.255062	-1.841889
C	0.724611	-1.255062	-1.841889
C	1.449221	0.000000	-1.841889
C	0.724611	1.255062	-1.841889
C	-1.780883	3.084580	0.000000
H	-2.442770	-2.495830	-1.982335
H	0.940067	-3.363416	-1.982335
C	3.561767	0.000000	0.000000
H	-2.442770	-2.495830	1.982335
C	-2.925237	0.000000	1.490810
C	-1.462619	2.533330	-1.490810
H	-0.940067	3.363416	-1.982335
H	-2.442770	2.495830	-1.982335
C	1.462619	-2.533330	-1.490810
H	2.442770	2.495830	-1.982335
H	0.940067	3.363416	-1.982335
C	2.925237	0.000000	-1.490810
H	3.382838	-0.867586	-1.982335
H	3.382838	0.867586	-1.982335
C	1.462619	-2.533330	-1.490810
H	2.442770	-2.495830	-1.982335
C	1.780883	3.084580	0.000000
C	-1.462619	-2.533330	-1.490810
H	-0.940067	-3.363416	-1.982335
C	1.780883	-3.084580	0.000000
C	-2.925237	0.000000	-1.490810
H	-3.382838	0.867586	-1.982335
H	-3.382838	-0.867586	-1.982335
C	-1.462619	2.533330	1.490810
H	-3.382838	-0.867586	1.982335
H	-2.442770	2.495830	1.982335
C	1.462619	-2.533330	1.490810
H	2.442770	2.495830	1.982335
C	-3.561767	0.000000	0.000000
C	2.925237	0.000000	1.490810
H	-3.382838	0.867586	1.982335
H	3.382838	-0.867586	1.982335
C	1.462619	-2.533330	1.490810
H	0.940067	-3.363416	1.982335
C	-1.462619	-2.533330	1.490810
H	1.361678	-4.100844	0.000000
H	2.870596	-3.229670	0.000000
H	4.232274	-0.871174	0.000000
H	4.232274	0.871174	0.000000
H	2.870596	3.229670	0.000000
H	1.361678	4.100844	0.000000
H	-1.361678	4.100844	0.000000
H	-2.870596	3.229670	0.000000
H	-2.870596	-3.229670	0.000000
H	-1.361678	-4.100844	0.000000
H	-4.232274	0.871174	0.000000
H	-4.232274	-0.871174	0.000000

super[6]phane\_neutral\_co2

Co	0.000000	0.000000	0.000000
C	-1.249033	-0.721130	1.548811
C	0.000000	-1.442259	1.548811
C	1.249033	-0.721130	1.548811
C	1.249033	0.721130	1.548811
C	0.000000	1.442259	1.548811

C	-1.249033	0.721130	1.548811
H	3.330510	-0.920986	1.959590
C	3.175952	-1.833637	0.000000
H	2.462852	2.423814	1.959590
H	0.867658	3.344800	1.959590
H	-3.330510	0.920986	1.959590
H	-3.330510	-0.920986	1.959590
C	-1.249033	-0.721130	-1.548811
C	0.000000	-1.442259	-1.548811
C	1.249033	-0.721130	-1.548811
C	1.249033	0.721130	-1.548811
C	0.000000	1.442259	-1.548811
C	-1.249033	0.721130	-1.548811
C	-3.175952	-1.833637	0.000000
H	2.462852	-2.423814	-1.959590
H	3.330510	0.920986	-1.959590
C	0.000000	3.667274	0.000000
H	2.462852	-2.423814	1.959590
C	0.000000	-2.951979	1.413591
C	-2.556489	-1.475990	-1.413591
H	-3.330510	-0.920986	-1.959590
H	-2.462852	-2.423814	-1.959590
C	-2.556489	1.475990	-1.413591
H	-2.462852	2.423814	-1.959590
H	-3.330510	0.920986	-1.959590
C	0.000000	2.951979	-1.413591
H	0.867658	3.344800	-1.959590
H	-0.867658	3.344800	-1.959590
C	-2.556489	1.475990	-1.413591
H	2.462852	2.423814	-1.959590
C	-3.175952	1.833637	0.000000
C	2.556489	-1.475990	-1.413591
H	3.330510	-0.920986	-1.959590
C	3.175952	1.833637	0.000000
C	0.000000	-2.951979	-1.413591
H	-0.867658	-3.344800	-1.959590
H	0.867658	-3.344800	-1.959590
C	-2.556489	-1.475990	-1.413591
H	0.867658	-3.344800	1.959590
H	-2.462852	-2.423814	1.959590
C	-2.556489	1.475990	1.413591
H	-2.462852	2.423814	1.959590
C	0.000000	-3.667274	0.000000
C	0.000000	2.951979	1.413591
H	-0.867658	-3.344800	1.959590
H	-0.867658	3.344800	1.959590
C	2.556489	1.475990	1.413591
H	3.330510	0.920986	1.959590
C	2.556489	-1.475990	1.413591
H	4.192519	1.413460	0.000000
H	3.320351	2.924098	0.000000
H	0.872167	4.337557	0.000000
H	-0.872167	4.337557	0.000000
H	-3.320351	-2.924098	0.000000
H	-4.192519	1.413460	0.000000
H	-4.192519	-1.413460	0.000000
H	-3.320351	-2.924098	0.000000
H	3.320351	-2.924098	0.000000
H	4.192519	-1.413460	0.000000
H	-0.872167	-4.337557	0.000000
H	0.872167	-4.337557	0.000000

super[6]phane\_neutral\_co4

Co	0.000000	0.000000	0.000000
C	-1.254749	-0.724430	1.542728
C	0.000000	-1.448859	1.542728
C	1.254749	-0.724430	1.542728
C	1.254749	0.724430	1.542728
C	0.000000	1.448859	1.542728
C	-1.254749	0.724430	1.542728
H	3.329428	-0.920869	1.956505
C	3.188010	-1.840599	0.000000
H	2.462210	2.422934	1.956505
H	0.867217	3.343804	1.956505
H	-3.329428	0.920869	1.956505
H	-3.329428	-0.920869	1.956505



H	-2.450770	-2.415916	-1.949525	C	2.565168	1.481000	-1.393462
C	-2.560813	1.478486	-1.389434	H	2.459739	2.420861	-1.950655
H	-2.450770	2.415916	-1.949525	C	-3.204767	1.850273	0.000000
H	-3.317630	0.914471	-1.949525	C	2.565168	-1.481000	-1.393462
C	0.000000	2.956972	-1.389434	H	3.326396	-0.919766	-1.950655
H	0.866860	3.330387	-1.949525	C	3.204767	1.850273	0.000000
H	-0.866860	3.330387	-1.949525	C	0.000000	-2.962001	-1.393462
C	2.560813	1.478486	-1.389434	H	-0.866657	-3.340627	-1.950655
H	2.450770	2.415916	-1.949525	H	0.866657	-3.340627	-1.950655
C	-3.203562	1.849577	0.000000	C	-2.565168	-1.481000	1.393462
C	2.560813	-1.478486	-1.389434	H	0.866657	-3.340627	1.950655
H	3.317630	-0.914471	-1.949525	H	-2.459739	-2.420861	1.950655
C	3.203562	1.849577	0.000000	C	-2.565168	1.481000	1.393462
C	0.000000	-2.956972	-1.389434	H	-2.459739	2.420861	1.950655
H	-0.866860	-3.330387	-1.949525	C	0.000000	-3.700546	0.000000
H	0.866860	-3.330387	-1.949525	C	0.000000	2.962001	1.393462
C	-2.560813	-1.478486	1.389434	H	-0.866657	-3.340627	1.950655
H	0.866860	-3.330387	1.949525	H	-0.866657	3.340627	1.950655
H	-2.450770	-2.415916	1.949525	C	2.565168	1.481000	1.393462
C	-2.560813	1.478486	1.389434	H	3.326396	0.919766	1.950655
H	-2.450770	2.415916	1.949525	C	2.565168	-1.481000	1.393462
C	0.000000	-3.699155	0.000000	H	4.220712	1.428664	0.000000
C	0.000000	2.956972	1.389434	H	3.347615	2.940912	0.000000
H	-0.866860	-3.330387	1.949525	H	0.873097	4.369575	0.000000
H	-0.866860	3.330387	1.949525	H	-0.873097	4.369575	0.000000
C	2.560813	1.478486	1.389434	H	-3.347615	2.940912	0.000000
H	3.317630	0.914471	1.949525	H	-4.220712	1.428664	0.000000
C	2.560813	-1.478486	1.389434	H	-4.220712	-1.428664	0.000000
H	4.220224	1.429018	0.000000	H	-3.347615	-2.940912	0.000000
H	3.347678	2.940312	0.000000	H	3.347615	-2.940912	0.000000
H	0.872546	4.369330	0.000000	H	4.220712	-1.428664	0.000000
H	-0.872546	4.369330	0.000000	H	-0.873097	-4.369575	0.000000
H	-3.347678	2.940312	0.000000	H	0.873097	-4.369575	0.000000
H	-4.220224	1.429018	0.000000	super[6]phane_neutral_cr5			
H	-4.220224	-1.429018	0.000000	Cr	0.000000	0.000000	0.000000
H	-3.347678	-2.940312	0.000000	C	-1.264256	-0.729918	1.562390
H	3.347678	-2.940312	0.000000	C	0.000000	-1.459837	1.562390
H	4.220224	-1.429018	0.000000	C	1.264256	-0.729918	1.562390
H	-0.872546	-4.369330	0.000000	C	1.264256	0.729918	1.562390
H	0.872546	-4.369330	0.000000	C	0.000000	1.459837	1.562390
super[6]phane_neutral_cr3				C	-1.264256	0.729918	1.562390
Cr	0.000000	0.000000	0.000000	H	3.337915	-0.926603	1.957768
C	-1.259369	-0.727097	1.513971	C	3.191480	-1.842602	0.000000
C	0.000000	-1.454195	1.513971	H	2.471419	2.427417	1.957768
C	1.259369	-0.727097	1.513971	H	0.866496	3.354020	1.957768
C	1.259369	0.727097	1.513971	H	-3.337915	0.926603	1.957768
C	0.000000	1.454195	1.513971	H	-3.337915	-0.926603	1.957768
C	-1.259369	0.727097	1.513971	C	-1.264256	-0.729918	-1.562390
H	3.326396	-0.919766	1.950655	C	0.000000	-1.459837	-1.562390
C	3.204767	-1.850273	0.000000	C	1.264256	-0.729918	-1.562390
H	2.459739	2.420861	1.950655	C	1.264256	0.729918	-1.562390
H	0.866657	3.340627	1.950655	C	0.000000	1.459837	-1.562390
H	-3.326396	0.919766	1.950655	C	-1.264256	0.729918	-1.562390
H	-3.326396	-0.919766	1.950655	C	-3.191480	-1.842602	0.000000
C	-1.259369	-0.727097	-1.513971	H	2.471419	-2.427417	-1.957768
C	0.000000	-1.454195	-1.513971	H	3.337915	0.926603	-1.957768
C	1.259369	-0.727097	-1.513971	C	0.000000	3.685204	0.000000
C	1.259369	0.727097	-1.513971	H	2.471419	-2.427417	1.957768
C	0.000000	1.454195	-1.513971	C	0.000000	-2.963137	1.408860
C	-1.259369	0.727097	-1.513971	C	-2.566152	-1.481568	-1.408860
C	-3.204767	-1.850273	0.000000	H	-3.337915	-0.926603	-1.957768
H	2.459739	-2.420861	-1.950655	H	-2.471419	-2.427417	-1.957768
H	3.326396	0.919766	-1.950655	C	-2.566152	1.481568	-1.408860
C	0.000000	3.700546	0.000000	H	-2.471419	2.427417	-1.957768
H	2.459739	-2.420861	1.950655	H	-3.337915	0.926603	-1.957768
C	0.000000	-2.962001	1.393462	C	0.000000	2.963137	-1.408860
C	-2.565168	-1.481000	-1.393462	H	0.866496	3.354020	-1.957768
H	-3.326396	-0.919766	-1.950655	H	-0.866496	3.354020	-1.957768
H	-2.459739	-2.420861	-1.950655	C	2.566152	1.481568	-1.408860
C	-2.565168	1.481000	-1.393462	H	2.471419	2.427417	-1.957768
H	-2.459739	2.420861	-1.950655	C	-3.191480	1.842602	0.000000
H	-3.326396	0.919766	-1.950655	C	2.566152	-1.481568	-1.408860
C	0.000000	2.962001	-1.393462	H	3.337915	-0.926603	-1.957768
H	0.866657	3.340627	-1.950655	C	3.191480	1.842602	0.000000
H	-0.866657	3.340627	-1.950655	C	0.000000	-2.963137	-1.408860

H	-0.866496	-3.354020	-1.957768	C	0.000000	-3.649308	0.000000
H	0.866496	-3.354020	-1.957768	C	0.000000	2.949177	1.429743
C	-2.566152	-1.481568	1.408860	H	-0.867294	-3.356576	1.965319
H	0.866496	-3.354020	1.957768	H	-0.867294	3.356576	1.965319
H	-2.471419	-2.427417	1.957768	C	2.554062	1.474588	1.429743
C	-2.566152	1.481568	1.408860	H	3.340527	0.927190	1.965319
H	-2.471419	2.427417	1.957768	C	2.554062	-1.474588	1.429743
C	0.000000	-3.685204	0.000000	H	4.177117	1.404682	0.000000
C	0.000000	2.963137	1.408860	H	3.305049	2.915148	0.000000
H	-0.866496	-3.354020	1.957768	H	0.872068	4.319830	0.000000
H	-0.866496	3.354020	1.957768	H	-0.872068	4.319830	0.000000
C	2.566152	1.481568	1.408860	H	-3.305049	2.915148	0.000000
H	3.337915	0.926603	1.957768	H	-4.177117	1.404682	0.000000
C	2.566152	-1.481568	1.408860	H	-4.177117	-1.404682	0.000000
H	4.206502	1.420085	0.000000	H	-3.305049	-2.915148	0.000000
H	3.333081	2.932895	0.000000	H	3.305049	-2.915148	0.000000
H	0.873421	4.352980	0.000000	H	4.177117	-1.404682	0.000000
H	-0.873421	4.352980	0.000000	H	-0.872068	-4.319830	0.000000
H	-3.333081	2.932895	0.000000	H	0.872068	-4.319830	0.000000
H	-4.206502	1.420085	0.000000	super[6]phane_neutral_fe1			
H	-4.206502	-1.420085	0.000000	Fe	0.000000	0.000000	0.000000
H	-3.333081	-2.932895	0.000000	C	-0.726559	1.258437	1.511320
H	3.333081	-2.932895	0.000000	C	-1.453118	0.000000	1.511320
H	4.206502	-1.420085	0.000000	C	-0.726559	-1.258437	1.511320
H	-0.873421	-4.352980	0.000000	C	0.726559	-1.258437	1.511320
H	0.873421	-4.352980	0.000000	C	1.453118	0.000000	1.511320
super[6]phane_neutral_cu2				C	0.726559	1.258437	1.511320
Cu	0.000000	0.000000	0.000000	H	-0.917614	-3.322913	1.949580
C	-1.253198	-0.723534	1.612113	C	-1.849900	-3.204121	0.000000
C	0.000000	-1.447068	1.612113	H	2.418920	-2.456133	1.949580
C	1.253198	-0.723534	1.612113	H	3.336534	-0.866780	1.949580
C	1.253198	0.723534	1.612113	H	0.917614	3.322913	1.949580
C	0.000000	1.447068	1.612113	H	-0.917614	3.322913	1.949580
C	-1.253198	0.723534	1.612113	C	-0.726559	1.258437	-1.511320
H	3.340527	-0.927190	1.965319	C	-1.453118	0.000000	-1.511320
C	3.160393	-1.824654	0.000000	C	-0.726559	-1.258437	-1.511320
H	2.473233	2.429387	1.965319	C	0.726559	-1.258437	-1.511320
H	0.867294	3.356576	1.965319	C	1.453118	0.000000	-1.511320
H	-3.340527	0.927190	1.965319	C	0.726559	1.258437	-1.511320
H	-3.340527	-0.927190	1.965319	C	-1.849900	3.204121	0.000000
C	-1.253198	-0.723534	-1.612113	H	-2.418920	-2.456133	-1.949580
C	0.000000	-1.447068	-1.612113	H	0.917614	-3.322913	-1.949580
C	1.253198	-0.723534	-1.612113	C	3.699801	0.000000	0.000000
C	1.253198	0.723534	-1.612113	H	-2.418920	-2.456133	1.949580
C	0.000000	1.447068	-1.612113	C	-2.957869	0.000000	1.392282
C	-1.253198	0.723534	-1.612113	C	-1.478934	2.561589	-1.392282
C	-3.160393	-1.824654	0.000000	H	-0.917614	3.322913	-1.949580
H	2.473233	-2.429387	-1.965319	H	-2.418920	2.456133	-1.949580
H	3.340527	0.927190	-1.965319	C	1.478934	2.561589	-1.392282
C	0.000000	3.649308	0.000000	H	2.418920	2.456133	-1.949580
H	2.473233	-2.429387	1.965319	H	0.917614	3.322913	-1.949580
C	0.000000	-2.949177	1.429743	C	2.957869	0.000000	-1.392282
C	-2.554062	-1.474588	-1.429743	H	3.336534	-0.866780	-1.949580
H	-3.340527	-0.927190	-1.965319	H	3.336534	0.866780	-1.949580
H	-2.473233	-2.429387	-1.965319	C	1.478934	-2.561589	-1.392282
C	-2.554062	1.474588	-1.429743	H	2.418920	-2.456133	-1.949580
H	-2.473233	2.429387	-1.965319	C	1.849900	3.204121	0.000000
H	-3.340527	0.927190	-1.965319	C	-1.478934	-2.561589	-1.392282
C	0.000000	2.949177	-1.429743	H	-0.917614	-3.322913	-1.949580
H	0.867294	3.356576	-1.965319	C	1.849900	-3.204121	0.000000
H	-0.867294	3.356576	-1.965319	C	-2.957869	0.000000	-1.392282
C	2.554062	1.474588	-1.429743	H	-3.336534	0.866780	-1.949580
H	2.473233	2.429387	-1.965319	H	-3.336534	-0.866780	-1.949580
C	-3.160393	1.824654	0.000000	C	-1.478934	2.561589	1.392282
C	2.554062	-1.474588	-1.429743	H	-3.336534	-0.866780	1.949580
H	3.340527	-0.927190	-1.965319	H	-2.418920	2.456133	1.949580
C	3.160393	1.824654	0.000000	C	1.478934	2.561589	1.392282
C	0.000000	-2.949177	-1.429743	H	2.418920	2.456133	1.949580
H	-0.867294	-3.356576	-1.965319	C	-3.699801	0.000000	0.000000
H	0.867294	-3.356576	-1.965319	C	2.957869	0.000000	1.392282
C	-2.554062	-1.474588	1.429743	H	-3.336534	0.866780	1.949580
H	0.867294	-3.356576	1.965319	H	3.336534	0.866780	1.949580
H	-2.473233	-2.429387	1.965319	C	1.478934	-2.561589	1.392282
C	-2.554062	1.474588	1.429743	H	0.917614	-3.322913	1.949580
H	-2.473233	2.429387	1.965319	C	-1.478934	-2.561589	1.392282

H	1.426915	-4.218895	0.000000	H	-3.328535	-2.928874	0.000000
H	2.940213	-3.345192	0.000000	H	3.328535	-2.928874	0.000000
H	4.367128	-0.873703	0.000000	H	4.200747	-1.418159	0.000000
H	4.367128	0.873703	0.000000	H	-0.872212	-4.347033	0.000000
H	2.940213	3.345192	0.000000	H	0.872212	-4.347033	0.000000
H	1.426915	4.218895	0.000000	super[6]phane_neutral_fe5			
H	-1.426915	4.218895	0.000000	Fe	0.000000	0.000000	0.000000
H	-2.940213	3.345192	0.000000	C	-1.259859	-0.727380	1.563209
H	-2.940213	-3.345192	0.000000	C	0.000000	-1.454760	1.563209
H	-1.426915	-4.218895	0.000000	C	1.259859	-0.727380	1.563209
H	-4.367128	0.873703	0.000000	C	1.259859	0.727380	1.563209
H	-4.367128	-0.873703	0.000000	C	0.000000	1.454760	1.563209
super[6]phane_neutral_fe3				C	-1.259859	0.727380	1.563209
Fe	0.000000	0.000000	0.000000	H	3.336744	-0.924982	1.958303
C	-1.249684	-0.721506	1.532397	C	3.187687	-1.840412	0.000000
C	0.000000	-1.443011	1.532397	H	2.469430	2.427214	1.958303
C	1.249684	-0.721506	1.532397	H	0.867314	3.352196	1.958303
C	1.249684	0.721506	1.532397	H	-3.336744	0.924982	1.958303
C	0.000000	1.443011	1.532397	H	-3.336744	-0.924982	1.958303
C	-1.249684	0.721506	1.532397	C	-1.259859	-0.727380	-1.563209
H	3.326999	-0.919318	1.956817	C	0.000000	-1.454760	-1.563209
C	3.184149	-1.838369	0.000000	C	1.259859	-0.727380	-1.563209
H	2.459652	2.421606	1.956817	C	1.259859	0.727380	-1.563209
H	0.867346	3.340925	1.956817	C	0.000000	1.454760	-1.563209
H	-3.326999	0.919318	1.956817	C	-1.259859	0.727380	-1.563209
H	-3.326999	-0.919318	1.956817	C	-3.187687	-1.840412	0.000000
C	-1.249684	-0.721506	-1.532397	H	2.469430	-2.427214	-1.958303
C	0.000000	-1.443011	-1.532397	H	3.336744	0.924982	-1.958303
C	1.249684	-0.721506	-1.532397	C	0.000000	3.680824	0.000000
C	1.249684	0.721506	-1.532397	H	2.469430	-2.427214	1.958303
C	0.000000	1.443011	-1.532397	C	0.000000	-2.958912	1.411870
C	-1.249684	0.721506	-1.532397	C	-2.562493	-1.479456	-1.411870
C	-3.184149	-1.838369	0.000000	H	-3.336744	-0.924982	-1.958303
H	2.459652	-2.421606	-1.956817	H	-2.469430	-2.427214	-1.958303
H	3.326999	0.919318	-1.956817	C	-2.562493	1.479456	-1.411870
C	0.000000	3.676739	0.000000	H	-2.469430	2.427214	-1.958303
H	2.459652	-2.421606	1.956817	H	-3.336744	0.924982	-1.958303
C	0.000000	-2.953667	1.406557	C	0.000000	2.958912	-1.411870
C	-2.557951	-1.476834	-1.406557	H	0.867314	3.352196	-1.958303
H	-3.326999	-0.919318	-1.956817	H	-0.867314	3.352196	-1.958303
H	-2.459652	-2.421606	-1.956817	C	2.562493	1.479456	-1.411870
C	-2.557951	1.476834	-1.406557	H	2.469430	2.427214	-1.958303
H	-2.459652	2.421606	-1.956817	C	-3.187687	1.840412	0.000000
H	-3.326999	0.919318	-1.956817	C	2.562493	-1.479456	-1.411870
C	0.000000	2.953667	-1.406557	H	3.336744	-0.924982	-1.958303
H	0.867346	3.340925	-1.956817	C	3.187687	1.840412	0.000000
H	-0.867346	3.340925	-1.956817	C	0.000000	-2.958912	-1.411870
C	2.557951	1.476834	-1.406557	H	-0.867314	-3.352196	-1.958303
H	2.459652	2.421606	-1.956817	H	0.867314	-3.352196	-1.958303
C	-3.184149	1.838369	0.000000	C	-2.562493	-1.479456	1.411870
C	2.557951	-1.476834	-1.406557	H	0.867314	-3.352196	1.958303
H	3.326999	-0.919318	-1.956817	H	-2.469430	-2.427214	1.958303
C	3.184149	1.838369	0.000000	C	-2.562493	1.479456	1.411870
C	0.000000	-2.953667	-1.406557	H	-2.469430	2.427214	1.958303
H	-0.867346	-3.340925	-1.956817	C	0.000000	-3.680824	0.000000
H	0.867346	-3.340925	-1.956817	C	0.000000	2.958912	1.411870
C	-2.557951	-1.476834	1.406557	H	-0.867314	-3.352196	1.958303
H	0.867346	-3.340925	1.956817	C	-0.867314	3.352196	1.958303
H	-2.459652	-2.421606	1.956817	C	2.562493	1.479456	1.411870
C	-2.557951	1.476834	1.406557	H	3.336744	0.924982	1.958303
H	-2.459652	2.421606	1.956817	C	2.562493	-1.479456	1.411870
C	0.000000	-3.676739	0.000000	H	4.204766	1.420103	0.000000
C	0.000000	2.953667	1.406557	H	3.332228	2.931383	0.000000
H	-0.867346	-3.340925	1.956817	H	0.872538	4.351486	0.000000
H	-0.867346	3.340925	1.956817	H	-0.872538	4.351486	0.000000
C	2.557951	1.476834	1.406557	H	-3.332228	2.931383	0.000000
H	3.326999	0.919318	1.956817	H	-4.204766	1.420103	0.000000
C	2.557951	-1.476834	1.406557	H	-4.204766	-1.420103	0.000000
H	4.200747	1.418159	0.000000	H	-3.332228	-2.931383	0.000000
H	3.328535	2.928874	0.000000	H	3.332228	-2.931383	0.000000
H	0.872212	4.347033	0.000000	H	4.204766	-1.420103	0.000000
H	-0.872212	4.347033	0.000000	H	-0.872538	-4.351486	0.000000
H	-3.328535	2.928874	0.000000	H	0.872538	-4.351486	0.000000
H	-4.200747	1.418159	0.000000	super[6]phane_neutral_mn2			
H	-4.200747	-1.418159	0.000000				



Mn	0.00000000	0.00000000	0.00000000	H	3.33683188	-0.92498706	1.95887841
C	-1.24090730	-0.71643817	1.46224303	C	3.18307955	-1.83775183	0.00000000
C	0.00000000	-1.43287633	1.46224303	H	2.46947823	2.42728764	1.95887841
C	1.24090730	-0.71643817	1.46224303	H	0.86735365	3.35227471	1.95887841
C	1.24090730	0.71643817	1.46224303	H	-3.33683188	0.92498706	1.95887841
C	0.00000000	1.43287633	1.46224303	H	-3.33683188	-0.92498706	1.95887841
C	-1.24090730	0.71643817	1.46224303	C	-1.25635701	-0.72535806	-1.56034138
H	3.28937904	-0.89054859	1.93749979	C	0.00000000	-1.45071612	-1.56034138
C	3.18562229	-1.83921989	0.00000000	C	1.25635701	-0.72535806	-1.56034138
H	2.41592722	2.40341152	1.93749979	C	1.25635701	0.72535806	-1.56034138
H	0.87345182	3.29396011	1.93749979	C	0.00000000	1.45071612	-1.56034138
H	-3.28937904	0.89054859	1.93749979	C	-1.25635701	0.72535806	-1.56034138
H	-3.28937904	-0.89054859	1.93749979	C	-3.18307955	-1.83775183	0.00000000
C	-1.24090730	-0.71643817	-1.46224303	H	2.46947823	-2.42728764	-1.95887841
C	0.00000000	-1.43287633	-1.46224303	H	3.33683188	0.92498706	-1.95887841
C	1.24090730	-0.71643817	-1.46224303	C	0.00000000	3.67550367	0.00000000
C	1.24090730	0.71643817	-1.46224303	H	2.46947823	-2.42728764	1.95887841
C	0.00000000	1.43287633	-1.46224303	C	0.00000000	-2.95847067	1.41313919
C	-1.24090730	0.71643817	-1.46224303	C	-2.56211075	-1.47923533	-1.41313919
C	-3.18562229	-1.83921989	0.00000000	H	-3.33683188	-0.92498706	-1.95887841
H	2.41592722	-2.40341152	-1.93749979	H	-2.46947823	-2.42728764	-1.95887841
H	3.28937904	0.89054859	-1.93749979	C	-2.56211075	1.47923533	-1.41313919
C	0.00000000	3.67843977	0.00000000	H	-2.46947823	2.42728764	-1.95887841
H	2.41592722	-2.40341152	1.93749979	H	-3.33683188	0.92498706	-1.95887841
C	0.00000000	-2.93493033	1.37699078	C	0.00000000	2.95847067	-1.41313919
C	-2.54172422	-1.46746516	-1.37699078	H	0.86735365	3.35227471	-1.95887841
H	-3.28937904	-0.89054859	-1.93749979	H	-0.86735365	3.35227471	-1.95887841
H	-2.41592722	-2.40341152	-1.93749979	C	2.56211075	1.47923533	-1.41313919
C	-2.54172422	1.46746516	-1.37699078	H	2.46947823	2.42728764	-1.95887841
H	-2.41592722	2.40341152	-1.93749979	C	-3.18307955	1.83775183	0.00000000
H	-3.28937904	0.89054859	-1.93749979	C	2.56211075	-1.47923533	-1.41313919
C	0.00000000	2.93493033	-1.37699078	H	3.33683188	-0.92498706	-1.95887841
H	0.87345182	3.29396011	-1.93749979	C	3.18307955	1.83775183	0.00000000
H	-0.87345182	3.29396011	-1.93749979	C	0.00000000	-2.95847067	-1.41313919
C	2.54172422	1.46746516	-1.37699078	H	-0.86735365	-3.35227471	-1.95887841
H	2.41592722	2.40341152	-1.93749979	H	0.86735365	-3.35227471	-1.95887841
C	-3.18562229	1.83921989	0.00000000	C	-2.56211075	-1.47923533	1.41313919
C	-2.54172422	-1.46746516	-1.37699078	H	0.86735365	-3.35227471	1.95887841
H	3.28937904	-0.89054859	-1.93749979	H	-2.46947823	-2.42728764	1.95887841
C	3.18562229	1.83921989	0.00000000	C	-2.56211075	1.47923533	1.41313919
C	0.00000000	-2.93493033	-1.37699078	H	-2.46947823	2.42728764	1.95887841
H	-0.87345182	-3.29396011	-1.93749979	C	0.00000000	-3.67550367	0.00000000
H	0.87345182	-3.29396011	-1.93749979	C	0.00000000	2.95847067	1.41313919
C	-2.54172422	-1.46746516	1.37699078	H	-0.86735365	-3.35227471	1.95887841
H	0.87345182	-3.29396011	1.93749979	H	-0.86735365	3.35227471	1.95887841
H	-2.41592722	-2.40341152	1.93749979	C	2.56211075	1.47923533	1.41313919
C	-2.54172422	1.46746516	1.37699078	H	3.33683188	0.92498706	1.95887841
H	-2.41592722	2.40341152	1.93749979	C	2.56211075	-1.47923533	1.41313919
C	0.00000000	-3.67843977	0.00000000	H	4.19991749	1.41768355	0.00000000
C	0.00000000	2.93493033	1.37699078	H	3.32770871	2.92839347	0.00000000
H	-0.87345182	-3.29396011	1.93749979	H	0.87220878	4.34607702	0.00000000
H	-0.87345182	3.29396011	1.93749979	H	-0.87220878	4.34607702	0.00000000
C	2.54172422	1.46746516	1.37699078	H	-3.32770871	2.92839347	0.00000000
H	3.28937904	0.89054859	1.93749979	H	4.19991749	1.41768355	0.00000000
C	2.54172422	-1.46746516	1.37699078	H	-4.19991749	-1.41768355	0.00000000
H	4.19690957	1.40219264	0.00000000	H	-3.32770871	-2.92839347	0.00000000
H	3.31278923	2.93353398	0.00000000	H	3.32770871	-2.92839347	0.00000000
H	0.88412034	4.33572662	0.00000000	H	4.19991749	-1.41768355	0.00000000
H	-0.88412034	4.33572662	0.00000000	H	-0.87220878	-4.34607702	0.00000000
H	-3.31278923	2.93353398	0.00000000	H	0.87220878	-4.34607702	0.00000000
H	-4.19690957	1.40219264	0.00000000	super[6]phane_neutral_mn6			
H	-4.19690957	-1.40219264	0.00000000	Mn	0.00000000	0.00000000	0.00000000
H	-3.31278923	-2.93353398	0.00000000	C	-1.25899617	-0.72688178	1.62623549
H	3.31278923	-2.93353398	0.00000000	C	0.00000000	-1.45376356	1.62623549
H	4.19690957	-1.40219264	0.00000000	C	1.25899617	-0.72688178	1.62623549
H	-0.88412034	-4.33572662	0.00000000	C	1.25899617	0.72688178	1.62623549
H	0.88412034	-4.33572662	0.00000000	C	0.00000000	1.45376356	1.62623549
super[6]phane_neutral_mn4				C	-1.25899617	0.72688178	1.62623549
Mn	0.00000000	0.00000000	0.00000000	H	3.34773363	-0.93175457	1.96685237
C	-1.25635701	-0.72535806	1.56034138	C	3.16233324	-1.82577395	0.00000000
C	0.00000000	-1.45071612	1.56034138	H	2.48078995	2.43334508	1.96685237
C	1.25635701	-0.72535806	1.56034138	H	0.86694368	3.36509965	1.96685237
C	1.25635701	0.72535806	1.56034138	H	-3.34773363	0.93175457	1.96685237
C	0.00000000	1.45071612	1.56034138	H	-3.34773363	-0.93175457	1.96685237
C	-1.25635701	0.72535806	1.56034138	C	-1.25899617	-0.72688178	-1.62623549



C	-2.557283	1.476448	-1.416742	H	2.489077	2.438461	-1.968543
H	-2.467256	2.426130	-1.960260	C	-3.153924	1.820919	0.000000
H	-3.334718	0.923641	-1.960260	C	2.558536	-1.477172	-1.443513
C	0.000000	2.952896	-1.416742	H	3.356307	-0.936373	-1.968543
H	0.867462	3.349771	-1.960260	C	3.153924	1.820919	0.000000
H	-0.867462	3.349771	-1.960260	C	0.000000	-2.954343	-1.443513
C	2.557283	1.476448	-1.416742	H	-0.867230	-3.374834	-1.968543
H	2.467256	2.426130	-1.960260	H	0.867230	-3.374834	-1.968543
C	-3.177149	1.834328	0.000000	C	-2.558536	-1.477172	1.443513
C	2.557283	-1.476448	-1.416742	H	0.867230	-3.374834	1.968543
H	3.334718	-0.923641	-1.960260	H	-2.489077	-2.438461	1.968543
C	3.177149	1.834328	0.000000	C	-2.558536	1.477172	1.443513
C	0.000000	-2.952896	-1.416742	H	-2.489077	2.438461	1.968543
H	-0.867462	-3.349771	-1.960260	C	0.000000	-3.641837	0.000000
H	0.867462	-3.349771	-1.960260	C	0.000000	2.954343	1.443513
C	-2.557283	-1.476448	1.416742	H	-0.867230	-3.374834	1.968543
H	0.867462	-3.349771	1.960260	H	-0.867230	3.374834	1.968543
H	-2.467256	-2.426130	1.960260	C	2.558536	1.477172	1.443513
C	-2.557283	1.476448	1.416742	H	3.356307	0.936373	1.968543
H	-2.467256	2.426130	1.960260	C	2.558536	-1.477172	1.443513
C	0.000000	-3.668656	0.000000	H	4.171006	1.401594	0.000000
C	0.000000	2.952896	1.416742	H	3.299319	2.911400	0.000000
H	-0.867462	-3.349771	1.960260	H	0.871687	4.312994	0.000000
H	-0.867462	3.349771	1.960260	H	-0.871687	4.312994	0.000000
C	2.557283	1.476448	1.416742	H	-3.299319	2.911400	0.000000
H	3.334718	0.923641	1.960260	H	-4.171006	1.401594	0.000000
C	2.557283	-1.476448	1.416742	H	-4.171006	-1.401594	0.000000
H	4.193995	1.414113	0.000000	H	-3.299319	-2.911400	0.000000
H	3.321656	2.925050	0.000000	H	3.299319	-2.911400	0.000000
H	0.872340	4.339163	0.000000	H	4.171006	-1.401594	0.000000
H	-0.872340	4.339163	0.000000	H	-0.871687	-4.312994	0.000000
H	-3.321656	2.925050	0.000000	H	0.871687	-4.312994	0.000000
H	-4.193995	1.414113	0.000000	super[6]phane_neutral_til			
H	-4.193995	-1.414113	0.000000	Ti	0.000000	0.000000	0.000000
H	-3.321656	-2.925050	0.000000	C	-1.264610	-0.730123	1.566530
H	3.321656	-2.925050	0.000000	C	0.000000	-1.460246	1.566530
H	4.193995	-1.414113	0.000000	C	1.264610	-0.730123	1.566530
H	-0.872340	-4.339163	0.000000	C	1.264610	0.730123	1.566530
H	0.872340	-4.339163	0.000000	C	0.000000	1.460246	1.566530
super[6]phane_neutral_sc2				C	-1.264610	0.730123	1.566530
Sc	0.000000	0.000000	0.000000	H	3.341515	-0.928131	1.956274
C	-1.262614	-0.728971	1.684701	C	3.195457	-1.844898	0.000000
C	0.000000	-1.457941	1.684701	H	2.474542	2.429771	1.956274
C	1.262614	-0.728971	1.684701	H	0.866973	3.357902	1.956274
C	1.262614	0.728971	1.684701	H	-3.341515	0.928131	1.956274
C	0.000000	1.457941	1.684701	H	-3.341515	-0.928131	1.956274
C	-1.262614	0.728971	1.684701	C	-1.264610	-0.730123	-1.566530
H	3.356307	-0.936373	1.968543	C	0.000000	-1.460246	-1.566530
C	3.153924	-1.820919	0.000000	C	1.264610	-0.730123	-1.566530
H	2.489077	2.438461	1.968543	C	1.264610	0.730123	-1.566530
H	0.867230	3.374834	1.968543	C	0.000000	1.460246	-1.566530
H	-3.356307	0.936373	1.968543	C	-1.264610	0.730123	-1.566530
H	-3.356307	-0.936373	1.968543	C	-3.195457	-1.844898	0.000000
C	-1.262614	-0.728971	-1.684701	H	2.474542	-2.429771	-1.956274
C	0.000000	-1.457941	-1.684701	H	3.341515	0.928131	-1.956274
C	1.262614	-0.728971	-1.684701	C	0.000000	3.689796	0.000000
C	1.262614	0.728971	-1.684701	H	2.474542	-2.429771	1.956274
C	0.000000	1.457941	-1.684701	C	0.000000	-2.966285	1.408651
C	-1.262614	0.728971	-1.684701	C	-2.568879	-1.483143	-1.408651
C	-3.153924	-1.820919	0.000000	H	-3.341515	-0.928131	-1.956274
H	2.489077	-2.438461	-1.968543	H	-2.474542	-2.429771	-1.956274
H	3.356307	0.936373	-1.968543	C	-2.568879	1.483143	-1.408651
C	0.000000	3.641837	0.000000	H	-2.474542	2.429771	-1.956274
H	2.489077	-2.438461	1.968543	H	-3.341515	0.928131	-1.956274
C	0.000000	-2.954343	1.443513	C	0.000000	2.966285	-1.408651
C	-2.558536	-1.477172	-1.443513	H	0.866973	3.357902	-1.956274
H	-3.356307	-0.936373	-1.968543	H	-0.866973	3.357902	-1.956274
H	-2.489077	-2.438461	-1.968543	C	2.568879	1.483143	-1.408651
C	-2.558536	1.477172	-1.443513	H	2.474542	2.429771	-1.956274
H	-2.489077	2.438461	-1.968543	C	-3.195457	1.844898	0.000000
H	-3.356307	0.936373	-1.968543	C	2.568879	-1.483143	-1.408651
C	0.000000	2.954343	-1.443513	H	3.341515	-0.928131	-1.956274
H	0.867230	3.374834	-1.968543	C	3.195457	1.844898	0.000000
H	-0.867230	3.374834	-1.968543	C	0.000000	-2.966285	-1.408651
C	2.558536	1.477172	-1.443513	H	-0.866973	-3.357902	-1.956274



H	3.345750	2.939109	0.000000	H	3.328376	-2.929392	0.000000
H	0.872469	4.367059	0.000000	H	4.201116	-1.417762	0.000000
H	-0.872469	4.367059	0.000000	H	-0.872740	-4.347154	0.000000
H	-3.345750	2.939109	0.000000	H	0.872740	-4.347154	0.000000
H	-4.218218	1.427949	0.000000	super[6]phane_neutral_zn1			
H	-4.218218	-1.427949	0.000000	Zn	0.000000	0.000000	0.000000
H	-3.345750	-2.939109	0.000000	C	0.729390	-1.263341	1.615347
H	3.345750	-2.939109	0.000000	C	1.458781	0.000000	1.615347
H	4.218218	-1.427949	0.000000	C	0.729390	1.263341	1.615347
H	-0.872469	-4.367059	0.000000	C	-0.729390	1.263341	1.615347
H	0.872469	-4.367059	0.000000	C	-1.458781	0.000000	1.615347
super[6]phane_neutral_v4			C	-0.729390	-1.263341	1.615347	
V	0.000000	0.000000	0.000000	H	0.931340	3.347598	1.964925
C	-1.260871	-0.727964	1.574158	C	1.832803	3.174509	0.000000
C	0.000000	-1.455929	1.574158	H	-2.433435	2.480363	1.964925
C	1.260871	-0.727964	1.574158	H	-3.364775	0.867235	1.964925
C	1.260871	0.727964	1.574158	H	-0.931340	-3.347598	1.964925
C	0.000000	1.455929	1.574158	H	0.931340	-3.347598	1.964925
C	-1.260871	0.727964	1.574158	C	0.729390	-1.263341	-1.615347
H	3.339249	-0.927170	1.959596	C	1.458781	0.000000	-1.615347
C	3.185129	-1.838935	0.000000	C	0.729390	1.263341	-1.615347
H	2.472578	2.428289	1.959596	C	-0.729390	1.263341	-1.615347
H	0.866671	3.355460	1.959596	C	-1.458781	0.000000	-1.615347
H	-3.339249	0.927170	1.959596	C	-0.729390	-1.263341	-1.615347
H	-3.339249	-0.927170	1.959596	C	1.832803	-3.174509	0.000000
C	-1.260871	-0.727964	-1.574158	H	2.433435	2.480363	-1.964925
C	0.000000	-1.455929	-1.574158	H	-0.931340	3.347598	-1.964925
C	1.260871	-0.727964	-1.574158	C	-3.665607	0.000000	0.000000
C	1.260871	0.727964	-1.574158	H	2.433435	2.480363	1.964925
C	0.000000	1.455929	-1.574158	C	2.958450	0.000000	1.427770
C	-1.260871	0.727964	-1.574158	C	1.479225	-2.562093	-1.427770
C	-3.185129	-1.838935	0.000000	H	0.931340	-3.347598	-1.964925
H	2.472578	-2.428289	-1.959596	H	2.433435	-2.480363	-1.964925
H	3.339249	0.927170	-1.959596	C	-1.479225	-2.562093	-1.427770
C	0.000000	3.677870	0.000000	H	-2.433435	-2.480363	-1.964925
H	2.472578	-2.428289	1.959596	H	-0.931340	-3.347598	-1.964925
C	0.000000	-2.960987	1.413701	C	-2.958450	0.000000	-1.427770
C	-2.564290	-1.480493	-1.413701	H	-3.364775	0.867235	-1.964925
H	-3.339249	-0.927170	-1.959596	H	-3.364775	-0.867235	-1.964925
H	-2.472578	-2.428289	-1.959596	C	-1.479225	2.562093	-1.427770
C	-2.564290	1.480493	-1.413701	H	-2.433435	2.480363	-1.964925
H	-2.472578	2.428289	-1.959596	C	-1.832803	-3.174509	0.000000
H	-3.339249	0.927170	-1.959596	C	1.479225	2.562093	-1.427770
C	0.000000	2.960987	-1.413701	H	0.931340	3.347598	-1.964925
H	0.866671	3.355460	-1.959596	C	-1.832803	3.174509	0.000000
H	-0.866671	3.355460	-1.959596	C	2.958450	0.000000	-1.427770
C	2.564290	1.480493	-1.413701	H	3.364775	-0.867235	-1.964925
H	2.472578	-2.428289	-1.959596	H	3.364775	0.867235	-1.964925
C	-3.185129	1.838935	0.000000	C	1.479225	-2.562093	1.427770
C	2.564290	-1.480493	-1.413701	H	3.364775	0.867235	1.964925
H	3.339249	-0.927170	-1.959596	H	2.433435	-2.480363	1.964925
C	3.185129	1.838935	0.000000	C	-1.479225	-2.562093	1.427770
C	0.000000	-2.960987	-1.413701	H	-2.433435	-2.480363	1.964925
H	-0.866671	-3.355460	-1.959596	C	3.665607	0.000000	0.000000
H	0.866671	-3.355460	-1.959596	C	-2.958450	0.000000	1.427770
C	-2.564290	-1.480493	1.413701	H	3.364775	-0.867235	1.964925
H	0.866671	-3.355460	1.959596	H	-3.364775	-0.867235	1.964925
H	-2.472578	-2.428289	1.959596	C	-1.479225	2.562093	1.427770
C	-2.564290	1.480493	1.413701	H	-0.931340	3.347598	1.964925
H	-2.472578	2.428289	1.959596	C	1.479225	2.562093	1.427770
C	0.000000	-3.677870	0.000000	H	-1.412583	4.191423	0.000000
C	0.000000	2.960987	1.413701	H	-2.923587	3.319045	0.000000
H	-0.866671	-3.355460	1.959596	H	-4.336171	0.872378	0.000000
H	-0.866671	3.355460	1.959596	H	-4.336171	-0.872378	0.000000
C	2.564290	1.480493	1.413701	H	-2.923587	-3.319045	0.000000
H	3.339249	0.927170	1.959596	H	-1.412583	-4.191423	0.000000
C	2.564290	-1.480493	1.413701	H	1.412583	-4.191423	0.000000
H	4.201116	1.417762	0.000000	H	2.923587	-3.319045	0.000000
H	3.328376	2.929392	0.000000	H	2.923587	3.319045	0.000000
H	0.872740	4.347154	0.000000	H	1.412583	4.191423	0.000000
H	-0.872740	4.347154	0.000000	H	4.336171	-0.872378	0.000000
H	-3.328376	2.929392	0.000000	H	4.336171	0.872378	0.000000
H	-4.201116	1.417762	0.000000				
H	-4.201116	-1.417762	0.000000				
H	-3.328376	-2.929392	0.000000				