

Supplementary Information

H₂ Physisorption on Covalent Organic Framework Linkers and Metalated Linkers: A Strategy to Enhance Binding Strength

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Figure S4: The different H_2 adsorption sites in the Linker 2; a) H_2 adsorption at the benzene ring site; b) H_2 adsorption at the C_3N_3 ring site c) H_2 adsorption at the BO_2C_2 ring site.

1. H₂-H₂ interactions

In the present calculations, we have considered the weak van der Waals (vdW) interactions by incorporating semi-empirical Grimmes' “-D3” dispersion corrections. To compute the binding enthalpy with the dispersion effects, we have used the equation below:

$$\Delta H_{nH_2} = H_{(\text{linker}+nH_2)} - (H_{\text{linker}} + H_{nH_2})$$

Here, we have included the dispersion correction in every terms. The dispersion interaction between the H₂ - H₂ molecules becomes more negative as the number of H₂ molecules increases in the system. The Grimme's dispersion interaction energies for the number of 2, 3, and 4 H₂ molecules are presented in Table S1 which indicates that the maximum and optimum H₂-H₂ dispersion energy can be -3.867 kJ/mol when the four number of H₂ physisorbed in the linkers. The value of ΔH may decrease due the decreasing value of the dispersion energies (as more negative value of ΔH). We have calculated the dispersion energy for the H₂ complexes and found that the dispersion energy is one of the dominant factors in the weak interaction of H₂ molecules adsorbed in the linkers.

Table S1: The Grimme's dispersion interaction energies for the 2H₂, 3H₂, and 4H₂ molecules are reported.

H ₂ -H ₂	2H ₂	3H ₂	4H ₂
Dispersion Energy (kJ/mol)	-0.038	-2.422	-3.867

The Figure S1 a) shows the electrostatic potential map of H₂-H₂ molecules. The red color in the electrostatic potential map indicates the positive value of electrostatic potential whereas the blue color indicates the negative value of electrostatic potential. The Figure S1 b) shows the electrostatic potential contour plot of H₂-H₂ molecule. The denser area in molecular electrostatic potential contour lines represents the stronger electrostatic field than the region with less contour lines.

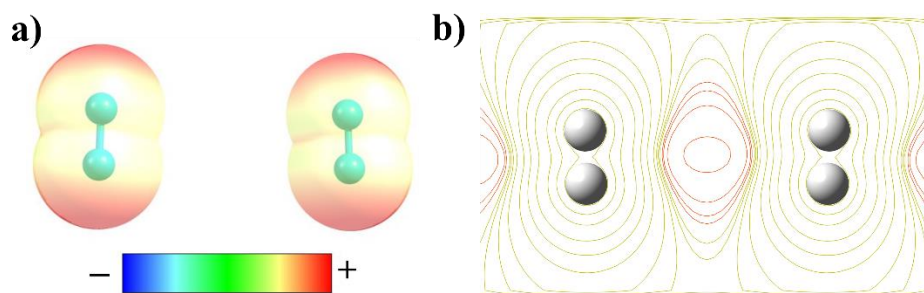
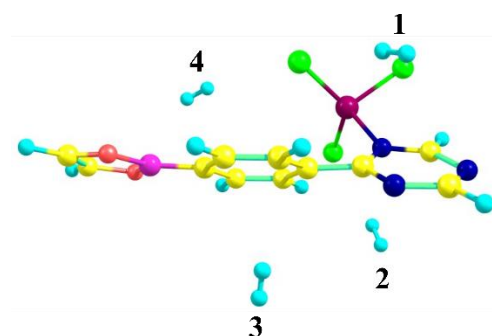


Figure S1: a) The electrostatic potential map of $\text{H}_2\text{-H}_2$ molecules and b) the electrostatic potential contour plot of $\text{H}_2\text{-H}_2$ molecule.

2. Different binding sites in the TM-chelated Linker-2:

The optimized equilibrium structure of the TM-chelated Linker-2 interacting with four H_2 molecules is shown in Figure S2. The numbers (near to the H_2 molecules) represent the sequence of the H_2 addition to the linker. Similarly, we chose the H_2 bindings at four different binding sites i.e., near to the transition metals of the TM-chelated linker, and at the BO_2C_2 ring, C_6H_4 ring, C_3N_3 ring of the pristine linkers.



Linker-2-TiCl₃-4H₂

Figure S2: The optimized equilibrium structure of the TM chelated Linker-2 interacting with four H_2 molecules is shown here.

Among all the H_2 complexes, the Sc chelated linkers have the most stable configurations because these Sc-chelated linkers have low binding enthalpy. The stable configurations and equilibrium structure of the H_2 adsorbed complexes are shown in Figure S3. In the present calculations, we have observed that the Sc chelated Linker-5 has the lowest binding enthalpy during physisorption process when four H_2 molecules physisorbed.

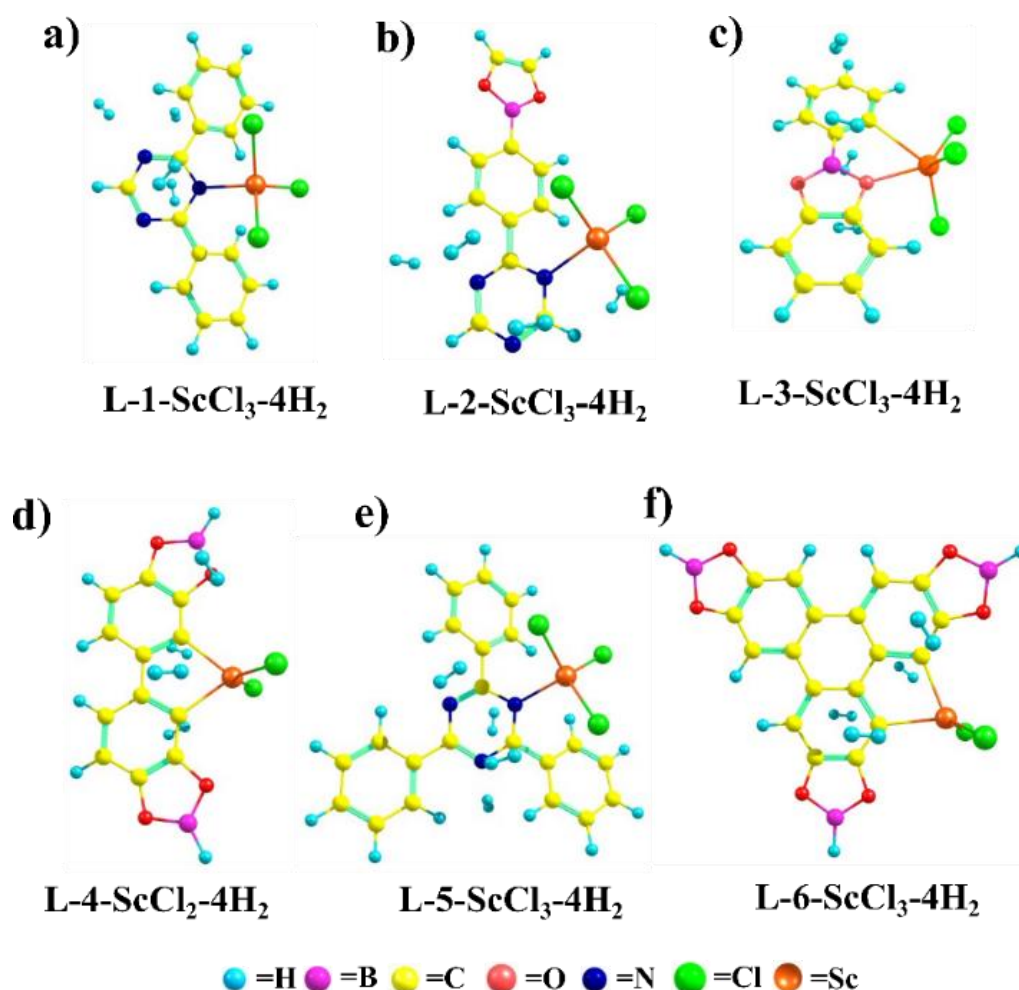


Figure S3: The equilibrium geometry of the physisorbed four H_2 molecules; a) $\text{L-1-ScCl}_3\text{-4H}_2$ b) $\text{L-2-ScCl}_3\text{-4H}_2$ c) $\text{L-3-ScCl}_3\text{-4H}_2$ d) $\text{L-4-ScCl}_2\text{-4H}_2$ e) $\text{L-5-ScCl}_3\text{-4H}_2$ f) $\text{L-6-ScCl}_3\text{-4H}_2$.

In the case of pristine linkers, we have also studied the stable binding sites and their H_2 binding energy in terms of enthalpy computed here. To examine the different binding sites in a linker, we have chosen linker-2 because among all the linkers the Linker-2 has all the binding sites (i.e., BO_2C_2 ring, C_6H_4 ring, C_3N_3 ring). The binding enthalpies (ΔH) of H_2 molecules at different adsorption sites are tabulated in Table S2.

Table S2: The binding enthalpies (ΔH) of H_2 molecules adsorption at different binding sites in the Linker-2.

H_2 Binding Enthalpy in kJ/mol	H_2 binding at different adsorption sites		
	BO_2C_2	C_6H_4	C_3N_3
	-2.29	-1.72	-1.56

The present calculations reveal that H₂ molecules adsorbed at all the binding sites of a linker are in equilibrium thermodynamically and all the structures are energetically and thermodynamically stable. We found that all the H₂ binding sites are stable at room temperature as there was no imaginary or negative frequency present in the computations. We observed that among all the binding sites, the BO₂C₂ ring is the most favorable site for the H₂ adsorption. Figure S4 a-c) shows the different H₂ adsorption sites i.e. BO₂C₂ ring, C₆H₄ ring, C₃N₃ ring in Linkers 2.

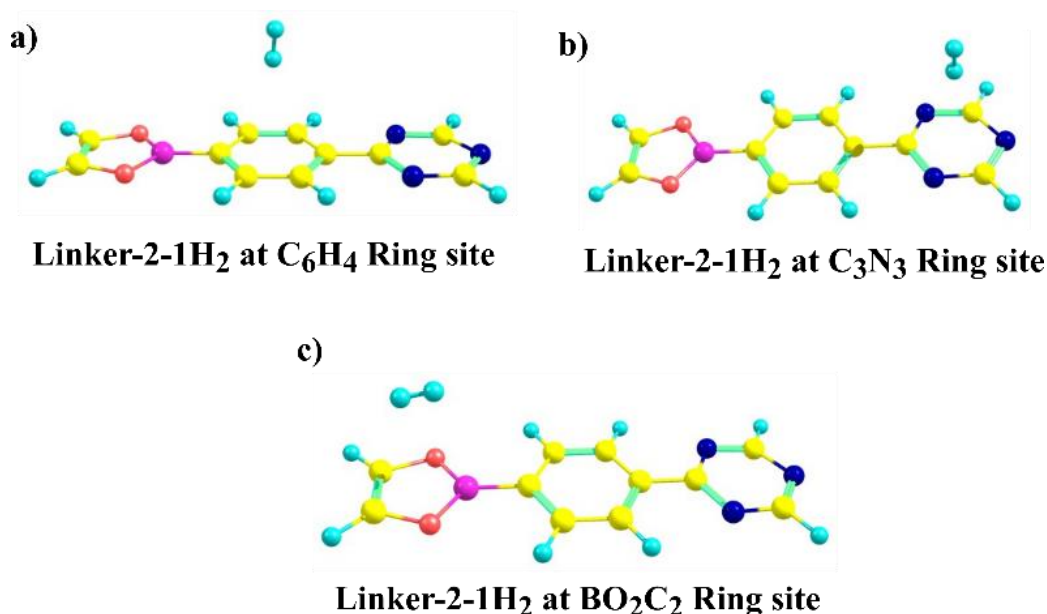


Figure S4: The different H₂ adsorption sites in Linkers 2; a) H₂ adsorption at benzene ring site; b) H₂ adsorption at C₃N₃ ring site; c) H₂ adsorption at BO₂C₂ ring site.

3. Binding Enthalpy of H₂ Molecules in the Pristine and TM-Chelated Linkers.

Table S3: The Binding Enthalpy of nH₂ molecules (n = 1 to 4 H₂ molecules) in the Linker-1-TM-Cl₃ in kJ/mol

linker/nH ₂	1H ₂	2H ₂	3H ₂	4H ₂
Linker -1	-2.59	-7.38	-11.03	-11.80
Linker-1- ScCl₃	-7.33	-13.77	-17.43	-18.25
Linker-1- TiCl₃	-6.79	-13.34	-15.04	-18.02
Linker-1- VCl₃	-4.33	-13.98 ^a	-14.30	-15.63

^a We have got two optimized geometries with different binding enthalpy during the recalculation of the binding energy of 2H₂ in the Linker-1-VCl₃, i.e., ~13.98 and ~19.31 kJ/mol.

Table S4: The Binding Enthalpy of nH₂ molecules (n = 1 to 4 H₂ molecules) in the Linker-2-TM-Cl₃ in kJ/mol.

linker/nH ₂	1H ₂	2H ₂	3H ₂	4H ₂
Linker -2	-1.38	-6.57	-10.10	-11.99
Linker-2- ScCl₃	-6.57	-12.95	-15.75	-17.69
Linker-2- TiCl₃	-6.40	-12.85	-17.54	-17.95
Linker-2- VCl₃	-5.85	-12.68	-16.87	-16.04

Table S5: The Binding Enthalpy of nH₂ molecules (n = 1 to 4 H₂ molecules) in the Linker-3-TM-Cl₃ in kJ/mol.

linker/nH ₂	1H ₂	2H ₂	3H ₂	4H ₂
Linker -3	-2.79	-5.74	-9.42	-10.54
Linker-3- ScCl₃	-1.81	-5.92	-14.63	-20.21
Linker-3- TiCl₃	-2.88	-8.06	-15.87	-21.09
Linker-3- VCl₃	-5.18	-12.04	-13.44	-17.23

Table S6: The Binding Enthalpy of nH₂ molecules (n = 1 to 4 H₂ molecules) in the Linker-4-TM-Cl₂ in kJ/mol.

linker/nH ₂	1H ₂	2H ₂	3H ₂	4H ₂
Linker -4	-2.22	-6.93	-10.35	-11.24
Linker-4- ScCl₂	-4.44	-11.25	-16.42	-18.66
Linker-4- TiCl₂	-3.75	-9.70	-14.62	-17.48
Linker-4- VCl₂	-3.52	-10.12	-15.46	-17.15

Table S7: The Binding Enthalpy of nH₂ molecules (n = 1 to 4 H₂ molecules) in the Linker-5-TM-Cl₃ in kJ/mol.

linker/nH ₂	1H ₂	2H ₂	3H ₂	4H ₂
Linker -5	-2.69	-7.15	-12.81	-13.44
Linker-5- ScCl₃	-8.08	-14.78	-19.50	-21.63
Linker-5- TiCl₃	-8.00	-14.78	-18.21	-20.43
Linker-5- VCl₃	-7.72	-14.48	-18.83	-20.49

Table S8: The Binding Enthalpy of nH₂ molecules (n = 1 to 4 H₂ molecules) in the Linker-6-TM-Cl₂ in kJ/mol.

linker/nH ₂	1H ₂	2H ₂	3H ₂	4H ₂
Linker -6	-2.24	-6.86	-10.88	-11.62
Linker-6- ScCl₂	-4.78	-11.89	-17.24	-19.12
Linker-6- TiCl₂	-4.05	-10.65	-15.87	-18.63

Linker-6- VCl₂	-4.04	-10.36	-16.40	-19.31
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4. The Distance and HOMO-LUMO Data Plotted of Figure 1

4.1 Distance between 1st H₂ and transition metal site in the complex

Table S9: The distance of 1H₂ molecule from the chelated TM atom site in Å.

Linkers/ TM	Pure	Sc	Ti	V
Linker-1	3.393	3.273	3.302	3.275
Linker-2	3.636	3.389	3.415	3.444
Linker-3	3.936	3.635	3.692	3.703
Linker-4	4.324	3.492	3.634	3.668
Linker-5	4.010	3.292	3.289	3.426
Linker-6	4.379	3.369	3.446	3.524

4.2 HOMO-LUMO values of all the H₂ complexes

Table S10: The HOMO-LUMO values (in eV) of the complexes where 1H₂ molecule is adsorbed.

TM/Linkers		Linker-1	Linker-2	Linker-3	Linker-4	Linker-5	Linker-6
Pure	LUMO	-2.04	-2.22	-1.22	-1.09	-1.97	-1.43
	HOMO	-6.86	-6.42	-6.30	-6.21	-6.80	-6.10
Sc	LUMO	-3.07	-3.29	-2.22	-2.49	-3.10	-2.41
	HOMO	-7.41	-6.82	-7.26	-6.75	-7.28	-6.69
Ti	LUMO	-3.19	-3.36	-3.37	-3.30	-3.17	-3.35
	HOMO	-5.63	-5.91	-6.91	-6.34	-5.48	-6.32
V	LUMO	-3.17	-3.53	-4.25	-3.86	-3.29	-3.94
	HOMO	-6.65	-5.50	-6.91	-6.30	-5.05	-6.28

Table S11: The HOMO-LUMO gap (in eV) of one H₂ molecule adsorbed complexes.

TM/Linkers	Linker-1	Linker-2	Linker-3	Linker-4	Linker-5	Linker-6
Pure	4.82	4.2	5.08	5.12	4.83	4.67
Sc	4.34	3.53	5.04	4.26	4.18	4.28

Ti	2.44	2.55	3.54	3.04	2.31	2.97
V	3.48	1.97	2.66	2.44	1.7	2.34

5. Uptake in weight percentage (%wt.) of H₂ molecules physisorbed in the linkers and the molecular wt. of the linkers.

Table S12: Weight percentage (%wt) up to 4H₂ molecules physisorbed in the pure linkers.

Linkers	1H₂ %wt	2H₂ %wt	3H₂ %wt	4H₂ %wt
Linker-1	1.69	1.67	2.49	3.29
Linker-2	1.75	1.73	2.58	3.41
Linker-3	1.99	1.97	2.93	3.86
Linker-4	1.66	1.64	2.44	3.23
Linker-5	1.28	1.27	1.90	2.51
Linker-6	1.12	1.12	1.67	2.21

Table S13: Weight percentage (%wt) up to 4H₂ molecules physisorbed in Sc chelated linkers.

Linkers	1H₂ %wt	2H₂ %wt	3H₂ %wt	4H₂ %wt
Linker-1- TM-Cl₃	1.03	1.03	1.54	2.04
Linker-2- TM-Cl₃	1.06	1.05	1.57	2.08
Linker-3- TM-Cl₃	1.14	1.13	1.69	2.24
Linker-4- TM-Cl₂	1.12	1.12	1.67	2.21
Linker-5- TM-Cl₃	0.87	0.86	1.29	1.71
Linker-6- TM-Cl₂	0.85	0.85	1.26	1.68

Table S14: Weight percentage (%wt) up to 4H₂ molecules physisorbed in Ti chelated linkers.

Linkers	1H₂ %wt	2H₂ %wt	3H₂ %wt	4H₂ %wt
Linker-1- TiCl₃	1.03	1.02	1.52	2.00
Linker-2- TiCl₃	1.05	1.04	1.55	2.04

Linker-3- TiCl₃	1.13	1.12	1.67	2.20
Linker-4- TiCl₂	1.11	1.11	1.64	2.17
Linker-5- TiCl₃	0.86	0.86	1.27	1.68
Linker-6- TiCl₃	0.84	0.84	1.25	1.65

Table S15: Weight percentage (%wt) up to 4H₂ molecules physisorbed in V chelated linkers.

Linkers	1H₂ %wt	2H₂ %wt	3H₂ %wt	4H₂ %wt
Linker-1- VCl₃	1.02	1.01	1.50	1.99
Linker-2- VCl₃	1.04	1.03	1.54	2.03
Linker-3- VCl₃	1.12	1.11	1.65	2.18
Linker-4- VCl₂	1.10	1.10	1.63	2.15
Linker-5- VCl₃	0.85	0.85	1.27	1.67
Linker-6- VCl₃	0.84	0.84	1.24	1.64

Table S16: Molecular wt. of the pristine as well as TM chelated Linkers.

Linkers	Molecular wt. of the Linkers (in g/mol)			
	TM $\equiv$ Pure	TM $\equiv$ Sc	TM $\equiv$ Ti	TM $\equiv$ V
Linker-1- TM-Cl₃	233.26	384.57	387.48	390.55
Linker-2- TM-Cl₃	225.01	376.31	379.23	382.30
Linker-3- TM-Cl₃	197.01	348.32	351.23	354.30
Linker-4- TM-Cl₂	237.80	353.66	356.57	359.65
Linker-5- TM-Cl₃	309.35	460.66	463.57	466.65
Linker-6- TM-Cl₂	353.68	469.54	472.45	475.52

6. Optimized Geometries

Geometries of pure linkers

1.1. Linker-1

C 0.14820700 0.00000100 0.13470900

N	0.05848800	0.00000100	1.46531200
C	1.24633100	0.00000000	2.10563000
N	2.43586100	-0.00000100	1.48284500
C	2.40424000	-0.00000300	0.14053800
N	1.26869700	-0.00000100	-0.58850400
H	-0.79593400	0.00000100	-0.42174600
C	1.23335500	0.00000000	3.58857700
C	2.43794500	-0.00000100	4.31395600
C	0.01106400	0.00000000	4.28432200
C	2.41863600	0.00000000	5.70853700
H	3.38118100	-0.00000100	3.76853500
C	-0.00339900	0.00000100	5.67901200
H	-0.91685000	0.00000100	3.71275300
C	1.19904400	0.00000000	6.39489300
H	3.35903000	-0.00000100	6.26403100
H	-0.95687800	0.00000100	6.21170600
H	1.18556500	0.00000000	7.48731900
C	3.69544600	-0.00000100	-0.58908600
C	4.91329800	0.00000000	0.11370100
C	3.71209000	-0.00000100	-1.99531700
C	6.12406400	0.00000100	-0.57860300
H	4.89258000	0.00000000	1.20307400
C	4.92526000	0.00000000	-2.68351500
H	2.76258400	-0.00000200	-2.53019900
C	6.13385900	0.00000100	-1.97807700
H	7.06549400	0.00000100	-0.02484900
H	4.92951600	0.00000000	-3.77568600
H	7.08314400	0.00000200	-2.51886900

1.2. Linker-2

C	0.01287100	0.00146200	0.01473900
N	0.03825800	0.00397200	1.35439000

C	1.27949000	0.00355600	1.85839400
N	2.41683300	0.00098600	1.16326000
C	2.26698800	-0.00130600	-0.17700400
N	1.06939700	-0.00125000	-0.79808100
H	1.36977200	0.00545300	2.95051700
H	-0.97419700	0.00159400	-0.46121700
C	3.48764600	-0.00442100	-1.01632300
C	3.38482500	-0.00718500	-2.41944300
C	4.76084200	-0.00463800	-0.41723000
C	4.53515200	-0.01009400	-3.20391700
H	2.39426600	-0.00697300	-2.87402000
C	5.90550700	-0.00753500	-1.20965900
H	4.82970100	-0.00250600	0.67052000
C	5.81561000	-0.01032400	-2.61590500
H	4.44725100	-0.01222900	-4.29290700
H	6.89064100	-0.00768100	-0.73735900
B	7.08820300	-0.01356600	-3.49077700
O	8.39134200	-0.01397200	-3.00694100
O	7.10296300	-0.01673900	-4.88072200
C	9.20064500	-0.01735100	-4.12847500
C	8.43987800	-0.01898100	-5.23492200
H	10.27703000	-0.01822400	-3.98497800
H	8.69115000	-0.02162400	-6.29137000

1.3. Linker-3

C	-0.06598400	0.00000000	-0.01801100
C	-0.06785700	0.00000000	1.38064600
C	1.10676500	0.00000000	2.11658700
C	2.30668900	0.00000000	1.38530200
C	2.30855500	0.00000000	-0.01635200
C	1.11058200	0.00000000	-0.75082900
O	-1.36834200	0.00000000	-0.47078100

B	-2.16189100	0.00000000	0.67852700
O	-1.37140800	0.00000000	1.82993500
H	1.08961700	0.00000000	3.20687300
H	3.25691300	0.00000000	1.92287700
H	3.26020800	0.00000000	-0.55139300
H	1.09633000	0.00000000	-1.84115600
C	-3.70228100	0.00000000	0.67624500
C	-4.42426300	0.00000000	1.88587200
C	-4.41999300	0.00000000	-0.53604700
C	-5.82014500	0.00000000	1.88511400
H	-3.87857900	0.00000000	2.83271100
C	-5.81576900	0.00000000	-0.54023200
H	-3.87093200	0.00000000	-1.48092000
C	-6.51689100	0.00000000	0.67121900
H	-6.36844500	0.00000000	2.83008600
H	-6.36080200	0.00000000	-1.48709900
H	-7.60968800	0.00000000	0.66919300

1.4. Linker-4

C	0.01828300	-0.21777300	0.02900200
C	0.01977400	0.17932400	1.36757900
C	1.19378300	0.51695700	2.02186200
C	2.37687800	0.44013500	1.27338800
C	2.39181400	0.03668500	-0.07893100
C	1.17902200	-0.30201700	-0.71962500
O	-1.27923300	-0.49951600	-0.35387500
B	-2.05150500	-0.26010500	0.77426600
O	-1.27514600	0.15837200	1.84652300
H	1.19120500	0.83655700	3.06416700
H	3.31707200	0.72713300	1.74682200
H	1.15206900	-0.64195200	-1.75491000
H	-3.23430400	-0.39695400	0.81771900

C	6.08987300	-0.18218200	-2.20166000
C	4.94628600	0.32420600	-2.82243400
C	3.72905500	0.41615400	-2.17084400
C	3.67315900	-0.03078300	-0.83175000
C	4.83646400	-0.54354200	-0.21886800
C	6.06498700	-0.62688200	-0.88938200
O	7.14357300	-0.14099600	-3.09316000
B	6.61314800	0.40003900	-4.25659400
O	5.26477500	0.69690600	-4.11431100
H	2.85892300	0.84138500	-2.67096900
H	4.77183400	-0.91273100	0.80581800
H	6.95669000	-1.03128300	-0.40993800
H	7.23880500	0.58771400	-5.25306200

1.5. Linker-5

C	0.07809600	-0.00018100	0.08987000
N	0.01554100	-0.00018700	1.43144700
C	1.19713900	-0.00022100	2.06984600
N	2.39023100	-0.00017400	1.45320400
C	2.35223400	-0.00019100	0.11070600
N	1.22171000	-0.00016400	-0.61430300
C	1.18357200	-0.00013000	3.55462300
C	2.38982100	-0.00008500	4.27721800
C	-0.03562700	-0.00011000	4.25513000
C	2.37508900	-0.00003700	5.67199300
H	3.33111900	-0.00009600	3.72856200
C	-0.04619700	-0.00004400	5.64994000
H	-0.96681500	-0.00015900	3.68945800
C	1.15804700	-0.00001400	6.36260900
H	3.31743700	-0.00000500	6.22433000
H	-0.99841800	-0.00001600	6.18508300
H	1.14804700	0.00004200	7.45512400

C	3.64500600	-0.00003300	-0.61990800
C	4.86104400	0.00004000	0.08602500
C	3.66774900	0.00003300	-2.02574000
C	6.07443400	0.00015800	-0.60198900
H	4.83620500	-0.00000300	1.17524500
C	4.88316800	0.00016400	-2.71017500
H	2.72197400	-0.00003200	-2.56663300
C	6.08961000	0.00022000	-2.00122400
H	7.01387500	0.00021300	-0.04471900
H	4.89057000	0.00021800	-3.80243300
H	7.04079800	0.00032400	-2.53876000
C	-1.20107700	-0.00011400	-0.66425200
C	-2.42979000	-0.00010300	0.01936000
C	-1.19823900	-0.00006200	-2.07028900
C	-3.63042600	-0.00004300	-0.69067700
H	-2.42486400	-0.00014400	1.10884900
C	-2.40097300	-0.00000100	-2.77678900
H	-0.24280000	-0.00007000	-2.59392900
C	-3.62015800	0.00000900	-2.08995700
H	-4.57985600	-0.00003600	-0.15060800
H	-2.38840600	0.00003900	-3.86899900
H	-4.56140000	0.00005600	-2.64472400

1.6. Linker-6

C	-0.00598300	-0.10846400	-0.00111100
C	0.00354300	-0.17899500	1.39640800
C	1.17506500	-0.17788900	2.11037100
C	2.40451000	-0.10331000	1.39863900
C	2.39483800	-0.03153400	-0.02851600
C	1.15571200	-0.03515200	-0.72729000
O	-1.31379500	-0.12802900	-0.44399600
B	-2.08470700	-0.21139400	0.70846600

O	-1.29812100	-0.24399100	1.85284800
H	1.13134400	-0.23378600	3.19471600
H	1.09707700	0.01712300	-1.81112600
H	-3.27525400	-0.25023700	0.71466400
C	6.07482900	0.18334200	-2.15233900
C	4.85869900	0.18371200	-2.84447300
C	3.65572500	0.11607800	-2.18840700
C	3.65953500	0.04416300	-0.76771000
C	4.90148300	0.04518100	-0.06064400
C	6.12500300	0.11590500	-0.78296700
O	7.11078400	0.25814800	-3.06233500
B	6.49614100	0.30320000	-4.30719700
O	5.11193400	0.25889800	-4.19980700
H	2.73783000	0.11888300	-2.77015400
H	7.09389400	0.11818800	-0.29092000
H	7.08428800	0.37163900	-5.34080400
C	4.90612500	-0.16157400	4.18877100
C	6.11273600	-0.08996700	3.48377500
C	6.14441200	-0.02246900	2.11384900
C	4.91131400	-0.02658700	1.40443700
C	3.67913100	-0.09953700	2.12455800
C	3.69445500	-0.16810200	3.54533800
O	5.17758700	-0.21757900	5.54148100
B	6.56302000	-0.17821100	5.63430700
O	7.16078100	-0.09986600	4.38289000
H	7.10640200	0.03299300	1.61147500
H	7.16501900	-0.20802100	6.66175500
H	2.78446900	-0.22465800	4.13664200

2. Geometries of Sc chelated linkers

2.1. Linker-1-ScCl₃

C	0.05820000	0.32387300	0.03323800
N	0.05244900	0.18551100	1.36030600
C	1.25995600	0.06602200	1.92863800
N	2.42412700	0.14762800	1.21591900
C	2.29622100	0.07210000	-0.14340500
N	1.11685600	0.19185000	-0.76802000
H	-0.90451400	0.52591600	-0.44761900
C	1.33553100	-0.15782800	3.37833800
C	2.42984300	-0.84290000	3.93854700
C	0.31145800	0.32347800	4.21429000
C	2.51674700	-1.01125300	5.31971800
H	3.20638600	-1.26243500	3.29795300
C	0.40745600	0.15656500	5.59290100
H	-0.53429200	0.84683700	3.76877700
C	1.51139500	-0.50410100	6.14787200
H	3.37331400	-1.53644900	5.74524800
H	-0.37613700	0.55133000	6.24238000
H	1.58473200	-0.62609000	7.23069300
C	3.50188300	-0.14536100	-0.95364200
C	4.60841800	-0.82984000	-0.41715100
C	3.55486100	0.34122400	-2.27258000
C	5.76579600	-0.99234100	-1.17711400
H	4.56303600	-1.25359200	0.58670800
C	4.71564900	0.18007800	-3.02377000
H	2.68961100	0.86395800	-2.67973000
C	5.82369300	-0.47995500	-2.47631800
H	6.62147400	-1.51716400	-0.74933700
H	4.76390400	0.57879700	-4.03884300
H	6.73414100	-0.59745000	-3.06796000
Sc	4.21050300	1.30892400	2.11345800
Cl	4.89916200	2.66176300	0.37574000
Cl	3.23162500	2.65140300	3.71445500

Cl	5.83450900	-0.15203300	2.92178400
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2.2. Linker-2-ScCl₃

C	-0.11592900	-0.28209100	-0.01613500
N	-0.14236400	-0.37236100	1.32412800
C	1.04807500	-0.25308700	1.89733200
N	2.22127200	-0.11103200	1.23718100
C	2.14411000	-0.16659600	-0.12521600
N	0.97163600	-0.19825700	-0.77835100
H	1.09688100	-0.24340200	2.98902300
H	-1.08216200	-0.29164100	-0.53091000
C	3.38469700	-0.18382600	-0.91106200
C	3.43357600	0.47647600	-2.15220600
C	4.52660700	-0.84811700	-0.42658700
C	4.62753400	0.51540000	-2.86424000
H	2.53895400	0.97399600	-2.52752900
C	5.71222000	-0.81549700	-1.15579000
H	4.48391100	-1.42355100	0.49995000
C	5.78701700	-0.12239900	-2.37762400
H	4.67260500	1.05287100	-3.81380700
H	6.59362600	-1.33120000	-0.76991400
B	7.11432400	-0.06319800	-3.17096300
O	8.30046400	-0.66546900	-2.78092600
O	7.29094400	0.60034200	-4.37589900
C	9.21320900	-0.35262800	-3.77216800
C	8.61696700	0.39542700	-4.71499700
H	10.22830600	-0.72427500	-3.67045000
H	8.98474100	0.83576600	-5.63678800
Sc	4.02343800	0.72105700	2.39934800
Cl	4.95067200	2.35753000	1.06598100
Cl	5.34506600	-1.05217800	3.08651600
Cl	2.80929200	1.59733800	4.16237100

2.3. Linker-3-ScCl₃

C	-0.06494100	0.00022300	0.01030200
C	-0.13167000	-0.00050900	1.40100400
C	0.98923000	-0.00088200	2.21064700
C	2.22342900	-0.00048300	1.54088800
C	2.30114100	0.00026400	0.14135200
C	1.14802500	0.00064500	-0.65921400
O	-1.34349000	0.00046000	-0.52859300
B	-2.20982500	-0.00017400	0.53629200
O	-1.49457100	-0.00075200	1.76648100
H	0.91096700	-0.00145400	3.29612000
H	3.14126800	-0.00076700	2.13083900
H	3.28046200	0.00057200	-0.34050200
H	1.19126200	0.00123500	-1.74828300
C	-3.73921300	-0.00001300	0.52244200
C	-4.45916600	-0.00065400	1.70928200
C	-4.51971800	0.00122700	-0.66112200
C	-5.82805400	-0.00023600	1.85342900
C	-5.91214400	0.00176600	-0.58782600
H	-4.01188700	0.00171900	-1.62896000
C	-6.56332400	0.00106600	0.65362400
H	-6.31077600	-0.00091600	2.83018700
H	-6.50198300	0.00273600	-1.50659200
H	-7.65542600	0.00154200	0.69957800
Sc	-2.34209800	-0.00147900	3.87790000
Cl	-1.17494000	-1.91120200	4.42600000
Cl	-4.40220300	-0.00220700	4.94069500
Cl	-1.17552300	1.90827400	4.42714300

2.4. Linker-4-ScCl₃

C	0.07421000	0.13350300	-0.05723700
C	-0.01609100	-0.32327900	1.27178800
C	1.12493900	-0.68069300	2.00489400
C	2.33705000	-0.55860700	1.34857500
C	2.42517100	-0.09079100	-0.01184100
C	1.23960800	0.27800800	-0.76585800
O	-1.22047700	0.40152300	-0.49540300
B	-2.04948600	0.10557500	0.56079700
O	-1.30946700	-0.34917400	1.67359400
H	1.04645100	-1.03313300	3.03300800
H	3.24025900	-0.82906500	1.89395000
H	-3.23395100	0.20909700	0.56519400
C	6.11223400	0.28694500	-2.02656400
C	4.89284500	0.61420700	-2.65032400
C	3.65562700	0.51927900	-2.06597900
C	3.69765200	0.03580700	-0.69680600
C	4.94355500	-0.30023300	-0.05479800
C	6.15915500	-0.18058500	-0.70506100
O	7.14608900	0.49303400	-2.87722800
B	6.55362900	0.96356300	-4.06898500
O	5.18667700	1.04121500	-3.94315800
H	4.94979800	-0.66117700	0.97284600
H	7.10694200	-0.43175300	-0.22965700
H	7.17979200	1.24785600	-5.03893000
Sc	1.60476700	0.98234800	-2.87366800
Cl	1.26902300	3.27701300	-3.06795900
Cl	0.92967800	-0.61388900	-4.42678600

2.5. Linker-5-ScCl₃

C	0.03698900	-0.09559300	0.02031900
N	0.04177500	-0.16624700	1.36529900
C	1.23143000	-0.12388200	1.96010200

N	2.40541400	0.03571300	1.27394400
C	2.31266600	-0.13014700	-0.08191100
N	1.15189600	-0.17252700	-0.73133000
C	1.29125300	-0.25765800	3.42482300
C	2.41902800	-0.83006000	4.04057300
C	0.22207300	0.19863100	4.21583400
C	2.48978900	-0.91534400	5.43086000
H	3.23689400	-1.22445500	3.43661700
C	0.30151700	0.11632700	5.60325800
H	-0.64601300	0.64311100	3.72944800
C	1.43600700	-0.43525000	6.21294700
H	3.37280900	-1.35347500	5.89887600
H	-0.51899400	0.49377900	6.21658500
H	1.49610000	-0.49089200	7.30202000
C	3.55727000	-0.27124900	-0.85508500
C	4.69887400	-0.84412400	-0.26588300
C	3.61142400	0.17778200	-2.18645500
C	5.88790600	-0.93718100	-0.98892100
H	4.65836200	-1.23287300	0.75218200
C	4.80294000	0.08771200	-2.90071800
H	2.72244600	0.62271800	-2.63306200
C	5.94336100	-0.46443800	-2.30271100
H	6.77011700	-1.37557100	-0.51963100
H	4.84970400	0.45943100	-3.92615400
H	6.87739700	-0.52626300	-2.86532600
C	-1.26088000	0.02708800	-0.66721300
C	-2.45423200	0.09429000	0.07701600
C	-1.31612300	0.08686800	-2.07285300
C	-3.67847900	0.22691300	-0.57544800
H	-2.40317600	0.03833000	1.16394700
C	-2.54360500	0.21946600	-2.71921700
H	-0.38869000	0.02521100	-2.64138200

C	-3.72605400	0.29077600	-1.97314000
H	-4.60088700	0.27967400	0.00638900
H	-2.58086100	0.26640400	-3.80942900
H	-4.68701400	0.39430600	-2.48221400
Sc	4.04990100	1.38301600	2.14132900
Cl	4.67977700	2.70891100	0.35835100
Cl	2.93088300	2.71879600	3.65703500
Cl	5.77073600	0.10430400	3.05641700

2.6. Linker-6-ScCl₃

C	-0.00088100	-0.02574600	0.00150800
C	-0.00082200	0.03145600	1.39799900
C	1.17043200	0.05854800	2.12049900
C	2.39885600	0.02698000	1.41317000
C	2.39879800	-0.03132900	-0.01345100
C	1.17031100	-0.05776100	-0.72088800
O	-1.30106400	-0.04148100	-0.44861500
B	-2.08493200	0.00718800	0.69966400
O	-1.30096600	0.05261900	1.84800900
H	1.12226200	0.10301800	3.20573000
H	1.12205200	-0.10207300	-1.80612200
H	-3.27474600	0.00968500	0.69961000
C	6.16178400	-0.12041500	-2.03048800
C	4.95752000	-0.14808100	-2.76118500
C	3.71036200	-0.12073200	-2.14403600
C	3.67352800	-0.06364000	-0.74408200
C	4.93135000	-0.03641300	-0.01388900
C	6.23415300	-0.06529500	-0.66828900
O	7.21092800	-0.15942900	-2.94661100
B	6.62615300	-0.20904600	-4.18991400
O	5.21813600	-0.20268200	-4.09137600
H	2.81869400	-0.14444200	-2.76566300

H	7.20469100	-0.25226400	-5.22791000
C	4.95782100	0.13305100	4.16112000
C	6.16201700	0.10010200	3.43053700
C	6.23425000	0.04464700	2.06834100
C	4.93140200	0.02129900	1.41383000
C	3.67365300	0.05395700	2.14391000
C	3.71061000	0.11103300	3.54386000
O	5.21854900	0.18672000	5.49132800
B	6.62657500	0.18704200	5.58999000
O	7.21124000	0.13469900	4.34674500
H	7.20519600	0.22788700	6.62803500
H	2.81900100	0.13868200	4.16540900
Sc	8.01907300	-0.01387200	0.70011100
Cl	9.09105000	2.05108600	0.61846100
Cl	9.08323300	-2.08286100	0.78179600

3. Geometries of Ti chelated linkers

3.1. Linker-1-TiCl₃

C	0.10319000	0.35400700	0.05723500
N	0.09081800	0.21250600	1.38330700
C	1.29409800	0.09354500	1.95948600
N	2.46314100	0.18504000	1.25090000
C	2.34069900	0.08836300	-0.11023300
N	1.16355300	0.20734100	-0.73815200
H	-0.85489800	0.56782800	-0.42774900
C	1.34985400	-0.14624000	3.40720400
C	2.43785400	-0.83031600	3.97926200
C	0.30088400	0.30686000	4.22834800
C	2.49113300	-1.02999000	5.35774300
H	3.23624300	-1.21746500	3.34675400
C	0.36344600	0.10975100	5.60489900

H	-0.53903500	0.83087100	3.77313800
C	1.45963300	-0.55291000	6.17218400
H	3.34124800	-1.55731300	5.79374100
H	-0.44066800	0.48144400	6.24282500
H	1.50673900	-0.70054300	7.25334700
C	3.53896700	-0.15766500	-0.92261800
C	4.64294800	-0.84233000	-0.38283200
C	3.57925700	0.28943500	-2.25619000
C	5.78367700	-1.04899900	-1.15670500
H	4.60634000	-1.22439000	0.63699100
C	4.72405200	0.08560300	-3.02139600
H	2.71611700	0.81415900	-2.66475300
C	5.82893200	-0.57803200	-2.47241400
H	6.63739600	-1.57688700	-0.72850400
H	4.76180200	0.45265700	-4.04879700
H	6.72683000	-0.73114600	-3.07513100
Ti	4.09631400	1.40885300	2.07650800
Cl	5.72592400	0.07399500	2.90123700
Cl	4.61304500	2.75431900	0.33391500
Cl	3.00131400	2.76510400	3.51679500

3.2. Linker-2-TiCl₃

C	-0.08677600	-0.31639600	-0.07412500
N	-0.14277500	-0.41137900	1.26468200
C	1.02912900	-0.25665000	1.86521900
N	2.21495300	-0.08006000	1.23297900
C	2.17485200	-0.14607000	-0.13140800
N	1.01646200	-0.20639900	-0.80839200
H	1.05220100	-0.24598600	2.95731900
H	-1.03967000	-0.34703400	-0.61243900
C	3.42277600	-0.15084900	-0.90813200
C	3.45890200	0.49226500	-2.15883500

C	4.57182000	-0.80375500	-0.42596200
C	4.64458500	0.52383600	-2.88546800
H	2.55859500	0.97944100	-2.53381900
C	5.74698500	-0.78370600	-1.17153200
H	4.54077000	-1.35504500	0.51463300
C	5.80876300	-0.10859800	-2.40484200
H	4.67725900	1.04741600	-3.84329600
H	6.63278100	-1.29666800	-0.79165800
B	7.12490300	-0.06629700	-3.21691200
O	8.31524800	-0.66577900	-2.83350700
O	7.28744300	0.57694600	-4.43516600
C	9.21469600	-0.37314500	-3.84302900
C	8.60753700	0.36101600	-4.78971900
H	10.22978500	-0.74712300	-3.74997300
H	8.96360300	0.78397100	-5.72418400
Ti	3.86000700	0.69153900	2.45860100
Cl	2.66164900	1.61845800	4.15542700
Cl	4.87625600	-1.17657000	3.20629700
Cl	4.70099300	2.33224300	1.17718000

3.3. Linker-3-TiCl₃

C	0.02225700	-0.00165500	-0.03582200
C	-0.09293600	-0.00051600	1.35572700
C	0.99874200	-0.00011000	2.20342100
C	2.25792700	-0.00091200	1.57996500
C	2.38408300	-0.00205300	0.18406400
C	1.25944700	-0.00245400	-0.65860500
O	-1.23900200	-0.00180300	-0.61608900
B	-2.13487900	-0.00071200	0.43253700
O	-1.44839800	0.00006300	1.66495200
H	0.87700800	0.00073300	3.28572800
H	3.15578100	-0.00064400	2.20027700

H	3.37989200	-0.00265200	-0.26291100
H	1.34510100	-0.00334000	-1.74531400
C	-3.65925100	-0.00022800	0.52532400
C	-4.19231900	0.00104800	1.85026400
C	-4.51086400	-0.00087100	-0.59005800
C	-5.59375400	0.00162200	1.99497100
C	-5.89663500	-0.00027000	-0.41867900
H	-4.08193600	-0.00183600	-1.59556300
C	-6.43179900	0.00097500	0.87284100
H	-6.04390800	0.00259300	2.98723400
H	-6.55841100	-0.00077100	-1.28766000
H	-7.51560800	0.00144800	1.01384200
Cl	-1.83992800	-1.92828800	3.90495000
Cl	-4.39008500	0.00376900	5.08488300
Cl	-1.84102700	1.93453200	3.89978600
Ti	-2.86466300	0.00233400	3.48304500

3.4. Linker-4-TiCl₃

C	0.05344200	0.17914800	-0.06868500
C	-0.07247900	-0.26416200	1.25013800
C	1.03663400	-0.63563200	1.99483500
C	2.29127400	-0.54795400	1.36994800
C	2.43257100	-0.10316800	0.04258600
C	1.27553900	0.27709800	-0.71399500
O	-1.20167500	0.47727000	-0.55935200
B	-2.07919400	0.20569100	0.48513500
O	-1.40349100	-0.25233200	1.60923900
H	0.93376100	-0.98111700	3.02382300
H	3.17165800	-0.83690900	1.94479400
H	-3.25934800	0.34756400	0.42370400
C	6.11525400	0.25952300	-2.09153100
C	4.89279300	0.58883600	-2.68210000

C	3.68362200	0.48082100	-2.01442400
C	3.73766000	0.00702000	-0.66229900
C	4.97573900	-0.32126500	-0.07994500
C	6.18415200	-0.20019200	-0.78515600
O	7.13100500	0.47087800	-2.99940000
B	6.50135200	0.93331700	-4.14817500
O	5.12358600	1.01355200	-3.97489900
H	5.01611400	-0.68194600	0.94830100
H	7.14040700	-0.45623800	-0.32822200
H	7.06901700	1.22405500	-5.15311200
Cl	1.44333200	3.03401500	-2.86689200
Cl	1.07485900	-0.55466300	-4.11011200
Ti	1.77809800	0.87338400	-2.58580200

3.5. Linker-5-TiCl₃

C	0.07367100	-0.07925700	0.04072300
N	0.07936500	-0.15631200	1.38479900
C	1.26756300	-0.10839800	1.98091800
N	2.44043700	0.06843900	1.29184300
C	2.34919500	-0.11760800	-0.06418000
N	1.18757300	-0.16597500	-0.71046000
C	1.31886900	-0.26289300	3.44354400
C	2.44732100	-0.82922600	4.06211100
C	0.22926300	0.15336700	4.22919600
C	2.49566500	-0.95360000	5.45020300
H	3.28322600	-1.18165100	3.45849000
C	0.28643200	0.03356600	5.61496900
H	-0.63849400	0.59526200	3.74034200
C	1.42000100	-0.51574500	6.22800000
H	3.37764000	-1.39023100	5.92184500
H	-0.55120600	0.37866400	6.22421900
H	1.46258200	-0.60312800	7.31589500

C	3.58647300	-0.28151500	-0.84401900
C	4.73111800	-0.84760900	-0.25576900
C	3.62391600	0.12601100	-2.18949000
C	5.90538900	-0.98016800	-0.99615800
H	4.70162100	-1.19328800	0.77714600
C	4.80117400	-0.00210800	-2.92135800
H	2.73289900	0.56804000	-2.63439900
C	5.94424700	-0.55098900	-2.32582300
H	6.79032500	-1.41630600	-0.52963000
H	4.83440900	0.33627000	-3.95881100
H	6.86722300	-0.64476400	-2.90226700
C	-1.22279800	0.05784300	-0.64574300
C	-2.41528100	0.13383100	0.09908200
C	-1.27767700	0.12415200	-2.05114300
C	-3.63821700	0.28153700	-0.55250300
H	-2.36433600	0.07286200	1.18574000
C	-2.50382700	0.27187900	-2.69664300
H	-0.35088800	0.05577300	-2.61992900
C	-3.68535000	0.35183500	-1.94993000
H	-4.55996400	0.34121700	0.02971600
H	-2.54084600	0.32404500	-3.78663000
H	-4.64532000	0.46724400	-2.45833900
Cl	4.34872400	2.78408000	0.27285100
Cl	2.68754600	2.79539100	3.43224500
Cl	5.65039700	0.33633300	2.98605500
Ti	3.92166600	1.47545300	2.06938300

3.6. Linker-6-TiCl₃

C	0.02682300	-0.02393500	-0.00066000
C	0.02658800	0.02323000	1.39887200
C	1.19357300	0.04601300	2.12180900
C	2.42670000	0.02061800	1.41630800

C	2.42693800	-0.02743500	-0.01706500
C	1.19405600	-0.04969400	-0.72309600
O	-1.27750300	-0.03745100	-0.45014200
B	-2.05800800	0.00225800	0.69866500
O	-1.27789200	0.04004300	1.84780000
H	1.14668400	0.08264500	3.20760800
H	1.14754900	-0.08623800	-1.80891600
H	-3.24884000	0.00377600	0.69841200
C	6.18301300	-0.09985800	-2.05195600
C	4.98392200	-0.12257200	-2.78206300
C	3.75002600	-0.10077500	-2.17333000
C	3.69643700	-0.05345200	-0.75170600
C	4.91600600	-0.03081400	-0.02642900
C	6.19882400	-0.05407300	-0.67521900
O	7.24177200	-0.13055200	-2.93398000
B	6.66575300	-0.17182800	-4.20032600
O	5.27877300	-0.16768800	-4.12908200
H	2.85545700	-0.12016400	-2.79212000
H	7.28469400	-0.20635500	-5.21623500
C	4.98278300	0.10920200	4.18237000
C	6.18211200	0.08335000	3.45275500
C	6.19838700	0.03753200	2.07602800
C	4.91576900	0.01759400	1.42671100
C	3.69596300	0.04340300	2.15147700
C	3.74908800	0.09063000	3.57312700
O	5.27719700	0.15358900	5.52950700
B	6.66415700	0.15415400	5.60132200
O	7.24058600	0.11129600	4.33521700
H	7.28275900	0.18707000	6.61749100
H	2.85431900	0.11238800	4.19154500
Cl	8.80003100	1.89216700	0.63780400
Cl	8.79507500	-1.91563900	0.76391900

Ti	7.69069700	-0.01029700	0.70071800
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4. Geometries of V chelated linkers

4.1. Linker-1-VCl₃

C	-0.00507600	0.02017600	-0.00414800
N	0.01104400	0.02797200	1.32857200
C	1.21719200	0.10948600	1.89821700
N	2.36940800	0.29242700	1.16369200
C	2.25069100	-0.06622700	-0.16217900
N	1.06718000	-0.15135700	-0.77698900
H	-0.97801100	0.09820100	-0.49881000
C	1.29566600	-0.02486800	3.36126200
C	2.43334500	-0.58467600	3.96964000
C	0.20533200	0.37322400	4.15645700
C	2.49152300	-0.71380700	5.35642000
H	3.27200100	-0.91968800	3.36040900
C	0.27424000	0.25057600	5.54172900
H	-0.67642000	0.79400000	3.67346800
C	1.41836300	-0.28793500	6.14488400
H	3.38069700	-1.14501700	5.81964400
H	-0.56463400	0.58093600	6.15759900
H	1.46981100	-0.37918900	7.23211700
C	3.45447600	-0.39226600	-0.94275200
C	4.58369000	-0.95169600	-0.31850000
C	3.46090500	-0.18043600	-2.33369700
C	5.71468500	-1.26423200	-1.07110700
H	4.57860700	-1.14328100	0.75387500
C	4.59756900	-0.48563800	-3.07773700
H	2.57568700	0.24183100	-2.80898300
C	5.72793000	-1.02301300	-2.44818100
H	6.58789500	-1.69361400	-0.57685100

H	4.60740600	-0.29947900	-4.15355800
H	6.61877900	-1.25785600	-3.03494100
Cl	5.56285900	0.47470400	2.74764300
Cl	4.56259400	2.57292500	-0.02940800
Cl	2.89208800	2.85641100	3.30693700
V	3.88037600	1.62251500	1.80817900

4.2. Linker-2-VCl₃

C	0.02658300	-0.04087900	0.00425100
N	0.02246800	-0.01318000	1.34726400
C	1.22943700	0.03674100	1.89135200
N	2.40044500	-0.00218800	1.20429400
C	2.28719000	-0.18541800	-0.14682400
N	1.10041900	-0.14322400	-0.77315300
H	1.30528500	0.14037400	2.97564000
H	-0.94586600	0.01074200	-0.49582400
C	3.47950600	-0.43538800	-0.97324400
C	3.53893300	0.10200200	-2.27161400
C	4.54026000	-1.22913400	-0.49951300
C	4.66625200	-0.11106200	-3.05898100
H	2.70378000	0.69826600	-2.63979700
C	5.65250400	-1.45566600	-1.30488100
H	4.48368400	-1.69573200	0.48450200
C	5.74299800	-0.88968700	-2.59061900
H	4.71954100	0.33047900	-4.05646900
H	6.46751100	-2.07929900	-0.93196000
B	6.99339700	-1.12269600	-3.47053900
O	8.09547200	-1.88042100	-3.10203200
O	7.17801300	-0.60457900	-4.74442800
C	8.96256000	-1.81377300	-4.17796300
C	8.42059300	-1.06017600	-5.14854100
H	9.90848600	-2.34225300	-4.10804000

H	8.77833100	-0.77072400	-6.13199300
Cl	3.28617900	1.70109500	3.97842900
Cl	4.58511600	-1.47553200	3.17343000
Cl	5.10086700	1.87660500	0.91821400
V	4.11730300	0.49147300	2.29208000

4.3. Linker-3-VCl₃

C	-0.02017600	0.00774100	0.00261600
C	-0.01782400	0.00257200	1.39950100
C	1.16450800	0.00839700	2.12094000
C	2.35403500	0.01981800	1.37273400
C	2.34193100	0.02487800	-0.02886300
C	1.13753900	0.01873500	-0.75253000
O	-1.34391900	-0.00052400	-0.41497800
B	-2.12756200	-0.00954000	0.75380300
O	-1.32236600	-0.00837700	1.87434600
H	1.16153700	0.00442100	3.21102500
H	3.31014800	0.02486500	1.89924800
H	3.28740600	0.03368100	-0.57379500
H	1.10585800	0.02200800	-1.84153300
C	-3.64211000	-0.01280100	0.54240200
C	-4.58163800	0.00126200	1.58270100
C	-4.07619800	-0.01134900	-0.81638800
C	-5.94964600	0.01773400	1.29610000
H	-4.23840700	0.00295900	2.62043500
C	-5.45780600	-0.00020900	-1.08516800
C	-6.38212200	0.01565300	-0.03391900
H	-6.67933000	0.03187800	2.10887700
H	-5.81749400	0.00067800	-2.11308600
H	-7.45131100	0.02754700	-0.25943200
V	-2.67815400	0.02349200	-2.28280800

C	-3.98211000	0.04732700	-4.05701500
C	-1.79050800	-1.95957300	-2.56835600
C	-1.85539800	2.04820700	-2.47083800
H	-4.43104200	3.22534800	0.06785100
H	-3.98026300	2.99438300	-0.50161800

4.4. Linker-4-VCl₃

C	0.02481400	-0.00000700	-0.03560200
C	-0.00451400	-0.00056700	1.36182500
C	1.16234700	-0.00053400	2.11236400
C	2.38085800	0.00009500	1.41250900
C	2.42100500	0.00066000	0.00797500
C	1.21028200	0.00061300	-0.75606700
O	-1.27042500	-0.00020900	-0.50775300
B	-2.07626200	-0.00083300	0.62630300
O	-1.31591100	-0.00113400	1.78859900
H	1.12841700	-0.00098100	3.20221000
H	3.30830000	0.00013500	1.98668200
H	-3.26628700	-0.00122400	0.60286800
C	5.85887300	0.00267800	-2.49955900
C	4.56350100	0.00249600	-3.02461100
C	3.43333400	0.00183400	-2.22012700
C	3.65704500	0.00133900	-0.80606100
C	4.96321800	0.00152200	-0.28815400
C	6.08747400	0.00220200	-1.13112700
O	6.76895400	0.00338600	-3.53572700
B	6.00153300	0.00356800	-4.69336500
O	4.64139000	0.00308700	-4.40102600
H	5.12436500	0.00113700	0.79066800
H	7.10210100	0.00235100	-0.73182100
H	6.45007300	0.00419800	-5.79587100
Cl	0.99622400	1.94794500	-3.49928800

Cl	0.99735000	-1.94464000	-3.50087100
V	1.51558500	0.00148200	-2.71232500

4.5. Linker-5-VCl₃

C	0.02760200	0.00465500	0.01388300
N	0.02698300	0.00037300	1.36014100
C	1.21503700	0.00792900	1.95791000
N	2.39669200	0.08289200	1.26133000
C	2.29510500	-0.19251800	-0.08067300
N	1.13242500	-0.20469400	-0.72635500
C	1.25099400	-0.07644900	3.42649000
C	2.33181300	-0.69214000	4.08109500
C	0.18580800	0.44668200	4.18119300
C	2.35537300	-0.76641100	5.47321500
H	3.14819100	-1.11798300	3.49942800
C	0.21937800	0.37832700	5.57143700
H	-0.64356400	0.92765600	3.66366100
C	1.30438200	-0.22513900	6.21983500
H	3.19864100	-1.24519300	5.97411500
H	-0.59850000	0.80471100	6.15559100
H	1.32890300	-0.27391700	7.31075800
C	3.51449600	-0.49694200	-0.84583300
C	4.61328500	-1.11470600	-0.22391700
C	3.57421800	-0.18459500	-2.21578300
C	5.76359500	-1.39895900	-0.95881100
H	4.56278000	-1.37822000	0.83160900
C	4.72906300	-0.46203800	-2.94236800
H	2.71927300	0.30020900	-2.68595200
C	5.82606700	-1.06657900	-2.31550700
H	6.61291000	-1.87793200	-0.46842300
H	4.78068100	-0.19877500	-4.00066500
H	6.73161000	-1.27968700	-2.88793200

C	-1.25466000	0.19935700	-0.68454900
C	-2.43865400	0.40292700	0.04992100
C	-1.30373500	0.19498000	-2.09178000
C	-3.64683700	0.60635900	-0.61396400
H	-2.39251100	0.39603500	1.13847900
C	-2.51511400	0.39908200	-2.74960600
H	-0.38409200	0.02804500	-2.65171300
C	-3.68781300	0.60597400	-2.01338200
H	-4.56191800	0.76515000	-0.03985900
H	-2.54762500	0.39625000	-3.84099000
H	-4.63626300	0.76539300	-2.53145800
Cl	4.21521300	2.62821000	0.01945800
Cl	2.61048500	2.92618100	3.05228500
Cl	5.46857800	0.38784600	2.85978800
V	3.82579000	1.47820800	1.88209300

4.6. Linker-6-VCl₃

C	-0.00496400	0.00031000	-0.00011200
C	-0.00495600	-0.00027800	1.40046500
C	1.16210300	-0.00055100	2.12432300
C	2.39461700	-0.00017000	1.41833700
C	2.39461000	0.00042400	-0.01801400
C	1.16208600	0.00063800	-0.72398500
O	-1.30956700	0.00032900	-0.44935000
B	-2.08982500	0.00031200	0.70018900
O	-1.30955400	-0.00063800	1.84971800
H	1.11748200	-0.00104800	3.21112600
H	1.11745100	0.00105700	-1.81078600
H	-3.28070100	-0.00019000	0.70019600
C	6.17604300	0.00149000	-2.01990100
C	4.98296400	0.00170900	-2.76369400
C	3.73732100	0.00139800	-2.17495500

C	3.66388400	0.00077800	-0.75326700
C	4.87622900	0.00056100	-0.02222000
C	6.17054900	0.00094000	-0.63976100
O	7.24256600	0.00203900	-2.88990400
B	6.68137700	0.00202600	-4.16387000
O	5.29420500	0.00240700	-4.10828300
H	2.85249500	0.00163600	-2.80853400
H	7.31258900	0.00294600	-5.17280200
C	4.98298800	-0.00111000	4.16399600
C	6.17606100	-0.00072700	3.42019400
C	6.17055800	-0.00015600	2.04005500
C	4.87623400	-0.00003000	1.42252200
C	3.66389500	-0.00041100	2.15357800
C	3.73734100	-0.00094200	3.57526500
O	5.29423700	-0.00149900	5.50858300
B	6.68140900	-0.00192000	5.56416100
O	7.24259000	-0.00088400	4.29019100
H	7.31262800	-0.00182000	6.57308800
H	2.85251700	-0.00120700	4.20884900
Cl	8.57896600	1.94521400	0.70092400
Cl	8.57939500	-1.94387200	0.69936700
V	7.63446200	0.00056400	0.70014300

5. Geometries of linkers-1 + nH₂

5.1. Linker-1 + H₂

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.33297000
C	1.22853300	0.00000000	1.89183200
N	2.37336500	-0.00036400	1.19045700
C	2.25366400	-0.00073600	-0.14673900
N	1.07038800	-0.00030500	-0.79591100

H	-0.97823200	0.00057900	-0.49417400
C	1.31529000	0.00041000	3.37199400
C	2.56603800	-0.00013500	4.01476000
C	0.14231300	0.00137100	4.14800300
C	2.64018600	0.00032700	5.40744200
H	3.47050400	-0.00099100	3.40714400
C	0.22137100	0.00183700	5.54055600
H	-0.82194700	0.00176100	3.64012300
C	1.46920600	0.00133600	6.17400500
H	3.61562400	-0.00013400	5.89887600
H	-0.69441500	0.00260900	6.13575700
H	1.52937100	0.00169200	7.26490200
C	3.49447700	-0.00182300	-0.95860600
C	4.75394200	0.00165400	-0.33247100
C	3.42534100	-0.00657100	-2.36346800
C	5.91995400	0.00049300	-1.09742000
H	4.80029500	0.00536300	0.75608500
C	4.59442800	-0.00786400	-3.12437000
H	2.44824300	-0.00937700	-2.84530000
C	5.84406300	-0.00430300	-2.49485300
H	6.89354300	0.00331000	-0.60234500
H	4.53093200	-0.01165400	-4.21469600
H	6.75845700	-0.00529500	-3.09279800
H	-0.08807300	0.06071600	-3.05439700
H	-0.53617700	0.07788500	-3.67294400

5.2. Linker-1+ 2H₂

C	0.48478300	1.02746300	0.24016800
N	0.44759400	0.80699700	1.55516400
C	1.59163800	0.31498500	2.07484600
N	2.69211900	0.05456800	1.35087100
C	2.61585500	0.30970300	0.03559600

N	1.51691900	0.80512400	-0.57303200
H	-0.42424400	1.43514100	-0.21645100
C	1.63403700	0.04181400	3.53110200
C	2.80851300	-0.45057100	4.12839000
C	0.49949600	0.27002000	4.33017400
C	2.84606100	-0.70926700	5.49798700
H	3.68349100	-0.62523700	3.50301100
C	0.54180000	0.00867000	5.69986000
H	-0.40856200	0.64927000	3.86242600
C	1.71326700	-0.48102900	6.28771200
H	3.76285900	-1.09076900	5.95284800
H	-0.34404300	0.18889600	6.31279300
H	1.74327400	-0.68544000	7.36051900
C	3.80752200	0.03190700	-0.80103500
C	4.99446100	-0.44236800	-0.21383100
C	3.76165300	0.23969000	-2.19108500
C	6.11392300	-0.70168600	-1.00389500
H	5.02185200	-0.60119700	0.86367800
C	4.88375400	-0.02259400	-2.97723900
H	2.83724200	0.60338200	-2.63849600
C	6.06200400	-0.49287100	-2.38686800
H	7.03214700	-1.06859900	-0.53996700
H	4.83985800	0.14075200	-4.05623000
H	6.93962400	-0.69721400	-3.00469900
H	0.69973300	2.09573700	-2.62761200
H	0.30821700	2.46079600	-3.17253600
H	-1.71350800	2.02197700	2.06664200
H	-2.39761400	2.36063600	2.10136100

5.3. Linker-1+ 3H₂

C	0.22027300	0.63284300	0.14129500
N	0.17357700	0.45241900	1.46183200

C	1.35961500	0.14386000	2.02817300
N	2.51007100	0.03237300	1.34444200
C	2.43944900	0.23257800	0.01804000
N	1.29862800	0.53445900	-0.63664800
H	-0.72203700	0.88979800	-0.35544700
C	1.39214600	-0.08223100	3.49217300
C	2.60663900	-0.35996200	4.14517400
C	0.20419800	-0.02337000	4.24346200
C	2.63177200	-0.56811600	5.52376500
H	3.52345600	-0.40832800	3.55880000
C	0.23478500	-0.23385100	5.62199200
H	-0.73461900	0.18512200	3.73156100
C	1.44712400	-0.50491000	6.26602900
H	3.57975500	-0.78054000	6.02280500
H	-0.69208900	-0.18648500	6.19773600
H	1.46872200	-0.66802000	7.34609500
C	3.68634500	0.11496400	-0.77377900
C	4.89867800	-0.22078200	-0.14498600
C	3.66863000	0.33910400	-2.16210000
C	6.07122200	-0.32697500	-0.89234200
H	4.90516800	-0.39786300	0.92982800
C	4.84389700	0.23159500	-2.90533400
H	2.72631600	0.59589000	-2.64461400
C	6.04777100	-0.10087900	-2.27354800
H	7.00852100	-0.58779800	-0.39610000
H	4.82179700	0.40890100	-3.98275000
H	6.96741600	-0.18416900	-2.85744600
H	0.27307500	1.23084900	-2.86351500
H	-0.16905300	1.43458500	-3.45160300
H	-1.06105100	2.49000900	2.51827900
H	-1.33789800	3.13805200	2.81289900
H	4.16436800	1.85259100	2.27714100

H	4.60975900	2.42083500	2.52473100
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5.4. Linker-1+ 4H₂

C	-0.03040900	0.19475400	0.00406600
N	-0.01621800	0.19538200	1.33731200
C	1.21505400	0.14102600	1.88725300
N	2.35101100	0.09123100	1.17222700
C	2.21895000	0.09035300	-0.16405100
N	1.03074200	0.14197200	-0.80162900
H	-1.01339000	0.24045900	-0.47828200
C	1.32022400	0.13783600	3.36537800
C	2.57686500	0.03752500	3.98959400
C	0.16331200	0.23377000	4.15984300
C	2.67255400	0.03442100	5.38071000
H	3.46971300	-0.03876200	3.37017600
C	0.26440800	0.23109500	5.55088000
H	-0.80822900	0.31122100	3.67305900
C	1.51771900	0.13157400	6.16517200
H	3.65244100	-0.04432300	5.85658600
H	-0.63907200	0.30717100	6.15973000
H	1.59463500	0.12953600	7.25498400
C	3.45031300	0.03289900	-0.98677000
C	4.71180600	-0.07396200	-0.37358900
C	3.37046200	0.09176100	-2.38979400
C	5.86939300	-0.11824700	-1.14995400
H	4.76854600	-0.11916300	0.71319700
C	4.53124200	0.04806500	-3.16178400
H	2.39207500	0.17732800	-2.86119200
C	5.78298400	-0.05638700	-2.54537400
H	6.84454600	-0.19898600	-0.66494600
H	4.45977700	0.09902300	-4.25031100
H	6.69107800	-0.08765700	-3.15186200

H	-0.15863400	0.08632200	-3.04812000
H	-0.61731300	0.08202500	-3.65898000
H	-2.51883700	0.23645600	1.78483000
H	-3.28229900	0.25540000	1.80290800
H	3.86295400	2.14240800	1.80955500
H	4.28685600	2.75920200	1.95790000
H	4.70288400	3.42437700	-1.53293100
H	4.72435800	2.66820200	-1.43697800

6. Geometries of linkers-2 + nH₂

6.1. Linker-2 + H₂

C	0.02116900	0.05957500	-0.00872500
N	0.02299000	0.07661100	1.33101200
C	1.25505800	0.05199100	1.85692900
N	2.40405100	0.01414600	1.18245700
C	2.27747000	0.00016500	-0.16034600
N	1.09139700	0.02219500	-0.80229000
H	1.32609000	0.06415100	2.95043000
H	-0.95723800	0.07820000	-0.50199300
C	3.51222600	-0.04188000	-0.97713300
C	3.43436100	-0.05806700	-2.38194400
C	4.77443400	-0.06592300	-0.35578700
C	4.59777200	-0.09760200	-3.14563300
H	2.45214600	-0.03902000	-2.85403800
C	5.93238300	-0.10539100	-1.12773400
H	4.82453600	-0.05296900	0.73293000
C	5.86723400	-0.12204600	-2.53502200
H	4.52908100	-0.10951600	-4.23593500
H	6.90877100	-0.12345200	-0.63787500
B	7.15449100	-0.16178400	-3.38650000
O	8.44836200	-0.18674600	-2.87882600

O	7.19377400	-0.18091600	-4.77591200
C	9.27693800	-0.21243500	-3.98533100
C	8.53626900	-0.20898200	-5.10533100
H	10.35046300	-0.23116300	-3.82308000
H	8.80717200	-0.22399700	-6.15676900
H	7.58667000	2.64119500	-4.11285300
H	8.00248600	2.63459400	-3.47500600

6.2. Linker-2+ 2H₂

C	0.00018400	-0.02479400	0.00613900
N	0.00190400	-0.01405300	1.34540600
C	1.23421300	-0.00129100	1.87135500
N	2.38360100	0.00174600	1.19670100
C	2.25934000	-0.00913100	-0.14609900
N	1.07228000	-0.02316700	-0.78630000
H	1.30504400	0.00757400	2.96482600
H	-0.97695500	-0.03602700	-0.48969400
C	3.49668000	-0.00415700	-0.95982500
C	3.42885900	-0.00923100	-2.36518400
C	4.75544400	0.01219500	-0.33068500
C	4.59798600	0.00346500	-3.12119200
H	2.45293800	-0.01964700	-2.84944100
C	5.91908900	0.02424300	-1.09491800
H	4.79833900	0.01829800	0.75826400
C	5.86364900	0.02082100	-2.50289600
H	4.53582300	0.00314200	-4.21182800
H	6.89200800	0.03974400	-0.59835600
B	7.15760900	0.04243100	-3.34581500
O	8.44729800	0.06275700	-2.82843800
O	7.20762400	0.04561800	-4.73452700
C	9.28504200	0.07926200	-3.92879800
C	8.55295800	0.06912600	-5.05443300

H	10.35721800	0.09704700	-3.75766800
H	8.83106100	0.07595400	-6.10410400
H	4.58731400	3.44428500	-1.70323800
H	4.70906400	2.69888600	-1.59805200
H	-0.56401800	-0.07508300	-3.65723900
H	-0.10295600	-0.06273900	-3.04843400

6.3. Linker-2+ 3H₂

C	0.06458000	-0.04472600	-0.03150500
N	0.05169900	-0.06080800	1.36708100
C	1.22892200	-0.05924800	1.90391400
N	2.39760600	-0.08575800	1.19459900
C	2.34904500	-0.09672300	-0.22656200
N	1.13176300	-0.05819600	-0.79918000
H	1.33411300	-0.04076800	2.99485700
H	-0.91410300	-0.01428300	-0.51500900
H	3.27699700	0.05763500	1.67552400
C	3.55950900	-0.15179600	-0.99666500
C	3.50495800	-0.01513100	-2.41156000
C	4.83668200	-0.33760500	-0.40012800
C	4.66212100	-0.04351700	-3.17055000
H	2.53024100	0.11951100	-2.88031900
C	5.98872500	-0.36425900	-1.17635800
H	4.93464300	-0.49769500	0.67636500
C	5.93761500	-0.21288000	-2.57776600
H	4.59044200	0.07023900	-4.25485800
H	6.95692400	-0.51327300	-0.69180500
B	7.22086100	-0.23724700	-3.41955400
O	8.50958300	-0.40633800	-2.91584900
O	7.28078700	-0.09652300	-4.80755100
C	9.34617100	-0.35905000	-4.01475100
C	8.62264500	-0.17686200	-5.13059100

H	10.41440300	-0.46935200	-3.85285200
H	8.90516300	-0.08646800	-6.17509300
H	4.87998700	1.90805600	1.54530100
H	4.72323900	2.16710100	2.24545500
H	8.27217200	2.59418300	-3.45784900
H	7.68904400	2.54763900	-3.94537600
H	5.12658700	0.60755400	-7.11161700
H	5.63387700	0.43627500	-6.56822200

6.4. Linker-2+4H₂

C	-0.03121600	0.02583100	0.02737900
N	-0.06124800	-0.20935500	1.34566700
C	1.14945400	-0.45045200	1.86617600
N	2.30682900	-0.46881200	1.20517200
C	2.21354200	-0.21261000	-0.11500800
N	1.05135700	0.03966500	-0.75036800
H	1.19353400	-0.65258100	2.94229800
H	-0.99105800	0.22887200	-0.46071800
C	3.46141100	-0.19656200	-0.91237900
C	3.41818000	0.06827700	-2.29332700
C	4.70226800	-0.43461600	-0.29382200
C	4.59498400	0.09891500	-3.03678100
H	2.45221100	0.25277200	-2.76306500
C	5.87428100	-0.40172600	-1.04444700
H	4.72542200	-0.63731700	0.77675600
C	5.84436200	-0.13238900	-2.42739400
H	4.55144800	0.31268600	-4.10679900
H	6.83490700	-0.57980100	-0.55569600
B	7.15316400	-0.06489400	-3.24301500
O	8.42721700	-0.26187800	-2.72500100
O	7.23887200	0.21339400	-4.60375500
C	9.29069300	-0.07614000	-3.78689400

C	8.58959900	0.20502900	-4.89787900
H	10.35682900	-0.17669700	-3.60655600
H	8.89343800	0.40941000	-5.92002000
H	5.02346900	3.20367800	-1.07285800
H	5.00665100	2.47183600	-1.28653600
H	1.85474800	2.63319100	1.14288300
H	1.63931400	2.67644000	0.41370200
H	8.22809800	2.68620200	-3.22502000
H	7.58935700	2.80464900	-2.82598300
H	5.09302400	0.99644200	-6.90749200
H	5.60104300	0.81584400	-6.36806400

7. Geometries of linkers-3 + nH₂

7.1. Linker-3+ H₂

C	0.01568200	-0.09586600	-0.00217200
C	0.01354100	-0.08593400	1.39633300
C	1.18794400	-0.08391300	2.13257500
C	2.38808500	-0.09286500	1.40168200
C	2.39026200	-0.10286200	0.00001300
C	1.19240200	-0.10434900	-0.73467300
O	-1.28599500	-0.09161000	-0.45552300
B	-2.07952100	-0.07231600	0.69362500
O	-1.28957200	-0.07527000	1.84549100
H	1.17059300	-0.07528100	3.22286000
H	3.33820000	-0.09161900	1.93950900
H	3.34204400	-0.10927200	-0.53482400
H	1.17849400	-0.11121500	-1.82501800
C	-3.61952800	-0.05379500	0.69105500
C	-4.34105400	-0.03474700	1.90064900
C	-4.33717700	-0.05197800	-0.52100200
C	-5.73684100	-0.01465100	1.90010500

H	-3.79508900	-0.03544500	2.84734900
C	-5.73295200	-0.03191400	-0.52523000
H	-3.78817000	-0.06612500	-1.46583800
C	-6.43375200	-0.01324200	0.68625000
H	-6.28499600	0.00010500	2.84510500
H	-6.27808200	-0.03061900	-1.47209100
H	-7.52648200	0.00256800	0.68438500
H	-1.20686600	2.72285100	1.05664600
H	-1.20842700	2.71970400	0.29519100

7.2. Linker-3+ 2H₂

C	-0.00199600	-0.16605700	-0.00289500
C	-0.00166600	-0.17158100	1.39577600
C	1.17377500	-0.16547000	2.13002000
C	2.37265800	-0.15292800	1.39691100
C	2.37234400	-0.14736900	-0.00502100
C	1.17309300	-0.15412600	-0.73761200
O	-1.30468200	-0.16598100	-0.45356000
B	-2.09608600	-0.16961500	0.69693800
O	-1.30413100	-0.17504900	1.84705300
H	1.15831200	-0.16569000	3.22027200
H	3.32366800	-0.14536100	1.93296700
H	3.32308800	-0.13555600	-0.54146700
H	1.15717200	-0.14569100	-1.82782600
C	-3.63653600	-0.16766600	0.69731000
C	-4.35580400	-0.16745800	1.90853000
C	-4.35636800	-0.15796800	-0.51353700
C	-5.75169700	-0.15715500	1.91059800
H	-3.80816300	-0.17213500	2.85412400
C	-5.75226000	-0.14764700	-0.51487500
H	-3.80916700	-0.15525600	-1.45939300
C	-6.45083000	-0.14704700	0.69804500
H	-6.29810000	-0.15417500	2.85659600

H	-6.29910500	-0.13725900	-1.46056400
H	-7.54352000	-0.13616200	0.69834200
H	0.90578800	3.21573500	0.71155400
H	1.20608600	2.51465700	0.70882100
H	-4.91057500	3.30051100	0.71155400
H	-4.93258600	2.53818800	0.70854200

7.3. Linker-3+ 3H₂

C	-0.14106700	0.01541400	-0.12611200
C	-0.06385100	-0.47464800	1.18133100
C	1.14658100	-0.80199600	1.77173100
C	2.29853400	-0.61602000	0.98856600
C	2.22012300	-0.12427900	-0.32190900
C	0.98639500	0.20365700	-0.90950900
O	-1.46264700	0.25946700	-0.43721000
B	-2.18649100	-0.08840300	0.70726100
O	-1.33346100	-0.54592300	1.71311300
H	1.19234100	-1.17873000	2.79391000
H	3.27475600	-0.85832300	1.41290200
H	3.13640900	0.00977800	-0.90003100
H	0.91129200	0.59127300	-1.92580500
C	-3.71665400	0.02084100	0.84379500
C	-4.35484500	-0.34594800	2.04513800
C	-4.50719600	0.49790600	-0.22039100
C	-5.73997600	-0.23886500	2.18038900
H	-3.75180000	-0.71436600	2.87859500
C	-5.89271300	0.60575600	-0.08790500
H	-4.02605000	0.78929100	-1.15687400
C	-6.50997200	0.23749500	1.11306700
H	-6.22245400	-0.52355600	3.11826600
H	-6.49427600	0.97976300	-0.91952700
H	-7.59414400	0.32439100	1.21848200

H	1.10765100	2.87007500	1.61443100
H	1.35235000	2.18783900	1.37701500
H	-4.63357600	3.35344700	2.12338100
H	-4.72822200	2.64947000	1.84569400
H	-2.00880200	1.13201600	-2.69951200
H	-2.17854300	1.39726300	-3.39410000

7.4. Linker-3+ 4H₂

C	-0.11158800	0.14484800	0.00543600
C	-0.11715900	0.15500800	1.40345600
C	1.05344900	0.20996800	2.14310900
C	2.25402600	0.25576200	1.41404800
C	2.25958200	0.24553700	0.01217500
C	1.06485400	0.18908100	-0.72560100
O	-1.41273500	0.09541000	-0.44980600
B	-2.21206200	0.07771600	0.69663400
O	-1.42187300	0.11213600	1.84902000
H	1.03409300	0.22156800	3.23314800
H	3.20187700	0.30226000	1.95364900
H	3.21168600	0.28429300	-0.52050300
H	1.05414500	0.18483900	-1.81581300
C	-3.75109100	0.02799900	0.69093300
C	-4.47551300	0.01847300	1.89957600
C	-4.46598500	-0.00017700	-0.52308200
C	-5.87090700	-0.01720800	1.89555600
H	-3.93510500	0.04292500	2.84867500
C	-5.86136800	-0.03590600	-0.52948300
H	-3.91815200	0.00971200	-1.46817600
C	-6.56489100	-0.04424100	0.68042500
H	-6.42071700	-0.02125700	2.83950000
H	-6.40374100	-0.05456100	-1.47754500
H	-7.65733300	-0.06937800	0.67632500

H	0.65636100	3.56005800	0.68269200
H	0.99418400	2.87678700	0.70871400
H	-5.13017500	3.44940500	0.65958700
H	-5.13176200	2.68678100	0.66588100
H	-1.79716600	0.10638900	-2.90909900
H	-1.91488600	0.10773900	-3.66256900
H	-1.82287700	0.14731300	4.30542000
H	-1.94373100	0.15631400	5.05834000

8. Geometries of linkers-4+ nH₂

8.1. Linker-4 + H₂

C	0.10028500	0.01933200	-0.01660200
C	0.15891600	0.16622600	1.37076700
C	1.36907400	0.25331500	2.04027000
C	2.52931000	0.18626000	1.25588100
C	2.48591800	0.03320500	-0.14633300
C	1.23749800	-0.05217400	-0.80187800
O	-1.22383900	-0.04834400	-0.40512600
B	-1.95403000	0.06532700	0.76995900
O	-1.12579700	0.19851900	1.87610600
H	1.41132600	0.37912900	3.12234800
H	3.50009800	0.28227300	1.74456600
H	1.16395100	-0.19431000	-1.88008700
H	-3.14422300	0.05063100	0.82273200
C	6.12577800	-0.16962400	-2.36731100
C	5.04038600	0.56230200	-2.85320200
C	3.84255400	0.65376100	-2.16650500
C	3.74535900	-0.03198000	-0.93503400
C	4.84902800	-0.77223900	-0.45969100
C	6.05873300	-0.85325700	-1.16402000
O	7.17632300	-0.06369800	-3.25681400

B	6.70436500	0.74646500	-4.28068300
O	5.39383600	1.14479500	-4.05470100
H	3.02197500	1.25830700	-2.55268100
H	4.75016400	-1.31918000	0.47913900
H	6.90531400	-1.42985000	-0.79087600
H	7.34424300	1.05997500	-5.23551500
H	6.03844300	2.67936200	-0.05433600
H	5.63613100	2.05718900	-0.23521100

8.2. Linker-4+ 2H₂

C	-0.00050300	-0.09461400	0.00497600
C	0.01529000	-0.08708400	1.40127200
C	1.20384300	-0.08433200	2.11330500
C	2.38813000	-0.08932100	1.36239100
C	2.38766600	-0.10003600	-0.04886800
C	1.16023000	-0.10288800	-0.74800900
O	-1.31177400	-0.09877100	-0.42888000
B	-2.07816700	-0.08815600	0.72858500
O	-1.28417700	-0.08149100	1.86743500
H	1.21247900	-0.06445000	3.20321000
H	3.34390800	-0.05420300	1.88743700
H	1.12031900	-0.12971300	-1.83689100
H	-3.26947400	-0.08593900	0.74290800
C	6.09607300	-0.08642000	-2.16067000
C	5.03177600	0.70674600	-2.59448700
C	3.81215500	0.73001700	-1.94119600
C	3.67097600	-0.09144300	-0.80045500
C	4.75344100	-0.89171000	-0.37724400
C	5.98538700	-0.90294700	-1.04682300
O	7.17611800	0.11006800	-2.99772300
B	6.74336400	1.03647500	-3.93695900
O	5.42843000	1.41904800	-3.70933200

H	3.00812200	1.38290100	-2.28060800
H	4.61990700	-1.54022100	0.48991500
H	6.81594000	-1.52643500	-0.71542100
H	7.41651200	1.45058500	-4.82846500
H	5.89837100	2.47623700	0.51259300
H	5.48594400	1.90341700	0.22364800
H	1.19083600	3.28446500	0.50554400
H	1.49097800	2.58511000	0.55585300

8.3. Linker-4+ 3H₂

C	-0.03358200	-0.27143600	-0.01061300
C	-0.01959000	-0.26826000	1.38609600
C	1.16833800	-0.23886800	2.09900700
C	2.35316900	-0.21608400	1.34948800
C	2.35455800	-0.22395200	-0.06187800
C	1.12823500	-0.25115100	-0.76229900
O	-1.34305300	-0.30473300	-0.44594800
B	-2.11073700	-0.31012900	0.71063100
O	-1.31775800	-0.29547900	1.85061400
H	1.17550600	-0.22180800	3.18898500
H	3.30744600	-0.16081000	1.87557400
H	1.09013200	-0.27573700	-1.85130800
H	-3.30168600	-0.33227000	0.72411400
C	6.06334000	-0.11251600	-2.16930900
C	4.98091700	0.65718400	-2.60046800
C	3.76049400	0.64833600	-1.94832800
C	3.63790600	-0.18208800	-0.81196800
C	4.73871300	-0.95819300	-0.39112900
C	5.97116300	-0.93679600	-1.05939800
O	7.13930500	0.11382200	-3.00410600
B	6.68558600	1.03426300	-3.93930000
O	5.36167600	1.38429800	-3.71132900

H	2.94198700	1.28483300	-2.28386700
H	4.61986600	-1.61350400	0.47306700
H	6.81612400	-1.54172000	-0.73002100
H	7.34960600	1.46868000	-4.82799700
H	5.80264100	2.43620600	0.51113500
H	5.39406000	1.87088800	0.20266900
H	1.81952900	3.28260600	0.01218900
H	1.88231300	2.54304200	0.18726800
H	-0.86623500	2.53547300	0.62270800
H	-1.42095800	2.54410700	1.14481200

8.4. Linker-4+ 4H₂

C	-0.02190500	-0.27489700	0.00701300
C	0.01893400	-0.23470600	1.40268300
C	1.22045000	-0.19221500	2.09175400
C	2.39082500	-0.19521200	1.31952700
C	2.36499700	-0.24111000	-0.09092400
C	1.12536400	-0.28084400	-0.76688600
O	-1.33963800	-0.31339300	-0.40211600
B	-2.08488800	-0.28436500	0.76869700
O	-1.27009000	-0.24352300	1.89248000
H	1.24862000	-0.14618200	3.18055400
H	3.35498000	-0.12923700	1.82570300
H	1.06639000	-0.33434200	-1.85393300
H	-3.27545900	-0.30037600	0.80552800
C	6.03429200	-0.20188900	-2.27024400
C	4.94713700	0.56235800	-2.70016100
C	3.73915300	0.57628900	-2.02466500
C	3.63391300	-0.22502400	-0.86605200
C	4.73976900	-0.99424500	-0.44544600
C	5.95973700	-0.99514800	-1.13645000
O	7.09313000	-0.00537000	-3.13168600

B	6.62765500	0.89775800	-4.07849500
O	5.30874600	1.25713600	-3.83679400
H	2.91695700	1.20732700	-2.36167200
H	4.63463200	-1.62602700	0.43783900
H	6.80819700	-1.59530000	-0.80729700
H	7.27721000	1.30670400	-4.98945900
H	5.23868400	2.40140500	0.91708100
H	5.04652300	1.82198900	0.46015200
H	1.82338300	3.26542100	-0.06065100
H	1.91937500	2.53301000	0.12873900
H	-0.80516500	2.55212200	0.60310300
H	-1.38303600	2.58882200	1.09827500
H	7.48609400	2.54161400	-1.76895500
H	6.77540200	2.65605700	-1.51969700

9. Geometries of linkers-5 + nH₂

9.1. Linker-5 + H₂

C	-0.00836500	0.00080400	-0.00647000
N	-0.01010800	0.00262800	1.33645400
C	1.19872600	0.00562200	1.92027600
N	2.36255700	0.00509200	1.25004800
C	2.26375700	0.00074700	-0.08930800
N	1.10195000	-0.00252400	-0.76187900
C	1.25288200	0.01613300	3.40393200
C	2.49077500	0.01692200	4.07076700
C	0.06685500	0.02737600	4.15904700
C	2.53957000	0.02858500	5.46475100
H	3.40602100	0.00820600	3.47976800
C	0.11973800	0.03912200	5.55287600
H	-0.88892400	0.02727100	3.63607400
C	1.35521000	0.03976200	6.20996100

H	3.50606500	0.02899800	5.97365700
H	-0.80714100	0.04806500	6.13072300
H	1.39501200	0.04903700	7.30175900
C	3.52196100	0.00584000	-0.87747800
C	4.76881100	0.00826300	-0.22754000
C	3.48090600	0.01028100	-2.28291300
C	5.94973100	0.01486500	-0.96990900
H	4.79366800	0.00488400	0.86168400
C	4.66398700	0.01691300	-3.02181200
H	2.51149600	0.00894400	-2.78016000
C	5.90140800	0.01923200	-2.36841300
H	6.91350500	0.01664700	-0.45586700
H	4.62174500	0.02054000	-4.11327500
H	6.82723300	0.02451800	-2.94851300
C	-1.32039200	0.00439600	-0.70179800
C	-2.51695900	0.00863100	0.03665700
C	-1.38108000	0.00501900	-2.10658100
C	-3.74846400	0.01344000	-0.61838400
H	-2.46285700	0.00819700	1.12482600
C	-2.61452800	0.00986200	-2.75796100
H	-0.45019000	0.00185300	-2.67268600
C	-3.80143400	0.01411100	-2.01673100
H	-4.67253400	0.01671100	-0.03599700
H	-2.65136100	0.01035800	-3.84962600
H	-4.76678800	0.01793800	-2.52836900
H	1.03671500	2.92384400	0.53518400
H	1.69715500	2.78922400	0.88995700

9.2. Linker-5+ 2H₂

C	-0.09798300	-0.01389700	0.02884200
N	-0.10298600	-0.02225300	1.37197700
C	1.10275100	0.03143000	1.96019900

N	2.26733200	0.09140600	1.29233400
C	2.17243500	0.09073400	-0.04784600
N	1.01358300	0.03980300	-0.72356900
C	1.15325000	0.02650000	3.44358500
C	2.38907600	0.03357500	4.11457900
C	-0.03534000	0.01422500	4.19487100
C	2.43282700	0.02965100	5.50871000
H	3.30741400	0.04121500	3.52867200
C	0.01273700	0.01152000	5.58876800
H	-0.98943500	0.00846200	3.66887200
C	1.24605900	0.01926200	6.24991500
H	3.39761900	0.03503600	6.02068800
H	-0.91604500	0.00354900	6.16352900
H	1.28227100	0.01704200	7.34186300
C	3.43141700	0.15365600	-0.83172900
C	4.67748000	0.13757900	-0.18028800
C	3.39169100	0.23504700	-2.23478300
C	5.85877400	0.20412800	-0.91935000
H	4.70333000	0.07327000	0.90673300
C	4.57500700	0.30342800	-2.96983200
H	2.42296000	0.24916400	-2.73305900
C	5.81156500	0.28844900	-2.31526900
H	6.82166000	0.19249400	-0.40404800
H	4.53352400	0.37162500	-4.05909700
H	6.73756900	0.34422300	-2.89223200
C	-1.40653200	-0.06943900	-0.67003200
C	-2.60405900	-0.12117900	0.06517000
C	-1.46298800	-0.07116100	-2.07500700
C	-3.83257200	-0.17247300	-0.59337600
H	-2.55301400	-0.12070900	1.15348100
C	-2.69347400	-0.12292700	-2.72983000
H	-0.53136200	-0.03215500	-2.63854000

C	-3.88134800	-0.17341500	-1.99186500
H	-4.75747200	-0.21222900	-0.01368600
H	-2.72729000	-0.12403700	-3.82156800
H	-4.84437600	-0.21393900	-2.50627700
H	4.53042100	2.90240500	-1.15688500
H	4.44158800	3.64999000	-1.27830600
H	3.88487300	2.91516700	2.17035700
H	3.53362800	2.26128400	1.99279900

9.3. Linker-5+ 3H₂

C	0.06617900	0.08072600	0.09796400
N	0.04991200	0.02020200	1.43988500
C	1.25217600	-0.01733000	2.03789200
N	2.42336400	0.00278300	1.38151500
C	2.34108500	0.07056200	0.04290300
N	1.18647700	0.11146200	-0.64250200
C	1.28790300	-0.08132300	3.51991400
C	2.51797800	-0.08799500	4.20144100
C	0.09334800	-0.13620400	4.25970800
C	2.55047000	-0.14592500	5.59458500
H	3.44001700	-0.04708800	3.62247200
C	0.13013400	-0.19452400	5.65278200
H	-0.85689600	-0.13357900	3.72727500
C	1.35765300	-0.19888200	6.32442700
H	3.51076700	-0.14967400	6.11502600
H	-0.80326900	-0.23678200	6.21840000
H	1.38482300	-0.24399600	7.41570400
C	3.60759800	0.10689700	-0.72950000
C	4.84552800	0.13576600	-0.06309200
C	3.58475400	0.11261900	-2.13545800
C	6.03541200	0.17312600	-0.78978000
H	4.85613200	0.13005200	1.02632700

C	4.77698900	0.14801400	-2.85852200
H	2.62352800	0.08633800	-2.64726900
C	6.00517800	0.17939100	-2.18880000
H	6.99201000	0.19758700	-0.26314000
H	4.74883000	0.15127000	-3.95037400
H	6.93809000	0.20822500	-2.75670300
C	-1.23674400	0.11919100	-0.61115500
C	-2.44196900	0.07393300	0.11201500
C	-1.28103500	0.19933200	-2.01444500
C	-3.66561900	0.11234500	-0.55621600
H	-2.40259100	0.00818700	1.19852900
C	-2.50681000	0.23801000	-2.67876200
H	-0.34507400	0.23119600	-2.57061600
C	-3.70214900	0.19567700	-1.95253000
H	-4.59620200	0.07747000	0.01453600
H	-2.53076300	0.30179400	-3.76885600
H	-4.66147700	0.22669600	-2.47445400
H	1.21133300	2.33312000	-2.03606000
H	1.19006100	2.97611500	-2.44651700
H	1.81969000	2.81125000	1.17555200
H	1.10391800	2.98252900	0.98005100
H	-1.62178600	2.74742000	2.54810300
H	-1.24137900	2.12514400	2.32354100

9.4. Linker-5+ 4H₂

C	0.11323700	0.02330400	-0.07708700
N	0.12118300	0.05102700	1.26559100
C	1.33407400	0.02950300	1.84292800
N	2.49275600	-0.02193100	1.16719700
C	2.38677600	-0.03811600	-0.17096200
N	1.22003200	-0.01576200	-0.83717200
C	1.39650100	0.07343100	3.32504700

C	2.63885800	0.10799600	3.98289800
C	0.21503800	0.09455400	4.08737100
C	2.69625900	0.16942700	5.37503700
H	3.55007900	0.09206300	3.38598300
C	0.27698500	0.15548900	5.47950200
H	-0.74456900	0.06580200	3.57309600
C	1.51660200	0.19495500	6.12726700
H	3.66577500	0.20077700	5.87695900
H	-0.64616900	0.17461400	6.06279300
H	1.56337500	0.24609400	7.21754900
C	3.63866000	-0.07797400	-0.96643100
C	4.88909000	-0.01725300	-0.32609000
C	3.58966400	-0.17517600	-2.36841600
C	6.06551000	-0.04921900	-1.07461100
H	4.91997000	0.05733800	0.76038500
C	4.76846500	-0.20915100	-3.11324100
H	2.61895900	-0.22581100	-2.86010600
C	6.00925300	-0.14527900	-2.46956100
H	7.03199500	0.00138400	-0.56828900
H	4.71989200	-0.28560600	-4.20170500
H	6.93165900	-0.17060200	-3.05453400
C	-1.20174600	0.04293200	-0.76424500
C	-2.39311100	0.09918200	-0.01915900
C	-1.27166000	0.00353200	-2.16816400
C	-3.62809800	0.11941000	-0.66704700
H	-2.33415300	0.12743300	1.06810400
C	-2.50869700	0.02353900	-2.81215300
H	-0.34647600	-0.04284800	-2.74116800
C	-3.69000500	0.08224200	-2.06445300
H	-4.54769900	0.16487300	-0.07948800
H	-2.55245800	-0.00637700	-3.90308400
H	-4.65818700	0.09870100	-2.57043100

H	1.40236300	2.85495400	0.06731100
H	1.37088200	2.89417600	0.82726200
H	1.44675300	3.58627300	4.16438800
H	1.35309700	2.82959100	4.17959300
H	-1.44054200	2.85622300	2.35515600
H	-1.09770600	2.23140900	2.08294300
H	1.24891500	2.67400100	-2.89102000
H	1.24422000	2.04249200	-2.46257300

10. Geometries of linkers-6+ nH₂

10.1. Linker-6 + H₂

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39948500
C	1.16709200	0.00000000	2.12043000
C	2.40193200	-0.00019900	1.41419000
C	2.40194200	-0.00005800	-0.01477600
C	1.16708600	0.00006600	-0.72097100
O	-1.30534400	0.00056700	-0.45016700
B	-2.08458100	0.00130500	0.69975700
O	-1.30533800	0.00057400	1.84967300
H	1.11575700	0.00092800	3.20588200
H	1.11573900	0.00105300	-1.80642000
H	-3.27574700	0.00178400	0.69976000
C	6.09777100	0.02107800	-2.12126100
C	4.88572500	0.01627900	-2.82092200
C	3.67787300	0.00806800	-2.17064200
C	3.67205300	0.00425200	-0.74811500
C	4.90968400	0.00875900	-0.03370500
C	6.13868300	0.01759900	-0.75007800
O	7.14020700	0.02937200	-3.02669000

B	6.53386700	0.03024000	-4.27645200
O	5.14840800	0.02177700	-4.17645500
H	2.76348800	0.00553000	-2.75776800
H	7.10438100	0.02233300	-0.25185400
H	7.12934700	0.03643900	-5.30806700
C	4.88586400	0.01473500	4.22028300
C	6.09789200	0.01938100	3.52055400
C	6.13876200	0.01647500	2.14937100
C	4.90972600	0.00836200	1.43300700
C	3.67209000	0.00375700	2.14751100
C	3.67798300	0.00713100	3.57007000
O	5.14860600	0.02006900	5.57579900
B	6.53407900	0.02749900	5.67573600
O	7.14035900	0.02757900	4.42593800
H	7.10444000	0.02110900	1.65111200
H	7.12960400	0.03381600	6.70732000
H	2.76363100	0.00465700	4.15724400
H	3.65102100	3.41795700	0.70483600
H	3.72411500	2.66046300	0.75760300

10.2. Linker-6+ 2H₂

C	-0.00635900	0.17017500	0.00693000
C	-0.00664800	0.17704200	1.40614200
C	1.15978600	0.15830200	2.12766800
C	2.39452700	0.13324200	1.42209300
C	2.39507900	0.12755900	-0.00709100
C	1.16055400	0.14527600	-0.71364000
O	-1.31121600	0.18305400	-0.44358500
B	-2.09070000	0.19672600	0.70610500
O	-1.31151500	0.19445200	1.85614600
H	1.10821500	0.15981600	3.21304100
H	1.10974100	0.13701200	-1.79900600

H	-3.28176400	0.21031300	0.70581700
C	6.09159700	0.05379500	-2.11113500
C	4.87981000	0.06131600	-2.81138400
C	3.67161100	0.08528500	-2.16189900
C	3.66541900	0.10254900	-0.73977600
C	4.90302300	0.09345400	-0.02406700
C	6.13223300	0.06897800	-0.73980600
O	7.13409900	0.02811200	-3.01598200
B	6.52826900	0.02007100	-4.26606300
O	5.14283100	0.04026600	-4.16651800
H	2.75760200	0.08887300	-2.74963900
H	7.09774300	0.06022900	-0.24139200
H	7.12394100	-0.00135000	-5.29732800
C	4.87642800	0.09126400	4.22922800
C	6.08866000	0.07934700	3.53033600
C	6.13023100	0.08277600	2.15904200
C	4.90176900	0.09927500	1.44224100
C	3.66416200	0.11340500	2.15590700
C	3.66896200	0.10831600	3.57816100
O	5.13811700	0.08270100	5.58482500
B	6.52349200	0.06565200	5.68577700
O	7.13050500	0.06344400	4.43627600
H	7.09623000	0.07151000	1.66157400
H	7.11825100	0.05439900	6.71775300
H	2.75438800	0.11647100	4.16500600
H	3.88807700	-3.28891000	0.56944800
H	4.20638200	-2.61478700	0.41068500
H	1.18043000	-2.55647300	0.80374900
H	0.71070800	-3.15434300	0.74856600

10.3. Linker-6+ 3H₂

C	-0.04989100	0.20530200	0.08284800
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C	-0.04796000	0.26811200	1.48079100
C	1.11990300	0.28082900	2.20030300
C	2.35347400	0.22846700	1.49380000
C	2.35136400	0.16575200	0.06617600
C	1.11591300	0.15460600	-0.63824500
O	-1.35537700	0.20198000	-0.36580700
B	-2.13317800	0.26310300	0.78355200
O	-1.35212700	0.30540600	1.93160200
H	1.07028500	0.32617800	3.28478800
H	1.06325400	0.10349800	-1.72233900
H	-3.32418000	0.27859000	0.78459000
C	6.04292200	-0.01043800	-2.04003600
C	4.83011900	-0.01974900	-2.73790600
C	3.62365500	0.03844500	-2.08776700
C	3.62015100	0.10756000	-0.66713100
C	4.85858700	0.11395600	0.04605400
C	6.08616200	0.05551000	-0.67047200
O	7.08335500	-0.08093600	-2.94446500
B	6.47510900	-0.13372100	-4.19234700
O	5.09006400	-0.09669000	-4.09137400
H	2.70857000	0.02586600	-2.67362100
H	7.05247800	0.05686900	-0.17359300
H	7.06856600	-0.20148000	-5.22285000
C	4.83964700	0.26255100	4.29732500
C	6.05030100	0.20669300	3.59781600
C	6.08975600	0.16170000	2.22734300
C	4.86059200	0.17187000	1.51161400
C	3.62428800	0.22875200	2.22606300
C	3.63155800	0.27552900	3.64773900
O	5.10325700	0.29243800	5.65190100
B	6.48831400	0.25264000	5.75203100
O	7.09299800	0.20061300	4.50241000

H	7.05441300	0.11341100	1.72960200
H	7.08445700	0.26303300	6.78315500
H	2.71812400	0.31493200	4.23494600
H	4.75770000	-3.32567700	-1.12627700
H	4.69247200	-2.60418200	-0.88834100
H	1.50252400	-2.46652200	1.02854900
H	1.17327600	-3.14810000	0.93649800
H	4.69203700	-3.16371300	2.95494900
H	4.53674400	-2.46457700	2.69323800

10.4. Linker-6+ 4H₂

C	-0.02265900	0.00216300	0.03224200
C	-0.02282300	0.03511200	1.43113100
C	1.14429700	0.04534100	2.15219600
C	2.37905500	0.02223000	1.44653200
C	2.37915600	-0.01308100	0.01819100
C	1.14462500	-0.02244300	-0.68819900
O	-1.32704000	-0.00626100	-0.41823100
B	-2.10670900	0.01541800	0.73151300
O	-1.32729100	0.04762800	1.88117100
H	1.09307500	0.06925900	3.23736200
H	1.09365300	-0.04918600	-1.77332200
H	-3.29762300	0.01371700	0.73141100
C	6.07546300	-0.12556200	-2.08599300
C	4.86303600	-0.13655800	-2.78588900
C	3.65531000	-0.09796200	-2.13591200
C	3.64939900	-0.04474400	-0.71446300
C	4.88728400	-0.03393500	0.00004700
C	6.11590700	-0.07582700	-0.71537300
O	7.11651400	-0.17921700	-2.98859900
B	6.51009100	-0.23076400	-4.23740800
O	5.12473200	-0.19687700	-4.13828000

H	2.74105200	-0.11366100	-2.72302900
H	7.08159600	-0.07440200	-0.21721200
H	7.10514900	-0.28820200	-5.26751000
C	4.86255700	0.07028500	4.25242100
C	6.07458200	0.04711300	3.55368600
C	6.11590300	0.01662900	2.18291000
C	4.88705200	0.00801800	1.46620600
C	3.64917300	0.03303200	2.18003100
C	3.65495700	0.06536200	3.60198600
O	5.12447900	0.09202300	5.60762300
B	6.50994100	0.08069100	5.70859600
O	7.11659200	0.05416900	4.45918300
H	7.08169900	-0.00396000	1.68545600
H	7.10496400	0.09335500	6.74038400
H	2.74062200	0.08164300	4.18893700
H	4.34912200	-3.54111500	-0.41945600
H	4.30410500	-2.78026000	-0.43982200
H	-1.14851500	-2.79903400	1.17585100
H	-1.13739000	-2.80656600	0.41443400
H	4.87289300	-3.27725700	3.06976600
H	4.78446900	-2.65727900	2.63485800
H	6.03420100	-3.13611800	-3.43901900
H	5.69560800	-2.95258800	-2.78121900

11. Geometries of linkers-1-ScCl_x + nH₂

11.1. Linker-1-ScCl₃+ H₂

C	0.00783900	0.05912400	0.01672100
N	-0.00293200	0.06724300	1.35125700
C	1.20390900	0.03448500	1.93179100
N	2.36959700	0.06351800	1.21954100
C	2.25244300	-0.15367100	-0.12528900

N	1.07356700	-0.13373100	-0.76147000
H	-0.95634800	0.18543600	-0.48648000
C	1.28017000	-0.02339600	3.39775700
C	2.38428000	-0.62506300	4.03034500
C	0.25003400	0.53676100	4.17486800
C	2.47418000	-0.63238800	5.42170000
H	3.16560700	-1.10527400	3.43998500
C	0.34940900	0.53081400	5.56322300
H	-0.60306000	0.99399100	3.67397000
C	1.46267800	-0.04679700	6.18798400
H	3.33804800	-1.09352000	5.90298900
H	-0.43881900	0.98726400	6.16489300
H	1.53848100	-0.04203800	7.27745400
C	3.46747300	-0.41228900	-0.90877500
C	4.59468700	-1.00152200	-0.30702300
C	3.50722600	-0.06050000	-2.27053200
C	5.75785300	-1.20324400	-1.04839000
H	4.56174700	-1.31900900	0.73555100
C	4.67398200	-0.25921700	-3.00326200
H	2.62601200	0.38913900	-2.72765100
C	5.80156300	-0.82439900	-2.39322600
H	6.62941200	-1.65357200	-0.57066400
H	4.71111600	0.03564400	-4.05367900
H	6.71637600	-0.97224400	-2.97120900
Sc	4.09584200	1.37327600	2.02677300
Cl	4.74509000	2.56822500	0.15819800
Cl	3.15275800	2.84000100	3.53636400
Cl	5.76930600	0.03753100	2.94101100
H	1.78698700	2.90840900	0.28502600
H	1.09943500	2.82037700	0.60217400

11.2. Linker-1-ScCl₃+ 2H₂

C	-0.02525900	-0.02595600	-0.02223200
N	-0.03094600	-0.02577800	1.31244000
C	1.17868200	-0.01864600	1.88761200
N	2.33918000	0.05427800	1.17169100
C	2.22410600	-0.16634100	-0.17217500
N	1.04330700	-0.18046800	-0.80451500
H	-0.99496800	0.07039300	-0.52132300
C	1.26377100	-0.08497900	3.35250300
C	2.38385300	-0.66915100	3.97301600
C	0.22661600	0.44658800	4.14005800
C	2.48244100	-0.68612900	5.36377600
H	3.16957400	-1.12966500	3.37298500
C	0.33466100	0.43127300	5.52770200
H	-0.63884600	0.88998800	3.64792400
C	1.46369500	-0.12799600	6.14086200
H	3.35844300	-1.13345200	5.83608600
H	-0.45914400	0.86613500	6.13797100
H	1.54607500	-0.13060200	7.22986200
C	3.44293300	-0.39488400	-0.95891600
C	4.58268000	-0.96302500	-0.36072100
C	3.47248300	-0.03990800	-2.32001000
C	5.74782500	-1.14094800	-1.10516400
H	4.55794400	-1.28263200	0.68144600
C	4.64126900	-0.21434400	-3.05574300
H	2.58138300	0.39287800	-2.77425500
C	5.78100000	-0.75879800	-2.44938700
H	6.62906800	-1.57522100	-0.63031700
H	4.67026900	0.08310600	-4.10568900
H	6.69710600	-0.88793900	-3.02980100
Sc	4.03119300	1.39548000	1.98836700
Cl	4.63945600	2.61447800	0.12123200
Cl	3.05766400	2.82847500	3.51134000

Cl	5.74229000	0.09565200	2.88545000
H	1.67158400	2.88311900	0.26252700
H	0.98470300	2.77554000	0.57499200
H	1.07631900	-2.87470600	1.24000400
H	1.65853300	-2.94096000	0.75349000

11.3. Linker-1-ScCl₃+ 3H₂

C	0.00124100	0.11473600	0.02839000
N	0.00871800	0.08993700	1.36065300
C	1.22176400	0.05086100	1.92858800
N	2.37811800	0.10504800	1.20219500
C	2.24558400	-0.08067700	-0.14355800
N	1.06060500	-0.05061700	-0.76729700
H	-0.96948600	0.24220100	-0.46144600
C	1.30675400	-0.05247600	3.39062800
C	2.41704400	-0.66551500	3.99988900
C	0.27114800	0.46748300	4.18867900
C	2.50697700	-0.72605100	5.38960600
H	3.20483400	-1.11090500	3.39173600
C	0.37073300	0.40976400	5.57596600
H	-0.58742100	0.93352300	3.70560900
C	1.48950000	-0.18082800	6.17811100
H	3.37551700	-1.19680000	5.85295100
H	-0.42223400	0.83449300	6.19441900
H	1.56517500	-0.21823900	7.26700000
C	3.45829100	-0.31609700	-0.93774900
C	4.56806400	-0.96074300	-0.35963100
C	3.51889200	0.11589300	-2.27498300
C	5.73650500	-1.13807500	-1.09961400
H	4.51387900	-1.34393500	0.66006100
C	4.69076800	-0.05958200	-3.00531800
H	2.65413400	0.61268900	-2.71431200

C	5.80153900	-0.67996900	-2.41833000
H	6.59478500	-1.63137300	-0.64079900
H	4.74559200	0.29786400	-4.03525500
H	6.72042300	-0.80813200	-2.99442600
Sc	4.17275500	1.35952700	1.94184200
Cl	4.94167300	2.57666100	0.13982600
Cl	3.15455600	2.81458100	3.42082600
Cl	5.78852500	-0.01466100	2.90218100
H	1.52742500	3.00793200	0.92580700
H	1.34125500	2.84630300	0.20450500
H	1.41275100	-2.83214500	0.41062600
H	1.39371300	-2.83194600	1.17199300
H	0.36619300	-0.79527300	-3.17028600
H	0.10456300	-0.99013500	-3.86057000

11.4. Linker-1-ScCl₃+ 4H₂

C	0.03277900	0.46515900	-0.01062900
N	0.02691000	0.39635700	1.32124700
C	1.22855100	0.23085300	1.89035500
N	2.39108800	0.21219200	1.17401400
C	2.25483900	0.08435900	-0.17898500
N	1.07981800	0.23456000	-0.80447300
H	-0.91943400	0.69200900	-0.50077000
C	1.30184300	0.06949700	3.34820900
C	2.34567400	-0.67495800	3.92905700
C	0.33022400	0.66946900	4.16956300
C	2.43723400	-0.78529200	5.31591600
H	3.07607600	-1.18600000	3.30052400
C	0.43188100	0.56043000	5.55351700
H	-0.47741900	1.23718700	3.70777500
C	1.48715400	-0.16021200	6.12835700
H	3.25461100	-1.35730100	5.75778100

H	-0.30847900	1.04696400	6.19131000
H	1.56547000	-0.23636600	7.21498500
C	3.43985500	-0.23724200	-0.98327700
C	4.49107700	-0.99001300	-0.42950500
C	3.51950000	0.19738000	-2.31915700
C	5.62101700	-1.27930900	-1.19272600
H	4.41891100	-1.37133200	0.58922900
C	4.65317600	-0.09114600	-3.07394500
H	2.69923400	0.77818200	-2.74007600
C	5.70604900	-0.82497400	-2.51171800
H	6.43327300	-1.86034600	-0.75322100
H	4.72283800	0.26355300	-4.10391700
H	6.59435300	-1.04543500	-3.10753200
Sc	4.23913600	1.28304300	2.05335800
Cl	4.98799000	2.53436300	0.26034800
Cl	3.44539600	2.72393200	3.66985300
Cl	5.77613900	-0.27008600	2.85679600
H	2.07292700	3.14496200	0.43974700
H	1.36881800	3.09685900	0.72778700
H	1.32829400	-2.64129900	0.23095900
H	1.12943100	-2.63309200	0.96627900
H	0.44563500	-0.72709000	-3.15152900
H	0.23462700	-1.01961000	-3.82428400
H	2.76503200	-3.39655600	-2.44381400
H	2.83048500	-2.63894600	-2.49780300

12. Geometries of linkers-1-TiCl_x + nH₂

12.1. Linker-1- Ti Cl₃+ H₂

C	0.00181000	-0.17529900	0.00502500
N	0.00242900	-0.14463300	1.33815900
C	1.21225500	-0.09751500	1.91045500

N	2.37005700	-0.00934600	1.18449800
C	2.25289000	-0.27715400	-0.15413900
N	1.06949700	-0.33496800	-0.77742500
H	-0.97108700	-0.10410900	-0.49219000
C	1.28859100	-0.14311700	3.37650400
C	2.41324200	-0.69299100	4.01805200
C	0.22456500	0.36320700	4.14492100
C	2.48671000	-0.70607000	5.40998800
H	3.22457200	-1.12255400	3.43070900
C	0.30787300	0.35421000	5.53446700
H	-0.64407400	0.78073900	3.63644500
C	1.43963800	-0.17439400	6.16861500
H	3.36496300	-1.12999800	5.89964400
H	-0.50831600	0.76879600	6.12915400
H	1.50247700	-0.17443300	7.25899900
C	3.46535000	-0.51221500	-0.94882700
C	4.61830700	-1.05578900	-0.35474000
C	3.46912700	-0.19691000	-2.32008900
C	5.77030000	-1.25144200	-1.11497300
H	4.61165500	-1.33841700	0.69746400
C	4.62512800	-0.38747700	-3.07176800
H	2.56776900	0.21797300	-2.77039200
C	5.77793600	-0.90924800	-2.47050500
H	6.66187000	-1.66968400	-0.64482800
H	4.63344900	-0.12107000	-4.13039000
H	6.68392800	-1.05266300	-3.06341100
Ti	3.93019700	1.38250300	1.88344700
Cl	5.64563500	0.22356700	2.79606200
Cl	4.31887100	2.58642400	0.00439400
Cl	2.86280800	2.82570900	3.25275800
H	1.41281100	2.75246300	0.24178500
H	0.66579900	2.66595800	0.36721900

12.2. Linker-1- Ti Cl₃+ 2H₂

C	0.03697900	-0.03142700	0.01471500
N	0.03890200	-0.03970300	1.34790200
C	1.24848900	-0.01491600	1.92065600
N	2.40686100	0.07878300	1.19631600
C	2.28599400	-0.16036100	-0.14585700
N	1.10270200	-0.18184600	-0.77221600
H	-0.93527000	0.06458500	-0.47945900
C	1.32215100	-0.09665400	3.38505600
C	2.43625200	-0.68053900	4.01383000
C	0.26321000	0.40432100	4.16422700
C	2.50518700	-0.73333500	5.40524200
H	3.24187900	-1.10582800	3.41618100
C	0.34200200	0.35583700	5.55317300
H	-0.59755100	0.84838500	3.66490300
C	1.46378900	-0.20729800	6.17553500
H	3.37526700	-1.18437200	5.88524400
H	-0.46987400	0.76581300	6.15691300
H	1.52295300	-0.23896800	7.26568500
C	3.49581500	-0.41012400	-0.93997900
C	4.62589000	-1.00603700	-0.35150400
C	3.52052400	-0.05928400	-2.30199100
C	5.77737200	-1.21808700	-1.10805800
H	4.60037500	-1.31673200	0.69275100
C	4.67638100	-0.26639500	-3.04963800
H	2.63630600	0.39556600	-2.74778000
C	5.80700600	-0.84016700	-2.45375500
H	6.65146700	-1.67663600	-0.64274100
H	4.70225500	0.02778300	-4.10058800
H	6.71304400	-0.99616700	-3.04337700
Ti	4.01636300	1.41329900	1.88238400

Cl	5.66903700	0.20405700	2.84451800
Cl	4.58536600	2.61132600	0.05480400
Cl	2.86092200	2.87628100	3.16917400
H	1.32481800	2.90570100	0.68047600
H	0.94254900	2.77727900	0.03347400
H	1.65593900	-2.93090400	0.59320200
H	1.32581800	-2.88193500	1.27793000

12.3. Linker-1- Ti Cl₃+ 3H₂

C	0.21853500	0.16707900	0.04916300
N	0.16482700	0.12518900	1.37944300
C	1.34801000	0.04891900	2.00248000
N	2.54040200	0.08502900	1.32845300
C	2.46364100	-0.09801800	-0.02576200
N	1.30673900	-0.02948100	-0.69746000
H	-0.72232500	0.33775000	-0.48390700
C	1.35173900	-0.07795800	3.46493000
C	2.40276700	-0.73958100	4.12501600
C	0.28812200	0.46186500	4.21161200
C	2.40611000	-0.83194800	5.51582900
H	3.21056900	-1.19381400	3.55216300
C	0.30184900	0.37336400	5.60070400
H	-0.52359300	0.96678000	3.68863900
C	1.36179200	-0.26793800	6.25487800
H	3.22755100	-1.34351600	6.02017800
H	-0.51240200	0.81282100	6.17996900
H	1.37027800	-0.33089500	7.34523600
C	3.68976800	-0.38549800	-0.77987900
C	4.75221400	-1.08002500	-0.17358000
C	3.80086600	0.03111000	-2.11892100
C	5.92194400	-1.32981400	-0.88930300
H	4.65915100	-1.43759100	0.85171800

C	4.97522300	-0.21411900	-2.82480900
H	2.97349800	0.56913500	-2.58061200
C	6.03780100	-0.88993100	-2.21123800
H	6.74288300	-1.86621300	-0.41066900
H	5.06886100	0.12990500	-3.85651700
H	6.95850000	-1.07624400	-2.76841300
Ti	4.20871800	1.29606800	2.11420200
Cl	5.73526400	-0.04963700	3.10171000
Cl	4.94306400	2.51595800	0.36283600
Cl	3.08429700	2.78813000	3.39497900
H	1.32929900	2.88727000	0.16242400
H	1.67116500	2.97776600	0.83783600
H	-0.03352000	1.01376700	-3.56274900
H	0.36977600	0.69998600	-2.99601800
H	1.42534900	-2.23862500	-2.14441600
H	1.50405400	-2.96171900	-2.37405800

12.4. Linker-1- Ti Cl₃+ 4H₂

C	0.16818900	0.72502100	0.11528300
N	0.11571900	0.59305200	1.44017400
C	1.28408600	0.32582300	2.03826000
N	2.46849500	0.27391500	1.35434500
C	2.36292900	0.19888900	-0.00821900
N	1.22025700	0.45188800	-0.65768200
H	-0.74879300	1.04411500	-0.39041200
C	1.28093800	0.07511100	3.48489200
C	2.23920700	-0.77619900	4.06433700
C	0.30575600	0.68389700	4.29564800
C	2.24156400	-0.98981200	5.44179300
H	2.97327000	-1.28243500	3.43776000
C	0.31928100	0.47311200	5.67161000
H	-0.43529500	1.33591800	3.83395100

C	1.28881500	-0.35841100	6.24702200
H	2.99088800	-1.64836400	5.88411000
H	-0.42345900	0.96477300	6.30270300
H	1.29794400	-0.51698600	7.32759800
C	3.53700700	-0.18750700	-0.79994000
C	4.50264400	-1.05688400	-0.26318400
C	3.68048500	0.29066600	-2.11543300
C	5.61134200	-1.42436400	-1.02398200
H	4.37672900	-1.46166500	0.74035100
C	4.79375500	-0.07478800	-2.86717500
H	2.92619600	0.96342200	-2.52226100
C	5.76142000	-0.92911700	-2.32253900
H	6.35642600	-2.09950900	-0.59996600
H	4.91390300	0.31221300	-3.88074400
H	6.63361200	-1.21184200	-2.91596700
Ti	4.24967700	1.20106800	2.25573500
Cl	5.64238500	-0.40221200	3.03412900
Cl	4.96988800	2.51959900	0.56049200
Cl	3.42131300	2.65135000	3.77522700
H	2.14943200	3.26140800	0.74713600
H	1.39156000	3.32189200	0.80385800
H	0.97741700	-2.45945100	0.98803300
H	1.23525000	-2.46193600	0.27113000
H	0.32987300	-0.51055200	-3.76627600
H	0.55982500	-0.29157600	-3.07205200
H	2.68589100	-2.45310800	-2.39703600
H	2.55407100	-3.20320400	-2.36237600

13. Geometries of linkers-1-VCl_x + nH₂

13.1. Linker-1-VCl₃+ H₂

C	-0.05152400	-0.02474600	-0.02328500
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N	-0.03359300	0.00069700	1.30909900
C	1.17294500	0.09160300	1.87576900
N	2.32342700	0.26871000	1.13816000
C	2.20394500	-0.11049000	-0.18125600
N	1.02042200	-0.20579800	-0.79404500
H	-1.02502100	0.04472600	-0.51797200
C	1.25413400	-0.03429600	3.33939200
C	2.38853400	-0.60209800	3.94632800
C	0.16886100	0.37472700	4.13575200
C	2.44892200	-0.72786200	5.33340300
H	3.22192400	-0.94683300	3.33538700
C	0.24017500	0.25560900	5.52122900
H	-0.71074300	0.80083600	3.65345200
C	1.38130200	-0.29065800	6.12316400
H	3.33543100	-1.16554600	5.79568400
H	-0.59446400	0.59451400	6.13821100
H	1.43456000	-0.37929900	7.21052500
C	3.40633800	-0.45670800	-0.95519400
C	4.52686600	-1.02194400	-0.32075400
C	3.41816500	-0.26369100	-2.34873100
C	5.65554600	-1.35855000	-1.06655500
H	4.51599500	-1.19998600	0.75385700
C	4.55265900	-0.59268100	-3.08597300
H	2.53899000	0.16262800	-2.83162400
C	5.67485200	-1.13566500	-2.44664400
H	6.52210000	-1.79250700	-0.56461600
H	4.56718900	-0.42109300	-4.16416300
H	6.56395300	-1.38939900	-3.02816600
Cl	5.52088900	0.44274400	2.72240000
Cl	4.52834700	2.51221700	-0.07807600
Cl	2.85972200	2.83965100	3.26046700
V	3.84327400	1.58816300	1.77243200

H	1.39269000	-2.78021700	1.39964300
H	1.73791400	-2.85285300	0.72434300

13.2. Linker-1-VCl₃+ 2H₂

C	0.08825200	-0.15331100	0.06274100
N	0.08105400	-0.11448900	1.39463100
C	1.28806100	-0.10943500	1.97547000
N	2.45215200	-0.05283000	1.25409300
C	2.33407000	-0.34934900	-0.08027700
N	1.15347400	-0.37180400	-0.70925800
H	-0.87599800	-0.03943300	-0.44306600
C	1.34547700	-0.17278600	3.44192000
C	2.42850200	-0.79259500	4.09063300
C	0.29429100	0.37063000	4.20232000
C	2.47111400	-0.84463400	5.48272600
H	3.22917400	-1.24183200	3.50447600
C	0.34823400	0.32480600	5.59302400
H	-0.54190800	0.84274000	3.68745500
C	1.43709400	-0.27797600	6.23511300
H	3.31483400	-1.32676600	5.97952200
H	-0.45789300	0.76673300	6.18177900
H	1.47708700	-0.30925900	7.32617800
C	3.53604800	-0.65995100	-0.86370100
C	4.64845300	-1.27018900	-0.25852000
C	3.56260200	-0.36597400	-2.23954300
C	5.78328000	-1.55946000	-1.01467200
H	4.61862400	-1.52786400	0.79899000
C	4.70263800	-0.64790300	-2.98686000
H	2.69173100	0.10252300	-2.69701300
C	5.81524600	-1.24067500	-2.37581600
H	6.64355400	-2.03274900	-0.53820800
H	4.72994200	-0.39932400	-4.04951200

H	6.70881200	-1.45791000	-2.96523800
Cl	5.58092200	0.17859100	2.79243700
Cl	4.26318200	2.45794600	0.02099200
Cl	2.82357000	2.78208700	3.13609300
V	3.91906100	1.30966100	1.90016500
H	0.67588600	2.72064900	0.32847600
H	1.39276700	2.72031900	0.06867300
H	1.62303500	-3.06606100	0.76644000
H	1.28341400	-2.98800600	1.44385200

13.3. Linker-1-VCl₃+ 3H₂

C	0.24863700	-0.66845400	0.20673900
N	0.26940800	-0.54935400	1.53420300
C	1.47434100	-0.32815800	2.07625500
N	2.59914400	-0.14583400	1.31402300
C	2.49726500	-0.53879700	0.00481200
N	1.31647700	-0.76789900	-0.58555500
H	-0.73393000	-0.73859700	-0.27068900
C	1.57634700	-0.28912200	3.53964600
C	2.75808200	-0.69694500	4.18411000
C	0.47485100	0.13787300	4.30402700
C	2.84361100	-0.65757400	5.57457400
H	3.60263200	-1.05408700	3.59640200
C	0.57073000	0.18443200	5.69211700
H	-0.43503900	0.45344200	3.79467900
C	1.75444800	-0.20926800	6.32892100
H	3.76332900	-0.97580000	6.06844600
H	-0.27753400	0.53585300	6.28249900
H	1.82618400	-0.16897000	7.41806800
C	3.71375800	-0.72849200	-0.79304100
C	4.91317700	-1.13571300	-0.18224800
C	3.67183100	-0.52465900	-2.18458400

C	6.06140500	-1.31547700	-0.95131200
H	4.94095700	-1.32268000	0.89025800
C	4.82491800	-0.69597400	-2.94542500
H	2.73649800	-0.20967500	-2.64623600
C	6.02094100	-1.08771200	-2.33071300
H	6.98889800	-1.63244500	-0.47137200
H	4.79587600	-0.51734800	-4.02193100
H	6.92399600	-1.21905000	-2.93093600
Cl	5.67255300	0.68500400	2.74784100
Cl	4.02067400	2.51366600	-0.17834400
Cl	2.50387800	2.82529300	2.89676800
V	3.86382000	1.47218100	1.77750900
H	1.94716400	-3.20529900	1.64335700
H	2.11820100	-3.28569900	0.90528700
H	1.54130700	-2.97959300	-1.96200100
H	1.66733400	-3.69500300	-2.19571300
H	-1.82391000	-1.63886400	2.65160600
H	-2.45308700	-1.97485500	2.92391000

13.4. Linker-1-VCl₃+ 4H₂

C	-0.07292200	-0.08274100	-0.06123600
N	-0.09299800	-0.04770700	1.27095900
C	1.10310200	0.03111400	1.86773500
N	2.26964600	0.15719200	1.15937400
C	2.18543600	-0.13762000	-0.17698700
N	1.01400000	-0.22976300	-0.81811600
H	-1.03749600	-0.03603000	-0.57665600
C	1.15495200	-0.03211400	3.33272800
C	2.27127900	-0.59065100	3.98184600
C	0.07883400	0.46241900	4.09218400
C	2.32383400	-0.62479600	5.37392800
H	3.09401500	-1.00682700	3.40067400

C	0.14248800	0.43280400	5.48231700
H	-0.78165500	0.89232600	3.58024200
C	1.26537100	-0.10520700	6.12455500
H	3.19721200	-1.05055300	5.86985300
H	-0.68200800	0.83902100	6.07123200
H	1.31344100	-0.11947600	7.21553300
C	3.41457500	-0.37476000	-0.94317900
C	4.54750300	-0.92900300	-0.32083500
C	3.45461400	-0.05619400	-2.31326000
C	5.71599100	-1.13320500	-1.05283900
H	4.51379000	-1.21113900	0.73107100
C	4.62753900	-0.25462100	-3.03566500
H	2.57137100	0.37146500	-2.78686700
C	5.76026700	-0.78823100	-2.40672800
H	6.59222100	-1.55873400	-0.56108200
H	4.66490500	0.01465800	-4.09289100
H	6.67955900	-0.93792400	-2.97715800
Cl	5.50053200	0.37071600	2.82520900
Cl	4.35974800	2.64275500	0.07723100
Cl	2.78504900	2.85614900	3.28260600
V	3.80606700	1.47322800	1.88154400
H	1.41367100	2.87552700	0.14166200
H	0.66538700	2.79099700	0.26049300
H	-2.47253200	-0.67884000	2.13498800
H	-3.19848000	-0.84189800	2.30599400
H	-0.05400300	-1.18723500	-3.85784900
H	0.26248600	-1.00336400	-3.18786600
H	4.30764300	1.90273300	5.62795200
H	4.65634400	1.75985200	6.29088900

14. Geometries of linkers-2-ScCl_x + nH₂

14.1. Linker-2-ScCl₃+ H₂

C	-0.06010900	-0.25853000	0.03176200
N	-0.05157900	-0.22874700	1.37498400
C	1.16289000	-0.18757600	1.90757600
N	2.32074500	-0.22236800	1.20899300
C	2.19448900	-0.37598400	-0.14119800
N	1.00484800	-0.34964500	-0.76129700
H	1.24846800	-0.09252900	2.99278600
H	-1.03907700	-0.21567000	-0.45658800
C	3.40647400	-0.55842400	-0.94991600
C	3.48088300	0.01385600	-2.23252600
C	4.50033100	-1.28329900	-0.44160900
C	4.65752000	-0.09375200	-2.96606600
H	2.62263100	0.56139100	-2.62276000
C	5.66778400	-1.39726600	-1.19190200
H	4.43105500	-1.78992700	0.52278400
C	5.77136000	-0.79319100	-2.45806100
H	4.72555100	0.37606100	-3.94954600
H	6.51269300	-1.95814500	-0.78785500
B	7.08148200	-0.89446700	-3.27536800
O	8.22335100	-1.56541700	-2.86586100
O	7.28496400	-0.32633700	-4.52401100
C	9.13687600	-1.39234400	-3.89012800
C	8.58264800	-0.66016100	-4.87029900
H	10.12076300	-1.83827700	-3.78058900
H	8.96480800	-0.31135300	-5.82483300
Sc	4.22524700	0.56808300	2.21992700
Cl	5.24968100	2.00036500	0.72551800
Cl	5.43009800	-1.22911800	3.04292700
Cl	3.15459300	1.70898000	3.92242500
H	2.39543500	2.67940900	0.29861100
H	1.63564900	2.67050600	0.23316400

14.2. Linker-2-ScCl₃+ 2H₂

C	-0.00080800	-0.02421600	0.01411700
N	0.00130600	-0.01563200	1.35772000
C	1.21331400	0.00042000	1.89697100
N	2.37341500	-0.03909700	1.20310800
C	2.25232600	-0.17099800	-0.14892100
N	1.06699200	-0.11738400	-0.77526200
H	1.29486500	0.07471200	2.98403500
H	-0.97663200	0.03925700	-0.47825000
C	3.46655800	-0.36348100	-0.95222200
C	3.57173800	0.24516600	-2.21554200
C	4.53123000	-1.13817900	-0.45595200
C	4.75235000	0.12331000	-2.94055700
H	2.73490300	0.83078000	-2.59707600
C	5.70212300	-1.26647000	-1.19871200
H	4.43298800	-1.67358100	0.48980400
C	5.83808400	-0.62683800	-2.44403300
H	4.84563200	0.62086400	-3.90820200
H	6.52434200	-1.86695700	-0.80491600
B	7.15302900	-0.74439200	-3.25127500
O	8.26864800	-1.46387500	-2.85176700
O	7.38796000	-0.14455000	-4.47942400
C	9.19824900	-1.28835000	-3.86105200
C	8.67814600	-0.50876600	-4.82317900
H	10.16630200	-1.76866500	-3.75586700
H	9.08150400	-0.14289100	-5.76248100
Sc	4.29291500	0.64440400	2.24979800
Cl	5.43976200	2.05076100	0.82174600
Cl	5.36625900	-1.24452100	3.05873600
Cl	3.25111600	1.80165400	3.95831700
H	2.64345600	2.86433200	0.27616200

H	1.88536700	2.88639500	0.19568800
H	2.36412200	-3.17016100	1.98581500
H	2.97124400	-2.86000800	2.32798000

14.3. Linker-2-ScCl₃+ 3H₂

C	-0.00624800	-0.02397400	0.00516800
N	-0.00139900	-0.00619000	1.34818800
C	1.21265100	0.01304900	1.88317900
N	2.37069600	-0.02142500	1.18739400
C	2.24916400	-0.15827900	-0.16109900
N	1.06089600	-0.11533400	-0.78486000
H	1.29405900	0.08097000	2.97113200
H	-0.98320600	0.02924500	-0.48615500
C	3.45670100	-0.35766400	-0.97470300
C	3.50470200	0.14896400	-2.28789200
C	4.55747100	-1.06857800	-0.46252000
C	4.65647700	-0.01375100	-3.04881800
H	2.63864600	0.67915500	-2.68480300
C	5.70325200	-1.23285300	-1.23723000
H	4.50198500	-1.55389600	0.51570300
C	5.77671800	-0.69970200	-2.53599300
H	4.70035800	0.40062400	-4.05827000
H	6.55357900	-1.78046500	-0.82715700
B	7.06224900	-0.85966800	-3.38222300
O	8.20611000	-1.52583900	-2.97141300
O	7.23872800	-0.35409000	-4.66150900
C	9.09342900	-1.41493300	-4.02672000
C	8.52221300	-0.72263200	-5.02594500
H	10.07402000	-1.86922400	-3.92207900
H	8.88250500	-0.42555200	-6.00613200
Sc	4.26457400	0.38808400	2.43010700
Cl	6.29008000	1.11399300	1.58394300

Cl	4.35860400	-1.74338000	3.32989600
Cl	3.28769000	1.90076400	3.88254700
H	3.78634400	2.55912900	0.31334200
H	3.24153700	2.74117800	0.81572600
H	1.82481600	-3.12313500	0.86629200
H	2.29916700	-2.92910600	1.43107100
H	5.74601100	2.64781800	-1.66855100
H	5.98636900	2.37027000	-1.00017300

14.4. Linker-2-ScCl₃+ 4H₂

C	0.04296800	-0.14772600	-0.37573100
N	-0.00292000	-0.10730000	0.96540400
C	1.18849100	-0.10315900	1.54984400
N	2.37325900	-0.18428500	0.90242500
C	2.29983600	-0.32876200	-0.45260900
N	1.13898300	-0.26858800	-1.12209000
H	1.23283400	-0.00585000	2.63694000
H	-0.91228200	-0.08645900	-0.90698300
C	3.54202200	-0.54635400	-1.20450500
C	3.71370300	0.04520500	-2.46854300
C	4.57569500	-1.32210500	-0.64838300
C	4.92737700	-0.09595900	-3.13293800
H	2.90610600	0.63793200	-2.89699800
C	5.78398400	-1.46336100	-1.32635800
H	4.42488000	-1.85384100	0.29266000
C	5.98448500	-0.84187900	-2.57225400
H	5.07055900	0.38695800	-4.10187700
H	6.58190300	-2.06035600	-0.88094600
B	7.33744200	-0.97639000	-3.31155900
O	8.42842000	-1.69380000	-2.84631400
O	7.63537000	-0.39629200	-4.53531700
C	9.40769900	-1.53723700	-3.81076000

C	8.93938100	-0.77052100	-4.80918100
H	10.36716500	-2.01948600	-3.65032700
H	9.39029500	-0.42057900	-5.73279100
Sc	4.29572300	0.48273600	1.98585900
Cl	5.12127000	2.10872800	0.57300500
Cl	5.76329300	-1.18952800	2.64170600
Cl	3.26186700	1.37589300	3.85445500
H	1.18039600	3.03383400	1.39626100
H	1.63117400	2.88293700	1.99191900
H	2.37619800	-2.36734900	3.27917400
H	3.12609000	-2.23900100	3.33300500
H	2.00747300	2.67559100	-1.30034700
H	2.67531100	2.69337000	-0.93300400
H	0.57354800	-0.54146600	-3.66468900
H	0.33599900	-0.56692700	-4.38964100

15. Geometries of linkers-2-TiCl_x + nH₂

15.1. Linker-2- TiCl₃+ H₂

C	-0.00338700	-0.00406300	0.00344200
N	-0.00273800	0.02088700	1.34651400
C	1.20875900	0.02400700	1.88479100
N	2.37123700	-0.04845300	1.19306900
C	2.24936500	-0.20750300	-0.15814500
N	1.06230400	-0.13580400	-0.78103100
H	1.29120700	0.11638200	2.97004900
H	-0.97631900	0.07816800	-0.49192700
C	3.44203400	-0.45653500	-0.97970300
C	3.51332900	0.09075300	-2.27353000
C	4.50492100	-1.23894300	-0.49278200
C	4.65654900	-0.10133500	-3.04234100

H	2.67764600	0.68179300	-2.64865000
C	5.63538600	-1.44170700	-1.27915900
H	4.43707800	-1.71482600	0.48618600
C	5.73762200	-0.86557700	-2.55916800
H	4.72126600	0.34794300	-4.03561800
H	6.45418500	-2.05353600	-0.89535800
B	7.00805000	-1.07047600	-3.41793500
O	8.11550900	-1.81214800	-3.03475600
O	7.20679500	-0.53887700	-4.68373100
C	9.00153900	-1.72117900	-4.09328300
C	8.46479000	-0.96884200	-5.06782300
H	9.95524800	-2.23336300	-4.00941500
H	8.83590500	-0.66441000	-6.04173000
Ti	4.17230300	0.59032500	2.25979400
Cl	3.21981300	1.82770800	3.91244200
Cl	4.99866100	-1.31880700	3.12339700
Cl	5.12896000	2.00249900	0.79298200
H	1.52298500	2.86304200	0.31605600
H	2.26216900	2.79811700	0.49119400

15.2. Linker-2- $\text{TiCl}_3 + 2\text{H}_2$

C	-0.15288600	0.06712100	-0.17142900
N	-0.19060600	0.04272500	1.17104000
C	1.00386600	-0.01281400	1.74303600
N	2.18307700	-0.09477200	1.08181600
C	2.09710300	-0.19451300	-0.27687800
N	0.93169500	-0.06375600	-0.93001700
H	1.05682600	0.03202700	2.83308300
H	-1.10849700	0.19369200	-0.69059000
C	3.30596200	-0.44282300	-1.07539800
C	3.44096800	0.17858200	-2.32991800
C	4.31911900	-1.29871300	-0.60724700

C	4.59951600	-0.01501700	-3.07518100
H	2.64243500	0.82623000	-2.69247000
C	5.46469500	-1.50202700	-1.37141300
H	4.19838400	-1.83273500	0.33556900
C	5.63190200	-0.85362300	-2.60918500
H	4.71438500	0.49077400	-4.03623900
H	6.24430400	-2.17171200	-1.00287500
B	6.91934000	-1.06083200	-3.44154300
O	7.98261000	-1.87138200	-3.07279400
O	7.17987200	-0.46288000	-4.66590300
C	8.90465100	-1.75506000	-4.09756200
C	8.43053000	-0.92286800	-5.03907800
H	9.83325100	-2.31207400	-4.01778400
H	8.84447700	-0.57663800	-5.98124500
Ti	3.97354600	0.35213900	2.24588500
Cl	3.04980100	1.53978800	3.94955400
Cl	4.59340400	-1.67609100	3.01778200
Cl	5.09820300	1.77667300	0.91958500
H	1.59721500	2.88785800	0.22318600
H	2.31912600	2.76844600	0.43743100
H	2.22720800	-2.99555400	1.71828000
H	1.66544600	-3.25042100	1.27008400

15.3. Linker-2- Ti Cl₃+ 3H₂

C	-0.33714600	-0.16630100	-0.09140200
N	-0.32060100	-0.15763900	1.25169800
C	0.89656200	-0.14683400	1.77699400
N	2.05041800	-0.19430900	1.07012400
C	1.91515300	-0.32837500	-0.28141600
N	0.72148600	-0.26609600	-0.89120300
H	0.99107400	-0.07224700	2.86256700
H	-1.31758500	-0.09713500	-0.57379100

C	3.10931900	-0.52975600	-1.11353300
C	3.19511400	0.10811900	-2.36324100
C	4.16904900	-1.33937600	-0.66602400
C	4.35731200	-0.01189200	-3.11918600
H	2.36018500	0.71791400	-2.70940800
C	5.31785500	-1.46827500	-1.44029900
H	4.08472600	-1.88906900	0.27177100
C	5.44083600	-0.79059100	-2.66711400
H	4.43766100	0.51351100	-4.07321100
H	6.13920700	-2.09222100	-1.08337700
B	6.74972100	-0.88083100	-3.48546200
O	7.88131000	-1.58294300	-3.09648500
O	6.97150200	-0.26091400	-4.70635200
C	8.80548300	-1.37603200	-4.10533200
C	8.26816000	-0.59502100	-5.05652900
H	9.78311900	-1.83823100	-4.00793100
H	8.66242400	-0.20978100	-5.99195800
Ti	3.88031400	0.35157600	2.12765900
Cl	2.97464100	1.55559600	3.82985500
Cl	4.61778000	-1.62194000	2.93287800
Cl	4.91290400	1.79099600	0.73814800
H	1.35858400	2.74050600	0.11441000
H	2.09032500	2.65838900	0.31223900
H	2.24694900	-3.07084800	1.79384300
H	1.67566900	-3.36098400	1.38047700
H	7.50483900	0.62051900	-0.44522100
H	8.04714900	0.21610700	-0.79684400

15.4. Linker-2- $\text{TiCl}_3 + 4\text{H}_2$

C	-0.06090100	-0.02389000	-0.00554900
N	-0.03234400	0.02412400	1.33654600
C	1.18940800	0.03870400	1.85095800

N	2.33655900	-0.04066000	1.13599700
C	2.18798700	-0.21245500	-0.20962800
N	0.98982500	-0.15664100	-0.81100400
H	1.29418000	0.14401200	2.93304300
H	-1.04489600	0.03990100	-0.48134600
C	3.37176800	-0.45133600	-1.04650900
C	3.45019400	0.14500600	-2.31723200
C	4.42384100	-1.26392100	-0.58796300
C	4.59846100	-0.02119600	-3.08602400
H	2.62030700	0.75667900	-2.67196800
C	5.55836100	-1.43852000	-1.37408700
H	4.34279500	-1.78342900	0.36708000
C	5.67436600	-0.80485300	-2.62445100
H	4.67293900	0.46982800	-4.05860400
H	6.37321600	-2.06645500	-1.00954600
B	6.96630000	-0.95090100	-3.46135400
O	8.09093000	-1.66049300	-3.06623500
O	7.17752000	-0.38113300	-4.70817700
C	9.00012600	-1.51008900	-4.09844200
C	8.46066100	-0.75428500	-5.06861400
H	9.97012100	-1.98812800	-4.00114500
H	8.84492500	-0.41224700	-6.02476400
Ti	4.18224600	0.50809300	2.16373900
Cl	3.30623000	1.77765800	3.83338700
Cl	4.88937700	-1.45490800	3.01965900
Cl	5.23352700	1.88584400	0.72663000
H	1.69792700	2.87358400	0.06689400
H	2.42871900	2.78438300	0.26519500
H	2.49865700	-2.90334800	1.91059000
H	1.92838700	-3.19337000	1.49582300
H	7.79827300	0.63400600	-0.47314700
H	8.32433000	0.20853500	-0.82454000

H	3.00456000	-3.38484500	-3.12092800
H	3.05780800	-2.62825200	-3.04414800

16. Geometries of linkers-2-VCl_x + nH₂

16.1. Linker-2- VCl₃+ H₂

C	-0.01566400	0.03085800	-0.01747700
N	-0.01237800	-0.00879700	1.32554900
C	1.19799900	-0.01910100	1.86263300
N	2.36237200	-0.06497600	1.16511600
C	2.23486800	-0.20089200	-0.18899500
N	1.04882600	-0.08248200	-0.80631900
H	1.28415100	0.03635900	2.94936000
H	-0.98728800	0.14938100	-0.50757700
C	3.41208000	-0.48919900	-1.02375000
C	3.49920800	0.07113500	-2.31025200
C	4.43203700	-1.34374000	-0.56521400
C	4.61572300	-0.18168000	-3.10158800
H	2.69510000	0.71598500	-2.66539400
C	5.53274500	-1.60839500	-1.37448700
H	4.35150600	-1.82386200	0.41104500
C	5.65215400	-1.02159600	-2.64874000
H	4.69223800	0.27686300	-4.08985000
H	6.31620400	-2.27822000	-1.01427500
B	6.89089200	-1.29765700	-3.53261500
O	7.95427000	-2.11533600	-3.17867400
O	7.10234400	-0.76411500	-4.79592600
C	8.82511900	-2.06971600	-4.25270000
C	8.32198500	-1.27135100	-5.20826500
H	9.74410700	-2.64489700	-4.19284800
H	8.69490000	-0.98009800	-6.18552900

Cl	3.24796400	1.72065900	3.81556300
Cl	4.53885900	-1.52869600	3.14881600
Cl	5.15861800	1.73775500	0.83065400
V	4.10391700	0.41167500	2.20879000
H	1.91237800	2.84661300	1.36992100
H	1.51763400	2.96764100	0.72868300

16.2. Linker-2-VCl₃+ 2H₂

(i)	C	-0.00572700	0.01524500	0.02060300
	N	-0.00231400	0.03436200	1.36343000
	C	1.20798000	0.03918000	1.90169600
	N	2.37259100	-0.02934000	1.20824200
	C	2.24978200	-0.17438700	-0.14501200
	N	1.06174100	-0.09876900	-0.76429100
	H	1.29206800	0.12512800	2.98686700
	H	-0.97975100	0.08898500	-0.47366200
	C	3.43540300	-0.41018100	-0.98513600
	C	3.50690500	0.19849400	-2.25082000
	C	4.47866500	-1.25087400	-0.55704100
	C	4.63058100	0.00748900	-3.04905500
	H	2.68495400	0.83271500	-2.58364400
	C	5.58705500	-1.45417600	-1.37404800
	H	4.40986200	-1.77316400	0.39726300
	C	5.69058100	-0.81839900	-2.62557900
	H	4.69403400	0.50375200	-4.01987600
	H	6.38847800	-2.11479400	-1.03709400
	B	6.93681000	-1.02713100	-3.51735300
	O	8.02276900	-1.82690000	-3.19220600
	O	7.13338200	-0.44211000	-4.76014800
	C	8.89208700	-1.71778300	-4.26286700
	C	8.36679000	-0.89970900	-5.18937800
	H	9.82684400	-2.26878100	-4.22296200

	H	8.73141600	-0.56284400	-6.15504200
	Cl	3.36525900	1.48508300	4.07360100
	Cl	4.46428300	-1.70842800	3.08210900
	Cl	5.13822000	1.75331000	1.00922200
	V	4.10594400	0.33064400	2.31079700
	H	2.37424500	2.79586900	0.51592400
	H	1.65501100	2.92178900	0.29671600
	H	1.65994700	-3.12120900	0.95785200
	H	2.17826000	-2.91347500	1.47699800
(ii)	C	0.14448200	0.37665900	-0.06700500
	N	0.16376700	0.37000000	1.26680800
	C	1.35801700	0.13501900	1.82528100
	N	2.50031000	-0.01170800	1.08047200
	C	2.31054300	-0.23880700	-0.25976200
	N	1.13921300	-0.00648800	-0.86679500
	H	-0.78951200	0.68723200	-0.54669100
	C	1.43046700	0.03388200	3.28850900
	C	2.39639800	-0.78423400	3.90165700
	C	0.51357500	0.74695800	4.08273100
	C	2.45823200	-0.87014500	5.29138800
	H	3.08953300	-1.35987400	3.28975700
	C	0.58752600	0.66441700	5.47061400
	H	-0.22962200	1.38017100	3.59953800
	C	1.56057200	-0.14001400	6.07698300
	H	3.21037400	-1.50700400	5.76017300
	H	-0.11112400	1.23525000	6.08519400
	H	1.61657000	-0.19971400	7.16615800
	C	3.41767200	-0.75456300	-1.07290900
	C	4.42271600	-1.55200200	-0.49627700
	C	3.46302100	-0.46085600	-2.44861300

C	5.47271100	-2.02653200	-1.27961500
H	4.37656000	-1.80580400	0.56171600
C	4.51923000	-0.93148600	-3.22371100
H	2.67691400	0.15481800	-2.88448900
C	5.52709200	-1.71001100	-2.64071700
H	6.25197400	-2.63969200	-0.82415400
H	4.56401900	-0.68470200	-4.28616800
H	6.35713900	-2.07235700	-3.25118100
Cl	5.63600500	-0.32280900	2.58876700
Cl	4.77535800	2.12514600	-0.18742700
Cl	3.31622600	2.72881500	2.87240200
V	4.19912200	1.07452500	1.68917400
H	-2.82620300	1.66423600	1.92164000
H	-2.15947000	1.29519200	1.87551900
H	7.95106600	0.23601200	-0.28654700
H	7.29108300	0.61768600	-0.27118100

16.3. Linker-2-VCl₃+ 3H₂

C	0.11166200	-0.18636200	-0.12221100
N	0.09780700	-0.13867800	1.21967200
C	1.30092900	-0.09879600	1.77188900
N	2.47537900	-0.16539000	1.09484600
C	2.37233100	-0.33866300	-0.25710000
N	1.19084800	-0.29427700	-0.89193500
H	1.37001700	0.01404700	2.85571800
H	-0.85743600	-0.14345600	-0.62965500
C	3.57079800	-0.57577000	-1.07883900
C	3.64964600	0.00840100	-2.35570300
C	4.61848000	-1.39653100	-0.62398700
C	4.78384700	-0.18556200	-3.13786900

H	2.82529500	0.62743000	-2.70942700
C	5.73838000	-1.60286100	-1.42450900
H	4.54430700	-1.90439000	0.33760800
C	5.84882100	-0.99029500	-2.68676000
H	4.85212900	0.29222700	-4.11759500
H	6.54308000	-2.24784800	-1.06581400
B	7.10746200	-1.20126100	-3.56038800
O	8.19916700	-1.98123600	-3.20757300
O	7.31130600	-0.63786800	-4.81198900
C	9.07938000	-1.88209900	-4.27026800
C	8.55502200	-1.08842600	-5.21828700
H	10.02018100	-2.42072600	-4.20914200
H	8.92669900	-0.76572800	-6.18610000
Cl	3.45984400	1.33882700	3.99830200
Cl	4.50202300	-1.86216300	3.00651900
Cl	5.26895000	1.59178600	0.95197200
V	4.19078900	0.18343500	2.23049100
H	1.54932200	2.82721600	2.44002400
H	0.99341900	3.01534400	1.95312900
H	2.20636700	2.70048900	-0.77417800
H	2.87941800	2.61872000	-0.42626700
H	2.25372600	-3.05244400	1.33636400
H	1.74966100	-3.24526100	0.79784700

16.4. Linker-2-VCl₃+ 4H₂

C	-0.29306100	0.28857100	-0.20843700
N	-0.36164200	0.12894200	1.12456800
C	0.81430300	-0.05292000	1.70386500
N	2.00590400	-0.11236600	1.06163200
C	1.94336300	-0.08847800	-0.29990200
N	0.79903300	0.16630300	-0.95535500
H	0.84233100	-0.14851900	2.79196100

H	-1.22762800	0.52340600	-0.72774100
C	3.14495300	-0.36266500	-1.09647000
C	3.32922400	0.30025000	-2.32529200
C	4.09580800	-1.30175000	-0.66098800
C	4.47645200	0.06292100	-3.07268300
H	2.57456300	1.01035200	-2.66417300
C	5.23480500	-1.54300200	-1.42488800
H	3.92663600	-1.87819900	0.24947300
C	5.45103000	-0.85805200	-2.63366100
H	4.63023200	0.59669100	-4.01297100
H	5.96844000	-2.27076400	-1.07493700
B	6.72863000	-1.11566800	-3.46673100
O	7.73324800	-2.00965700	-3.12665400
O	7.03888900	-0.48602000	-4.66382100
C	8.66905500	-1.91295500	-4.14048300
C	8.25916400	-1.01280600	-5.04907500
H	9.55784600	-2.53364900	-4.07913600
H	8.70294100	-0.65666500	-5.97382500
Cl	3.03611400	1.80395300	3.35516600
Cl	3.35470600	-2.07196600	3.04573300
Cl	5.85319400	0.09427800	1.82824200
V	3.72095200	0.01107000	2.31028300
H	1.65821300	2.82387800	0.91926600
H	1.26189300	2.93303800	0.27741200
H	1.08755400	-3.06648400	0.26068800
H	1.51638700	-2.97092600	0.88442500
H	4.16363000	2.66805700	-0.15077600
H	4.63704000	2.13583500	0.11948900
H	5.59403000	-3.27825100	1.57101100
H	6.00105300	-3.68194900	1.06806000

17. Geometries of linkers-3-ScCl_x + nH₂

17.1. Linker-3-ScCl₃+ H₂

C	-0.01582200	-0.05729000	-0.00551500
C	-0.01656200	-0.04192700	1.38672400
C	1.14060600	0.00697100	2.14197500
C	2.34099600	0.03965900	1.41409200
C	2.35236200	0.02364000	0.01251200
C	1.16336700	-0.02547800	-0.73214200
O	-1.31794000	-0.10526100	-0.48264400
B	-2.13189000	-0.11866500	0.62255600
O	-1.35973900	-0.08201800	1.81671200
H	1.11345900	0.01816500	3.22988300
H	3.28519500	0.07864400	1.95947200
H	3.30722600	0.05026700	-0.51548400
H	1.15505200	-0.03781800	-1.82196300
C	-3.65961700	-0.15775000	0.68308300
C	-4.32099200	-0.17192200	1.90298400
C	-4.49610900	-0.15824000	-0.46124600
C	-5.68105800	-0.18695900	2.11352100
C	-5.88349000	-0.17102600	-0.32069000
H	-4.03596600	-0.14321600	-1.45244700
C	-6.47377100	-0.18523500	0.95102500
H	-6.11565400	-0.19414800	3.11249300
H	-6.51718200	-0.16839000	-1.20973900
H	-7.56229800	-0.19327500	1.04965000
Sc	-2.11290000	-0.02787300	3.96329200
Cl	-0.83949700	-1.86135700	4.53667500
Cl	-4.11741600	-0.07849300	5.12701400
Cl	-1.00496700	1.94996800	4.37578000
H	-5.04000500	2.54597500	0.75777200
H	-4.76086600	3.21756200	0.98550100

17.2. Linker-3-ScCl₃+ 2H₂

C	-0.00288700	0.00821300	0.00221900
C	-0.00148300	0.00710900	1.39455100
C	1.15745400	-0.00028000	2.14860800
C	2.35741500	-0.00509600	1.41930500
C	2.36663700	-0.00281800	0.01760600
C	1.17585500	0.00372800	-0.72579800
O	-1.30652200	0.01249700	-0.47335800
B	-2.11889400	0.01243700	0.63294000
O	-1.34466300	0.01230800	1.82604100
H	1.13181800	-0.00146600	3.23662300
H	3.30301000	-0.01082900	1.96362600
H	3.32125500	-0.00666300	-0.51149100
H	1.16593400	0.00467700	-1.81567300
C	-3.64693000	0.00736900	0.69622500
C	-4.30602300	-0.00154300	1.91705100
C	-4.48478300	0.00437000	-0.44647900
C	-5.66582700	-0.01259000	2.12974100
C	-5.87200000	-0.00742800	-0.30400700
H	-4.02605800	0.01094300	-1.43836400
C	-6.46046900	-0.01584300	0.96848400
H	-6.09880200	-0.01955400	3.12937400
H	-6.50691400	-0.00893300	-1.19213100
H	-7.54877500	-0.02504600	1.06889700
Sc	-2.09574100	-0.00024500	3.97327500
Cl	-0.93921300	-1.93735500	4.44224500
Cl	-4.09958000	0.03495300	5.13937300
Cl	-0.86759200	1.87979200	4.49134600
H	-5.01084500	2.73135300	1.13271800
H	-4.76027600	3.40493300	0.87937000
H	-4.70634200	-3.35251400	1.01019200

H	-4.97604500	-2.73618600	0.65213000
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17.3. Linker-3-ScCl₃+ 3H₂

C	-0.00083000	-0.00017700	-0.00000900
C	-0.00084300	-0.00014600	1.39245000
C	1.15790000	-0.00044600	2.14688100
C	2.35854300	-0.00738200	1.41861900
C	2.36891400	-0.01199800	0.01701400
C	1.17853400	-0.00758800	-0.72692300
O	-1.30265400	0.01866600	-0.47732700
B	-2.11561300	0.04538600	0.62814300
O	-1.34395500	0.01289400	1.82266300
H	1.13200700	0.00115700	3.23486200
H	3.30366600	-0.00834900	1.96380800
H	3.32389600	-0.01694400	-0.51142700
H	1.16922500	-0.00647500	-1.81681200
C	-3.64234100	0.10658200	0.68843300
C	-4.30317000	0.16667200	1.90632800
C	-4.47634100	0.13159300	-0.45639300
C	-5.66125400	0.24345100	2.11538400
C	-5.86185000	0.20944500	-0.31857000
H	-4.01573800	0.09094300	-1.44658500
C	-6.45239200	0.26494200	0.95194700
H	-6.09574900	0.28675700	3.11334900
H	-6.49386600	0.22696500	-1.20862500
H	-7.53933200	0.32609300	1.04910600
Sc	-2.11385100	0.22561500	3.95016500
Cl	-0.83647100	-1.54725900	4.68607600
Cl	-4.11097800	0.22416200	5.12736700
Cl	-1.02504300	2.24407400	4.20270700
H	-4.88793500	2.93295900	0.64020800
H	-4.44310900	3.45666000	0.96942700

H	-4.90096000	-3.21844800	0.95454300
H	-5.26248800	-2.54946100	1.00929400
H	-1.36185700	2.83321800	0.55360900
H	-1.24914600	2.76942900	1.30542600

17.4. Linker-3-ScCl₃+ 4H₂

C	0.00218100	-0.00501200	-0.00075700
C	0.00156300	-0.00324900	1.39152300
C	1.15923100	-0.00742100	2.14729400
C	2.36059700	-0.01272900	1.42034200
C	2.37189400	-0.01382500	0.01863000
C	1.18224000	-0.01010700	-0.72659200
O	-1.29968100	-0.00211000	-0.47814400
B	-2.11251800	0.00027700	0.62760000
O	-1.34000000	0.00193700	1.82064100
H	1.13138700	-0.00634300	3.23522300
H	3.30537300	-0.01606800	1.96611500
H	3.32735600	-0.01794000	-0.50896700
H	1.17430500	-0.01146500	-1.81648800
C	-3.64015800	-0.00271800	0.69309200
C	-4.29673600	-0.01182300	1.91452400
C	-4.48080200	-0.00350300	-0.44679400
C	-5.65567500	-0.02273600	2.13170400
C	-5.86774100	-0.01415100	-0.30138100
H	-4.02418400	0.00250400	-1.43966100
C	-6.45337300	-0.02400700	0.97213400
H	-6.08621300	-0.03059300	3.13230100
H	-6.50457500	-0.01470600	-1.18815100
H	-7.54140700	-0.03269400	1.07558100
Sc	-2.11091100	0.01690600	3.94741900
Cl	-0.94373300	-1.91341900	4.43621800
Cl	-4.09820400	0.05437400	5.14087900

Cl	-0.89737500	1.92187300	4.42283800
H	-5.03098100	2.76042400	1.23771300
H	-4.62926600	3.31663200	0.90660100
H	-4.60690500	-3.36251800	0.97761100
H	-5.00419000	-2.74931700	0.76148800
H	-1.42441400	2.87426600	0.78465600
H	-1.29117500	2.73415100	1.52238800
H	-1.45655500	-2.87840600	0.79938000
H	-1.30483800	-2.73099000	1.53211700

18. Geometries of linkers-3-TiCl_x + nH₂

18.1. Linker-3- TiCl₃+ H₂

C	0.00365400	0.00057100	-0.00575800
C	0.01162500	-0.00012600	1.39051000
C	1.17363000	-0.00475400	2.13880500
C	2.37297700	-0.00851100	1.40685200
C	2.37561600	-0.00787700	0.00524200
C	1.18115000	-0.00339100	-0.73512100
O	-1.30389400	0.00592700	-0.47250100
B	-2.10360200	0.00947700	0.65100900
O	-1.31130600	0.00330400	1.81805300
H	1.14746100	-0.00645200	3.22764000
H	3.32200300	-0.01213100	1.94560800
H	3.32816900	-0.01085300	-0.52772400
H	1.17077800	-0.00269900	-1.82515000
C	-3.61373300	0.02423900	0.87805500
C	-4.02824200	0.03483600	2.24458500
C	-4.55987100	0.04215200	-0.15760700
C	-5.41112700	0.05712300	2.51263900
C	-5.92491000	0.06948700	0.13543800
H	-4.22142600	0.03756900	-1.19700400

C	-6.34447100	0.07482200	1.46889300
H	-5.77182700	0.06534800	3.54073300
H	-6.66043800	0.08646100	-0.67187700
H	-7.41145000	0.09502000	1.70464100
Cl	-1.49506800	-1.84104100	4.15126700
Cl	-3.94035900	0.12641800	5.48199200
Cl	-1.52686700	2.02503700	4.00009400
Ti	-2.56298800	0.07208800	3.75213900
H	-4.07535200	2.85502400	1.86620800
H	-4.27174800	3.49660100	1.50545000

18.2. Linker-3- $\text{TiCl}_3 + 2\text{H}_2$

C	-0.08995000	0.00086700	-0.04053100
C	-0.10850400	-0.00108600	1.35560500
C	1.03907300	-0.00229300	2.12582000
C	2.25204700	-0.00149000	1.41670700
C	2.28127900	0.00041900	0.01538200
C	1.10107800	0.00165400	-0.74752600
O	-1.38861500	0.00183700	-0.53197000
B	-2.20901700	0.00048800	0.57620300
O	-1.43932500	-0.00164700	1.75796000
H	0.99217300	-0.00370700	3.21394800
H	3.19069600	-0.00236000	1.97335300
H	3.24378000	0.00099800	-0.49940600
H	1.11129500	0.00318400	-1.83755000
C	-3.72333800	0.00069100	0.77505200
C	-4.16291400	0.00057700	2.13358000
C	-4.64971700	-0.00093500	-0.27819000
C	-5.55079900	-0.00146800	2.37570500
C	-6.02015800	-0.00308400	-0.01092100
H	-4.29094600	-0.00121900	-1.31070500
C	-6.46465900	-0.00342900	1.31450100

H	-5.93077400	-0.00164800	3.39683400
H	-6.74052400	-0.00489900	-0.83189200
H	-7.53600000	-0.00515700	1.53027400
Cl	-1.68088900	-1.92871800	4.02062500
Cl	-4.13766100	0.01165800	5.37175600
Cl	-1.67249500	1.93373300	4.01238400
Ti	-2.72520300	0.00383500	3.66980900
H	-4.24557500	-3.52816700	1.45252200
H	-4.27117000	-2.77808300	1.58384600
H	-4.25949400	2.78361500	1.65186200
H	-4.28230400	3.53419400	1.52305300

18.3. Linker-3- $\text{TiCl}_3 + 3\text{H}_2$

C	-0.00101000	-0.00343600	0.00082400
C	-0.00023300	-0.00063400	1.39700700
C	1.15752600	0.00149100	2.15163200
C	2.36086100	0.00129700	1.42633500
C	2.37098000	-0.00132000	0.02473900
C	1.18052300	-0.00395700	-0.72200100
O	-1.30521200	-0.01053200	-0.47315100
B	-2.11070100	-0.02171400	0.64561400
O	-1.32487700	-0.00433900	1.81763900
H	1.12521700	0.00223300	3.24029300
H	3.30697100	0.00275500	1.97019000
H	3.32639800	-0.00184300	-0.50308600
H	1.17609100	-0.00725600	-1.81206700
C	-3.62159000	-0.03559800	0.86740900
C	-4.03925900	-0.03905400	2.23276300
C	-4.56541800	-0.03870400	-0.16983400
C	-5.42290000	-0.04113300	2.49850400
C	-5.93138700	-0.04230200	0.12056800
H	-4.22492200	-0.03704600	-1.20851000

C	-6.35415000	-0.04197100	1.45297400
H	-5.78537000	-0.04329000	3.52595100
H	-6.66534200	-0.04457100	-0.68832800
H	-7.42178300	-0.04384700	1.68633700
Cl	-1.49639400	-1.97346800	4.04915700
Cl	-3.95867300	-0.09633800	5.46684000
Cl	-1.55625100	1.89653300	4.10198700
Ti	-2.57543000	-0.04752200	3.74115000
H	-4.43908700	-3.53880300	1.66984600
H	-4.36864000	-2.81242200	1.88816900
H	-4.12337300	2.76431100	1.85321400
H	-4.23258400	3.46271800	1.56917700
H	-1.25830000	-2.80846600	0.44718300
H	-1.32423000	-2.75507800	1.20464900

18.4. Linker-3- $\text{TiCl}_3 + 4\text{H}_2$

C	-0.20040100	0.01096000	0.07734800
C	-0.22580800	0.00725300	1.47318900
C	0.91736800	0.00547000	2.24957700
C	2.13425900	0.00764700	1.54732700
C	2.17083100	0.01137200	0.14617200
C	0.99467300	0.01310900	-0.62285900
O	-1.49462300	0.01193100	-0.42144300
B	-2.32133200	0.00891700	0.68145200
O	-1.55754500	0.00581400	1.86885100
H	0.86441400	0.00253200	3.33741400
H	3.06990300	0.00639700	2.10898700
H	3.13605500	0.01297600	-0.36350200
H	1.01089900	0.01599800	-1.71281800
C	-3.83596100	0.00859300	0.87682100
C	-4.27604100	0.00512500	2.23489400
C	-4.76285600	0.01161900	-0.17542100

C	-5.66367500	0.00472900	2.47855500
C	-6.13333300	0.01126700	0.09290500
H	-4.40569200	0.01423200	-1.20847600
C	-6.57784400	0.00780600	1.41824000
H	-6.04238900	0.00218800	3.50010500
H	-6.85406400	0.01368300	-0.72779000
H	-7.64910500	0.00755200	1.63423700
Cl	-1.79117700	-1.93562500	4.11712300
Cl	-4.24591600	-0.00283400	5.46790400
Cl	-1.79241100	1.93750200	4.12561200
Ti	-2.83469600	0.00140200	3.76386700
H	-4.68495600	-3.49321400	1.66018000
H	-4.62479000	-2.76326500	1.86949600
H	-4.63003700	2.77381400	1.88396200
H	-4.70586300	3.50065100	1.66897600
H	-1.47416800	-2.79857500	0.51643400
H	-1.55902100	-2.73562500	1.27123300
H	-1.56408800	2.75030100	1.28391200
H	-1.48497900	2.81594300	0.52871500

19. Geometries of linkers-3- $\text{VCl}_x + n\text{H}_2$

19.1. Linker-3- $\text{VCl}_3 + \text{H}_2$

C	0.08103300	0.27371200	0.02573600
C	0.04389100	-0.24855400	1.32214000
C	1.19770200	-0.52823700	2.03714800
C	2.41291900	-0.25814800	1.38762300
C	2.44941800	0.26459900	0.08593900
C	1.27287900	0.54309900	-0.62751900
O	-1.21136700	0.44820500	-0.42618600
B	-2.01782000	-0.00343200	0.60398600
O	-1.27612100	-0.41593000	1.70214100

H	1.15440900	-0.93784400	3.04656300
H	3.35012000	-0.46271000	1.90860000
H	3.41465100	0.45772900	-0.38583800
H	1.28297200	0.94544800	-1.64052000
C	-3.56911600	-0.00251900	0.57975700
C	-4.30230800	-0.21452300	1.76744200
C	-4.35281800	0.17828900	-0.56661900
C	-5.69642400	-0.10010600	1.78181200
H	-3.75460400	-0.43718400	2.68609400
C	-5.72174200	0.43859500	-0.58356400
C	-6.40792600	0.23073700	0.61993900
H	-6.23535100	-0.23117400	2.72277600
H	-6.24789100	0.70070400	-1.50192300
H	-7.49462800	0.33775000	0.64460000
V	-3.72660900	-0.88010400	-2.42253400
Cl	-5.59286600	-1.70162500	-3.27827600
Cl	-2.24291700	-2.41308000	-1.82015200
Cl	-3.13506700	1.12401800	-3.19343300
H	-2.39400100	2.81300000	-0.52479300
H	-2.64551900	3.37653500	-0.07746900

19.2. Linker-3-VCl₃+ 2H₂

C	0.00022200	0.00006500	-0.00013600
C	0.00012400	-0.00028500	1.39813000
C	1.17372900	-0.00056400	2.13535300
C	2.37009600	0.00030600	1.40043500
C	2.36967400	0.00281300	-0.00281000
C	1.17348500	0.00288700	-0.73750500
O	-1.30412300	-0.00244400	-0.45066700
B	-2.08009100	0.03126300	0.69409400
O	-1.30844600	0.00513400	1.84768500
H	1.15888500	0.00185200	3.22547200

H	3.32169100	0.00190500	1.93530700
H	3.32121700	0.00745700	-0.53771500
H	1.15521200	0.00908000	-1.82736900
C	-3.63181000	0.04174800	0.71360500
C	-4.33367200	-0.25371500	1.90290800
C	-4.44505100	0.35184300	-0.38216100
C	-5.72830900	-0.36221700	1.90643400
H	-3.76142700	-0.43183700	2.81629700
C	-5.81719700	0.12721600	-0.46737200
C	-6.47131700	-0.18285800	0.73130200
H	-6.24285000	-0.62918600	2.83211400
H	-6.36787400	0.27136400	-1.39727200
H	-7.55811400	-0.29068200	0.73899900
V	-3.84496900	2.08911000	-1.63390800
Cl	-5.70576600	3.23214700	-2.00033900
Cl	-3.37171800	0.55914300	-3.18224300
Cl	-2.24866800	3.20237500	-0.57453300
H	-4.52025600	-3.20278700	-0.32608700
H	-4.66916000	-2.70317200	0.22948700
H	-5.05390300	2.73014800	1.57044500
H	-5.45012600	2.98172200	0.96991900

19.3. Linker-3-VCl₃+ 3H₂

C	0.18007300	0.20320600	-0.09325200
C	0.12849600	-0.10395400	1.27006200
C	1.27137200	-0.18059200	2.05078500
C	2.48910800	0.06829500	1.39769100
C	2.53906200	0.37865000	0.02989800
C	1.37424200	0.45390100	-0.74976200
O	-1.10193000	0.20703000	-0.60008100
B	-1.92021200	-0.08343900	0.47635200
O	-1.19028300	-0.29122400	1.63990400

H	1.21778800	-0.41999200	3.11308000
H	3.41767800	0.02025600	1.96959400
H	3.50582900	0.56755200	-0.44043100
H	1.39412200	0.69676200	-1.81213600
C	-3.46446100	-0.19556300	0.41912600
C	-4.20026800	-0.35474600	1.61255300
C	-4.23386100	-0.14651200	-0.75303400
C	-5.58148000	-0.57315400	1.58409800
H	-3.66228900	-0.33498400	2.56314600
C	-5.57791900	-0.51600900	-0.84090100
C	-6.27144500	-0.65916400	0.36688700
H	-6.12096800	-0.72662000	2.52137800
H	-6.08669300	-0.61169100	-1.79992400
H	-7.34508300	-0.85922100	0.34879400
V	-3.66813900	1.15827300	-2.46366300
Cl	-5.56983300	1.74833900	-3.42279500
Cl	-2.84785600	-0.77359300	-3.25536300
Cl	-2.47036000	2.91553600	-1.85778900
H	-1.43055500	-2.49365700	-0.97503600
H	-1.24650100	-2.93094200	-0.37818400
H	-1.50810500	2.75353500	0.87824300
H	-1.29037700	2.57542400	1.58730100
H	-6.26943800	-1.94065000	-4.06528800
H	-5.54479500	-1.71119300	-4.00385400

19.4. Linker-3-VCl₃+ 4H₂

C	-0.02925100	-0.02250600	-0.02578900
C	-0.03212600	-0.00942300	1.36840100
C	1.14589000	0.00820400	2.09728600
C	2.33689100	0.01206500	1.35349500
C	2.32910200	-0.00134100	-0.04896800
C	1.12992100	-0.01920900	-0.77879000

O	-1.35812600	-0.03901200	-0.45369500
B	-2.13177500	-0.03591300	0.71722500
O	-1.33986200	-0.01744400	1.83925400
H	1.13733100	0.01828500	3.18720100
H	3.29129900	0.02575900	1.88295200
H	3.27653600	0.00210800	-0.59043600
H	1.09696200	-0.02978500	-1.86654400
C	-3.65853500	-0.05334800	0.57482700
C	-4.58038900	-0.05771600	1.65043000
C	-4.24057300	-0.06831800	-0.68232600
C	-5.95362500	-0.07515300	1.40908200
H	-4.18963900	-0.04721900	2.67101500
C	-5.57692000	-0.08481200	-1.00536500
C	-6.44994800	-0.08857100	0.09989900
H	-6.64996800	-0.07821500	2.25001600
H	-5.93594600	-0.09480900	-2.03238600
H	-7.52726000	-0.10206800	-0.08345700
V	-2.36047300	-0.06870400	-2.48387600
Cl	-4.00297700	-0.09499500	-3.99196000
Cl	-1.20280900	-1.94991700	-2.82131800
Cl	-1.22450000	1.81720300	-2.86670700
H	-3.69560600	2.92742700	-1.78930500
H	-4.32602400	2.95634600	-1.36162400
H	-1.27665900	-2.75332500	0.04010600
H	-1.33304400	-2.87304900	0.79134500
H	-1.33242600	2.68214600	-0.02500900
H	-1.39499500	2.81931400	0.72276200
H	-4.27354400	-3.12010300	-1.27285600
H	-3.64367200	-3.08558300	-1.70094400

20. Geometries of linkers-4-ScCl_x + nH₂

20.1. Linker-4-ScCl₃+ H₂

C	-0.00878400	-0.09053200	-0.00158500
C	-0.00816700	-0.06349000	1.40646200
C	1.18688400	-0.04432500	2.14011700
C	2.35787100	-0.05221900	1.40254200
C	2.35279600	-0.07749900	-0.03822400
C	1.11167600	-0.09879400	-0.79207900
O	-1.33783800	-0.10257300	-0.41838500
B	-2.09707300	-0.08314500	0.72785600
O	-1.27832700	-0.05884100	1.87742800
H	1.17895000	-0.02404100	3.22957000
H	3.30153600	-0.03768900	1.94627200
H	-3.28513700	-0.08602000	0.77486300
C	5.91185300	-0.03986000	-2.30161800
C	4.64540800	-0.07141400	-2.91679100
C	3.44517700	-0.08868300	-2.25370600
C	3.58168300	-0.07217700	-0.80794800
C	4.87563900	-0.04171500	-0.17451900
C	6.05026500	-0.02484400	-0.90615200
O	6.88990200	-0.02666100	-3.23886900
B	6.21304100	-0.05014200	-4.47729800
O	4.85049300	-0.07746400	-4.29452700
H	4.95295600	-0.03039700	0.91187800
H	7.03381300	-0.00075000	-0.43771700
H	6.77382000	-0.04631200	-5.52574000
Sc	1.33373200	-0.11447700	-3.03127300
Cl	0.75106900	1.94875400	-3.94515800
Cl	0.77876200	-2.18641200	-3.93262000
H	2.18770700	2.93419300	-1.55727000
H	2.57141200	3.12404100	-0.92571200

20.2. Linker-4-ScCl₃+ 2H₂

C	-0.02471300	0.00309300	-0.04458500
C	-0.02538200	0.02073400	1.36369000
C	1.16890400	0.03780700	2.09837400
C	2.34056900	0.03607300	1.36156400
C	2.33680100	0.01832000	-0.07903000
C	1.09648000	0.00112400	-0.83368300
O	-1.35339900	-0.01039400	-0.46270400
B	-2.11368800	-0.00077800	0.68309800
O	-1.29611100	0.01867800	1.83344200
H	1.16008800	0.05168900	3.18791500
H	3.28376900	0.04945200	1.90612900
H	-3.30179100	-0.00763400	0.72893300
C	5.89729500	0.01354400	-2.33938500
C	4.63085600	0.00398800	-2.95545400
C	3.43052300	0.00479300	-2.29292100
C	3.56585900	0.01751800	-0.84739700
C	4.85940600	0.02766400	-0.21318900
C	6.03488300	0.02558100	-0.94393400
O	6.87602400	0.00878300	-3.27615500
B	6.19972300	-0.00421000	-4.51490600
O	4.83665000	-0.00722100	-4.33310100
H	4.93608400	0.03651900	0.87327500
H	7.01832100	0.03265000	-0.47471500
H	6.76105100	-0.01135400	-5.56304700
Sc	1.32142000	-0.01836800	-3.07070100
Cl	0.73332300	2.03601700	-3.99951800
Cl	0.77350900	-2.10032800	-3.96182500
H	2.55687200	3.22297100	-0.98101800
H	2.17259400	3.03371200	-1.61243300
H	2.31954700	-3.03223400	-1.61589300
H	2.72297000	-3.20399200	-0.99147300

20.3. Linker-4-ScCl₃+ 3H₂

C	0.04154700	-0.03476600	0.01902000
C	0.03184800	-0.04207900	1.42665500
C	1.22148000	-0.05467500	2.16914200
C	2.39820500	-0.06010800	1.44042200
C	2.40374600	-0.05108000	-0.00008700
C	1.16807200	-0.03212800	-0.76189600
O	-1.28375300	-0.00633500	-0.40826300
B	-2.05165500	-0.00023400	0.73275600
O	-1.24184400	-0.02289300	1.88834800
H	1.20547900	-0.05872500	3.25869300
H	3.33784200	-0.07206200	1.99117000
H	-3.23986200	0.02035100	0.77051100
C	5.97495700	-0.06145400	-2.24320800
C	4.71211500	-0.04907800	-2.86506000
C	3.50937700	-0.03887200	-2.20759100
C	3.63696000	-0.05506900	-0.76160900
C	4.92726600	-0.06925800	-0.12132500
C	6.10589900	-0.07150100	-0.84701300
O	6.95833800	-0.04970400	-3.17523900
B	6.28800100	-0.02664700	-4.41691100
O	4.92385900	-0.02510800	-4.24144400
H	4.99876600	-0.07911200	0.96549600
H	7.08717700	-0.07956400	-0.37327800
H	6.85403600	-0.01158600	-5.46240700
Sc	1.41060900	0.10640700	-2.98853700
Cl	1.02858000	2.32013100	-3.61382400
Cl	0.70638600	-1.80360300	-4.12540900
H	1.19588000	3.18536300	0.12651400
H	1.12801600	2.98639900	-0.60663500
H	2.13882500	-3.01823700	-1.81516100
H	2.52014500	-3.24022400	-1.19290100

H	4.26935400	3.16842000	-1.73372600
H	3.65051800	2.97501200	-2.13536500

20.4. Linker-4-ScCl₃+ 4H₂

C	0.04413600	0.02408700	0.00195600
C	0.03537500	0.00018100	1.40931000
C	1.22524700	-0.03404100	2.15057200
C	2.40142100	-0.04543000	1.42069500
C	2.40569800	-0.02037800	-0.01927800
C	1.16985900	0.02332900	-0.77986700
O	-1.28124600	0.06770900	-0.42415800
B	-2.04825500	0.06816000	0.71768300
O	-1.23801800	0.02565100	1.87213100
H	1.21002600	-0.04905600	3.24003900
H	3.34164800	-0.07104400	1.97007200
H	-3.23622800	0.09871100	0.75637400
C	5.96961100	-0.08133400	-2.27288700
C	4.70701100	0.00499100	-2.88885700
C	3.50757100	0.02695700	-2.22645000
C	3.63752400	-0.03737700	-0.78268200
C	4.92819700	-0.11745400	-0.14766400
C	6.10368700	-0.14277700	-0.87805200
O	6.94895500	-0.09149000	-3.20894500
B	6.27551600	-0.00468000	-4.44655400
O	4.91397900	0.05883500	-4.26369900
H	5.00175400	-0.16664500	0.93800200
H	7.08503200	-0.20794400	-0.40887200
H	6.83785400	0.01207100	-5.49391700
Sc	1.41296800	0.15225700	-3.00734400
Cl	0.95784000	2.33439400	-3.69307800
Cl	0.84195700	-1.82767900	-4.10303400
H	1.10789800	3.27436200	0.02484000

H	1.04645300	3.05231000	-0.70216300
H	1.85551500	-2.97755900	-1.53524600
H	2.15612600	-3.21773800	-0.87687100
H	4.17412800	3.28453800	-1.84869100
H	3.56015600	3.06716200	-2.24542500
H	3.74382000	-2.79045800	-3.82157200
H	4.42039700	-3.12766300	-3.72159900

21. Geometries of linkers-4-TiCl_x + nH₂

21.1. Linker-4- TiCl₃+ H₂

C	0.01269200	-0.01119000	0.00376600
C	0.00982800	-0.00024600	1.40066900
C	1.19275500	0.01540900	2.12407800
C	2.39353200	0.01855600	1.39582500
C	2.41092800	0.00685300	-0.01093800
C	1.17891100	-0.00748500	-0.74421900
O	-1.29288400	-0.02585300	-0.44366400
B	-2.07587300	-0.02309900	0.70611100
O	-1.29237300	-0.00719100	1.85326100
H	1.18552600	0.02509600	3.21431700
H	3.33115300	0.03255400	1.95231800
H	-3.26604800	-0.03306600	0.70695000
C	5.90423500	-0.02903200	-2.46872700
C	4.62217000	0.00383600	-3.02158700
C	3.47255100	0.02048300	-2.24867100
C	3.65434600	0.00539900	-0.82672000
C	4.95119800	-0.02630400	-0.28341100
C	6.09674500	-0.04535800	-1.09564200
O	6.83723000	-0.04930300	-3.48342300
B	6.09653500	-0.03122700	-4.65859900
O	4.73035200	0.00128400	-4.39719300

H	5.08886500	-0.04304100	0.79813200
H	7.09948200	-0.07463300	-0.66850500
H	6.57022200	-0.04147800	-5.75038900
Cl	0.85254400	1.85749100	-3.69606000
Cl	0.97906800	-1.96405900	-3.63872100
Ti	1.50923400	-0.01951200	-2.74482400
H	3.74058200	-2.81880600	-2.11788700
H	4.26487300	-3.29505000	-1.83686900

21.2. Linker-4- $\text{TiCl}_3 + 2\text{H}_2$

C	0.09526500	-0.00039800	0.00704300
C	0.07947700	0.00260200	1.40391500
C	1.25568600	0.00648000	2.13836600
C	2.46319800	0.00732700	1.42133100
C	2.49348200	0.00438500	0.01478300
C	1.26836400	0.00029400	-0.73007100
O	-1.20614500	-0.00390100	-0.45257600
B	-1.99979400	-0.00301000	0.68992000
O	-1.22685900	0.00097400	1.84433400
H	1.23833900	0.00871200	3.22852400
H	3.39570100	0.01017600	1.98648800
H	-3.18994700	-0.00535800	0.67970300
C	6.00749400	0.00793000	-2.41327000
C	4.73000900	0.00113700	-2.97685900
C	3.57412700	-0.00043700	-2.21319000
C	3.74379700	0.00528400	-0.78960400
C	5.03603400	0.01212400	-0.23571300
C	6.18836000	0.01361800	-1.03856500
O	6.94921500	0.00809200	-3.41999800
B	6.21835000	0.00145800	-4.60138400
O	4.84933100	-0.00285800	-4.35117300
H	5.16515600	0.01667700	0.84696600

H	7.18783600	0.01903400	-0.60290400
H	6.70104000	-0.00030000	-5.68919100
Cl	1.04065700	1.91146400	-3.65726300
Cl	1.03812800	-1.91807400	-3.65284400
Ti	1.61642500	-0.00282100	-2.72776300
H	4.27823800	3.36148400	-1.80985600
H	3.80974800	2.82280500	-2.07623500
H	3.86039400	-2.79863800	-2.03479400
H	4.29234400	-3.38583700	-1.81286500

21.3. Linker-4- Ti Cl₃+ 3H₂

C	0.14632000	-0.04077900	-0.09569200
C	0.12357200	0.04509400	1.29815800
C	1.29602400	0.09122200	2.03679800
C	2.50722200	0.04650800	1.32735700
C	2.54453000	-0.03869200	-0.07593500
C	1.32316200	-0.08330700	-0.82544700
O	-1.15219400	-0.05712500	-0.56187300
B	-1.95193500	0.01834600	0.57417900
O	-1.18471900	0.08099400	1.73070000
H	1.27330700	0.16235100	3.12452600
H	3.43684500	0.08553900	1.89585500
H	-3.14191400	0.02691500	0.55715900
C	6.06958300	-0.13398500	-2.48537600
C	4.79418200	-0.14582800	-3.05472600
C	3.63439800	-0.11708600	-2.29675900
C	3.79909500	-0.07299500	-0.87305300
C	5.08877200	-0.06256500	-0.31328500
C	6.24424700	-0.09313800	-1.11045400
O	7.01578000	-0.16800900	-3.48682000
B	6.29056100	-0.20004000	-4.67131300
O	4.92058200	-0.18723400	-4.42770600

H	5.21308400	-0.03066800	0.76947200
H	7.24165600	-0.08515700	-0.67018300
H	6.77840400	-0.23448600	-5.75624200
Cl	1.09600600	1.79074400	-3.74921600
Cl	1.08007900	-2.03659800	-3.73046000
Ti	1.67571500	-0.12080500	-2.82016600
H	4.38925100	3.34157100	-2.09021800
H	4.22554300	2.60661700	-1.97349600
H	4.00031500	-2.85448400	-1.90512300
H	4.26891900	-3.56317300	-1.82552300
H	1.22785300	3.30094000	-0.04018600
H	1.30531600	2.72578500	-0.53363000

21.4. Linker-4- Ti Cl₃+ 4H₂

C	0.02940200	-0.00850100	0.00687600
C	0.02399300	-0.00323000	1.40315100
C	1.20576900	0.00454300	2.12830000
C	2.40835100	0.00691100	1.40292600
C	2.42849500	0.00164000	-0.00279100
C	1.19759400	-0.00638800	-0.73776700
O	-1.27426600	-0.01592900	-0.44380900
B	-2.06037000	-0.01493000	0.70473000
O	-1.27887100	-0.00712200	1.85325200
H	1.19651400	0.00867100	3.21855300
H	3.34472400	0.01301200	1.96150900
H	-3.25041900	-0.02011700	0.70262000
C	5.92009900	0.00674700	-2.46113200
C	4.63766300	-0.00143400	-3.01336300
C	3.48866400	-0.00333400	-2.23939900
C	3.67145900	0.00363500	-0.81746200
C	4.96840400	0.01185100	-0.27493800
C	6.11340200	0.01353300	-1.08814500

O	6.85271600	0.00657100	-3.47616500
B	6.11149000	-0.00186300	-4.65107600
O	4.74468500	-0.00691600	-4.38861200
H	5.10685000	0.01719300	0.80655900
H	7.11678500	0.01992800	-0.66161100
H	6.58445100	-0.00445800	-5.74311600
Cl	0.92584900	1.90119400	-3.64655300
Cl	0.94242100	-1.94419300	-3.62656000
Ti	1.52600800	-0.01421400	-2.73507700
H	4.29230500	3.35772500	-1.90249300
H	3.82167000	2.79835100	-2.11668000
H	3.85328800	-2.79825300	-2.09201000
H	4.32801100	-3.35428800	-1.87813300
H	1.15001100	3.35272600	0.14534100
H	1.15097000	2.78851800	-0.36648500
H	1.17042100	-2.80816100	-0.36725400
H	1.18242000	-3.35065900	0.16738700

22. Geometries of linkers-4-VCl_x + nH₂

22.1. Linker-4- VCl₂+ H₂

C	-0.01693800	-0.11613300	-0.03552800
C	-0.01743200	-0.06457600	1.36114000
C	1.16464000	-0.02372800	2.08635300
C	2.36838900	-0.03503300	1.36142400
C	2.37943900	-0.08520200	-0.04234300
C	1.15345100	-0.12858500	-0.78032100
O	-1.32139400	-0.14689600	-0.48012300
B	-2.10381500	-0.11321400	0.66987700
O	-1.31967700	-0.06264000	1.81512800
H	1.15304400	0.01654400	3.17593000
H	3.30741400	-0.00100700	1.91535800

H	-3.29397900	-0.12623400	0.67140600
C	5.76312900	-0.07144300	-2.62125400
C	4.45783500	-0.11995700	-3.11842800
C	3.34481800	-0.12878000	-2.29020300
C	3.59768600	-0.08524500	-0.88170100
C	4.91349800	-0.03728200	-0.39194200
C	6.01972500	-0.02966200	-1.25840200
O	6.65136800	-0.07336500	-3.67621700
B	5.86058600	-0.12338400	-4.81693100
O	4.50721400	-0.15286700	-4.49565600
H	5.09661500	-0.00317000	0.68280500
H	7.04204100	0.00832000	-0.88110200
H	6.28611700	-0.13920000	-5.92839200
Cl	0.83984000	1.72299800	-3.57891100
Cl	0.92559400	-2.16692900	-3.45595700
V	1.41889800	-0.18676300	-2.73995300
H	2.26728900	2.84846700	-1.21066900
H	2.64510700	3.15372100	-0.62381700

22.2. Linker-4-VCl₃+ 2H₂

C	0.03020200	-0.15975500	0.01540900
C	0.03444400	-0.24369700	1.41015600
C	1.21762800	-0.22991600	2.13453300
C	2.41778000	-0.12658400	1.41097000
C	2.42431300	-0.04375600	0.00884600
C	1.19706300	-0.06120100	-0.72825500
O	-1.27329400	-0.20747100	-0.42960700
B	-2.05101300	-0.31986300	0.71884600
O	-1.26421900	-0.34297000	1.86317800
H	1.20974600	-0.29960100	3.22265500
H	3.35779300	-0.11851400	1.96419100
H	-3.23931300	-0.38671900	0.71966600

C	5.79567500	0.25045100	-2.56938400
C	4.49277200	0.16571900	-3.06704800
C	3.38415600	0.06820500	-2.23891700
C	3.63901100	0.05261000	-0.83016500
C	4.95259000	0.13651900	-0.33997000
C	6.05419700	0.23877700	-1.20635500
O	6.67916600	0.34816000	-3.62365500
B	5.88754200	0.32333800	-4.76461900
O	4.53812900	0.21141400	-4.44374200
H	5.13718400	0.12991500	0.73503500
H	7.07461500	0.30913000	-0.82856700
H	6.30904600	0.38856200	-5.87574900
Cl	0.86771300	1.95470900	-3.41164300
Cl	0.99109200	-1.94804800	-3.49707500
V	1.45941300	0.00328100	-2.68702000
H	3.58576800	2.93353700	-2.07783800
H	4.16002800	3.34853800	-1.79681300
H	1.27554700	-2.92758000	-0.47903900
H	1.33437900	-3.34103700	0.15856900

22.3. Linker-4-VCl₃+ 3H₂

C	-0.08795400	-0.30967500	-0.17774200
C	-0.12787000	-0.27535900	1.21818000
C	1.02695200	-0.13345200	1.97374500
C	2.24458000	-0.02470400	1.28085500
C	2.29557800	-0.05877100	-0.12191200
C	1.09714100	-0.20603100	-0.89120200
O	-1.37151700	-0.45594200	-0.65682600
B	-2.18271700	-0.50930300	0.47296400
O	-1.43526800	-0.39987400	1.63843900
H	0.98451200	-0.10798600	3.06300100
H	3.16235800	0.08676300	1.85959000

H	-3.36601200	-0.63299200	0.44305100
C	5.72618100	0.26572600	-2.61637200
C	4.44594000	0.08089000	-3.14472500
C	3.31872500	-0.02953800	-2.34385300
C	3.52956800	0.05137300	-0.93005000
C	4.82066100	0.23603800	-0.40881300
C	5.94199900	0.34755200	-1.24830600
O	6.63583200	0.35108100	-3.64922700
B	5.88284400	0.21750500	-4.80863700
O	4.53186600	0.05010800	-4.51989200
H	4.97148700	0.30143600	0.66947000
H	6.94489200	0.49540100	-0.84672800
H	6.33487800	0.24207900	-5.90934900
Cl	0.74138800	1.67536800	-3.64662500
Cl	1.07035900	-2.22213600	-3.58107800
V	1.41450400	-0.21876400	-2.84087800
H	0.74989500	2.61718800	-0.58555400
H	0.70490300	3.07055100	0.02521500
H	3.39665600	2.85774000	-2.36218100
H	3.96061900	3.28288500	-2.07607100
H	1.42287800	-3.46795800	0.15266000
H	1.36548400	-3.00308300	-0.44858500

22.4. Linker-4-VCl₃+ 4H₂

C	-0.09552500	-0.19539600	-0.07884800
C	-0.12140200	-0.20681400	1.31793700
C	1.04435500	-0.12246800	2.06550000
C	2.25818800	-0.02710000	1.36392200
C	2.29500400	-0.01768600	-0.03965800
C	1.08533900	-0.10270100	-0.80035300
O	-1.38703200	-0.28454000	-0.54910300
B	-2.18820500	-0.35947300	0.58669600

O	-1.42693400	-0.30712900	1.74749700
H	1.01299800	-0.13108100	3.15540700
H	3.18423500	0.03914800	1.93641300
H	-3.37451300	-0.44960500	0.56506300
C	5.71092400	0.26352800	-2.55885300
C	4.41845700	0.15819400	-3.07933700
C	3.29512700	0.06397300	-2.27066000
C	3.52388400	0.07645700	-0.85701200
C	4.82707200	0.18136100	-0.34396700
C	5.94378300	0.27793700	-1.19124600
O	6.61326000	0.35075400	-3.59782800
B	5.84371000	0.29902700	-4.75295400
O	4.48950400	0.18046200	-4.45551100
H	4.99145900	0.19308900	0.73421700
H	6.95635000	0.36345400	-0.79590500
H	6.28584000	0.34876400	-5.85683300
Cl	0.76479900	1.92527500	-3.44924900
Cl	0.94433900	-1.97634600	-3.59137500
V	1.37913300	-0.03030200	-2.75168000
H	0.78019600	2.77722800	-0.37112800
H	0.78173100	3.02831200	0.34829500
H	-1.13920200	-3.13832900	0.93156900
H	-0.93787500	-3.05389700	0.20195500
H	3.55763800	2.86949300	-2.08070600
H	4.05911000	3.41017500	-1.88868400
H	2.20220500	-3.44772400	-0.34503000
H	1.95019900	-2.89914500	-0.80952300

23. Geometries of linkers-5-ScCl_x + nH₂

23.1. Linker-5-ScCl₃+ H₂

C	0.00883300	0.00112100	0.01061300
N	0.00438700	0.00255200	1.35764700
C	1.19294400	-0.00198200	1.95553300
N	2.37589200	0.04563900	1.27012200
C	2.27789200	-0.18073500	-0.07638500
N	1.11803200	-0.18856600	-0.72829900
C	1.24433000	-0.05554900	3.42579800
C	2.33406800	-0.66299100	4.07606400
C	0.20930000	0.51623800	4.18646000
C	2.40242500	-0.66952100	5.46921000
H	3.12263100	-1.14548200	3.49735400
C	0.28673200	0.51170100	5.57635200
H	-0.62859000	0.98736300	3.67296900
C	1.38424700	-0.07564700	6.21947300
H	3.25603200	-1.13554900	5.96402700
H	-0.50549800	0.97830200	6.16500200
H	1.44341400	-0.06963300	7.30998100
C	3.51330000	-0.42583200	-0.83789900
C	4.62536300	-1.02348100	-0.21821500
C	3.58806800	-0.05049100	-2.19109800
C	5.80653400	-1.21541100	-0.93446100
H	4.56731200	-1.35232600	0.81967200
C	4.77198200	-0.23893200	-2.89885200
H	2.72212800	0.41520300	-2.66110900
C	5.88360500	-0.81667500	-2.27163300
H	6.66622500	-1.67272200	-0.44196200
H	4.83569800	0.07527400	-3.94246000
H	6.81214000	-0.95625900	-2.82946400
C	-1.27540800	0.17618200	-0.69076300
C	-2.46413900	0.35966900	0.04111500
C	-1.32120200	0.17234400	-2.09796900
C	-3.67414800	0.54359100	-0.62537900

H	-2.42097600	0.35248500	1.12981100
C	-2.53440700	0.35676900	-2.75840400
H	-0.39783400	0.02141400	-2.65629400
C	-3.71204900	0.54363600	-2.02480900
H	-4.59299000	0.68647400	-0.05312600
H	-2.56431900	0.35420600	-3.84984800
H	-4.66181600	0.68773200	-2.54490300
Sc	4.06062800	1.36370000	2.09956000
Cl	4.72076200	2.57525100	0.24299900
Cl	3.08106200	2.82564600	3.59367900
Cl	5.73313500	0.04333000	3.04211500
H	1.73147200	2.85530800	0.31414400
H	1.00654900	2.74667000	0.52344500

23.2. Linker-5-ScCl₃+ 2H₂

C	0.01174900	0.00301200	0.00597600
N	0.01647600	-0.01497300	1.35159300
C	1.20736800	-0.01141800	1.94421200
N	2.38558100	0.05741200	1.25136400
C	2.28083900	-0.15594500	-0.09483900
N	1.11903000	-0.16341100	-0.74319200
C	1.26064500	-0.08780300	3.41293300
C	2.35538200	-0.69425200	4.05428800
C	0.21555300	0.45454600	4.18170100
C	2.41832300	-0.73079800	5.44708200
H	3.15376300	-1.15030800	3.46831500
C	0.28738600	0.42095600	5.57161500
H	-0.62678600	0.92505600	3.67499500
C	1.38950600	-0.16681900	6.20630200
H	3.27598400	-1.19673200	5.93504100
H	-0.51334000	0.86418300	6.16683800
H	1.44405400	-0.18483500	7.29696100
C	3.51743600	-0.38848200	-0.85836900

C	4.62192400	-1.00766600	-0.24545800
C	3.60337500	0.02071600	-2.20065200
C	5.80848900	-1.18460400	-0.95704500
H	4.55156000	-1.36834700	0.78133800
C	4.79248600	-0.15331500	-2.90324800
H	2.74263800	0.50166200	-2.66503000
C	5.89740200	-0.75047300	-2.28216400
H	6.66262400	-1.65797200	-0.47017200
H	4.86602100	0.18792500	-3.93766100
H	6.83014100	-0.87760600	-2.83586200
C	-1.27911300	0.16976300	-0.68525500
C	-2.46515400	0.32890400	0.05648900
C	-1.33432300	0.18116300	-2.09206900
C	-3.68199100	0.50382900	-0.59988300
H	-2.41422300	0.31020700	1.14469000
C	-2.55436000	0.35656600	-2.74240900
H	-0.41286300	0.04876200	-2.65826800
C	-3.72941000	0.51909700	-1.99895300
H	-4.59877100	0.62788300	-0.01998100
H	-2.59163100	0.36576600	-3.83359800
H	-4.68454900	0.65608000	-2.51107000
Sc	4.11116500	1.35414300	2.02044600
Cl	4.90159600	2.55463600	0.21378800
Cl	3.03028800	2.82607300	3.44040200
Cl	5.73216800	0.02847400	3.04328900
H	1.19120100	2.73537000	0.19139600
H	1.44208500	2.91600300	0.88819500
H	1.54224700	-2.90958400	1.21574400
H	1.40482400	-2.88970900	0.46697500

23.3. Linker-5-ScCl₃+ 3H₂

C	-0.00433100	0.00213800	0.01099800
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N	-0.00336300	0.01768500	1.35654300
C	1.18534900	0.01291100	1.95374700
N	2.36580300	0.05995800	1.26196200
C	2.26153500	-0.18122400	-0.07981300
N	1.10189400	-0.20225700	-0.73037000
C	1.23322700	-0.05369100	3.42284800
C	2.32144900	-0.66516100	4.07102000
C	0.18830100	0.49721400	4.18583700
C	2.37952700	-0.69650400	5.46397200
H	3.11793100	-1.13120100	3.49039400
C	0.25511300	0.46823200	5.57611100
H	-0.64774100	0.97232300	3.67462100
C	1.35155100	-0.12296100	6.21727600
H	3.23240100	-1.16624300	5.95663900
H	-0.54549000	0.91809000	6.16654600
H	1.40200800	-0.13702000	7.30820600
C	3.50058100	-0.42252500	-0.83662100
C	4.59838300	-1.04762600	-0.21790500
C	3.59641700	-0.00995300	-2.17707900
C	5.78879200	-1.22770400	-0.92243600
H	4.51926000	-1.41125700	0.80726300
C	4.78959400	-0.18666900	-2.87227700
H	2.74060200	0.47662900	-2.64481700
C	5.88793700	-0.79008700	-2.24564400
H	6.63786500	-1.70584100	-0.43140400
H	4.87152600	0.15753000	-3.90508100
H	6.82384500	-0.91911100	-2.79350000
C	-1.29005700	0.17747400	-0.68745000
C	-2.47443400	0.37717800	0.04726200
C	-1.34121300	0.15947100	-2.09428900
C	-3.68566000	0.56318800	-0.61647500
H	-2.42668100	0.38056700	1.13580300

C	-2.55577400	0.34551500	-2.75190400
H	-0.42089600	-0.00331400	-2.65440700
C	-3.72908700	0.54866600	-2.01570200
H	-4.60119500	0.71881000	-0.04224500
H	-2.59007400	0.33181100	-3.84314400
H	-4.67983300	0.69423100	-2.53359000
Sc	4.11818400	1.32524000	2.02166400
Cl	4.95986200	2.50450700	0.21881400
Cl	3.07814000	2.82689200	3.43916300
Cl	5.71189700	-0.01942200	3.06100700
H	2.12259000	2.87664300	-0.17590700
H	1.36615500	2.79762700	-0.12472100
H	1.35961900	-2.89060900	0.56499900
H	1.51489500	-2.89712500	1.31050000
H	0.33824600	3.17420000	2.38584800
H	-0.33991200	3.08946600	2.04741300

23.4. Linker-5-ScCl₃+ 4H₂

C	-0.05769200	0.01949300	0.06280600
N	-0.06281300	-0.02681300	1.40928600
C	1.12419600	-0.01074200	2.00962900
N	2.30657200	0.08378200	1.32970600
C	2.21474600	-0.10747100	-0.02271800
N	1.05726700	-0.11344400	-0.67824400
C	1.17022300	-0.09864000	3.47724400
C	2.24389600	-0.74572100	4.11476400
C	0.14538500	0.47830100	4.24718500
C	2.30715500	-0.78736700	5.50756900
H	3.02026000	-1.23508900	3.52556900
C	0.21839900	0.43947500	5.63684800
H	-0.67936200	0.98073800	3.74223900
C	1.30014800	-0.18802600	6.26856400

H	3.14780700	-1.28506800	5.99361300
H	-0.56492900	0.90987000	6.23429500
H	1.35565400	-0.20939500	7.35906700
C	3.45450700	-0.31916300	-0.78586900
C	4.55590700	-0.95729400	-0.18765000
C	3.54376100	0.12437100	-2.11711100
C	5.74237800	-1.12153600	-0.90193300
H	4.48444200	-1.34215600	0.83018500
C	4.73357100	-0.03577800	-2.82210800
H	2.68622400	0.62154400	-2.56916900
C	5.83502200	-0.65358400	-2.21546300
H	6.59368600	-1.61103700	-0.42614900
H	4.80980100	0.33183100	-3.84727700
H	6.76790300	-0.77071200	-2.77117800
C	-1.34475300	0.18459400	-0.63472200
C	-2.53474500	0.34907000	0.09978800
C	-1.39150000	0.19190000	-2.04199800
C	-3.74734500	0.52363600	-0.56455000
H	-2.49198800	0.33744800	1.18839400
C	-2.60748700	0.36633800	-2.70000200
H	-0.46670300	0.05560900	-2.60182100
C	-3.78658900	0.53319300	-1.96389700
H	-4.66711400	0.65218200	0.00955100
H	-2.63849200	0.37111500	-3.79140000
H	-4.73856600	0.66953000	-2.48201600
Sc	4.03403800	1.29695000	2.23032600
Cl	4.79495100	2.57536200	0.46080800
Cl	3.08912300	2.73272700	3.77663300
Cl	5.65158100	-0.11373600	3.13764600
H	1.54794500	2.81089100	-1.18985400
H	2.24333700	2.93091200	-0.90079300
H	1.67169800	-2.90457400	0.93811100

H	0.99543400	-2.84308300	1.28309500
H	0.84148000	3.06520800	1.99298100
H	0.26863700	2.93893800	1.50571000
H	-1.69125300	-2.59649200	2.78416400
H	-1.38576700	-1.94571300	2.52785000

24. Geometries of linkers-5-TiCl_x + nH₂

24.1. Linker-5- TiCl₃+ H₂

C	0.00457400	-0.05725200	0.01468000
N	0.00657700	-0.06585900	1.36054000
C	1.19538100	-0.05768700	1.95580200
N	2.37687700	0.00281700	1.26140400
C	2.27197100	-0.24616300	-0.08296400
N	1.10944000	-0.25279400	-0.72871500
C	1.23635300	-0.12246300	3.42553100
C	2.31629200	-0.73610700	4.08358800
C	0.18488400	0.43051400	4.17808100
C	2.35661800	-0.77320400	5.47715300
H	3.11989800	-1.19324400	3.50706000
C	0.23458800	0.39763600	5.56893700
H	-0.64500000	0.90818700	3.65802900
C	1.32114500	-0.20006600	6.22069700
H	3.20125600	-1.24787400	5.97940600
H	-0.57138200	0.84844000	6.15127500
H	1.35835100	-0.21914900	7.31212600
C	3.49606900	-0.52657700	-0.85045300
C	4.59609000	-1.15005900	-0.23565900
C	3.56572300	-0.17215100	-2.20938000
C	5.76023600	-1.39188200	-0.96434700
H	4.53899900	-1.45523600	0.80895900

C	4.73346000	-0.40885600	-2.92947700
H	2.70915000	0.31467300	-2.67482300
C	5.83317000	-1.01474800	-2.30823500
H	6.61084400	-1.87195500	-0.47758100
H	4.79371200	-0.11129100	-3.97815800
H	6.74903700	-1.19374500	-2.87576100
C	-1.28033900	0.13253700	-0.68056000
C	-2.46370200	0.32738300	0.05707000
C	-1.33200300	0.13373600	-2.08763100
C	-3.67427000	0.52711800	-0.60368000
H	-2.41535100	0.31695700	1.14550100
C	-2.54576900	0.33420900	-2.74231800
H	-0.41267700	-0.02627400	-2.65014200
C	-3.71804400	0.53201900	-2.00298700
H	-4.58898500	0.67900900	-0.02714900
H	-2.58041000	0.33545200	-3.83363100
H	-4.66831700	0.68860400	-2.51855100
Cl	4.59768000	2.49182800	0.13205400
Cl	2.82827300	2.82150500	3.21050700
Cl	5.58773800	0.08827400	2.96971100
Ti	3.97639300	1.31842100	1.96163400
H	0.87456200	2.69902000	0.06503600
H	1.32723600	2.81571100	0.66735800

24.2. Linker-5- Ti Cl₃+ 2H₂

C	0.01577000	-0.00896500	0.02563400
N	0.01598700	-0.01235500	1.37130800
C	1.20402900	-0.00161300	1.96782500
N	2.38579100	0.05915000	1.27545900
C	2.28300900	-0.19727000	-0.06689000
N	1.12186800	-0.20653300	-0.71487800
C	1.24321700	-0.06951100	3.43731500

C	2.31710300	-0.69574500	4.09323100
C	0.19565600	0.48897400	4.19106800
C	2.35562900	-0.73972600	5.48671600
H	3.11643200	-1.15764000	3.51458500
C	0.24381400	0.44945200	5.58182100
H	-0.62967000	0.97580800	3.67217900
C	1.32449400	-0.16080900	6.23180800
H	3.19542300	-1.22430300	5.98764700
H	-0.55871600	0.90458400	6.16554400
H	1.36037500	-0.18528300	7.32317500
C	3.50738400	-0.48879700	-0.82945400
C	4.59753600	-1.12384200	-0.20913900
C	3.58602200	-0.13748700	-2.18860500
C	5.76170000	-1.38018900	-0.93293600
H	4.53174600	-1.42693400	0.83554700
C	4.75391800	-0.38840300	-2.90365300
H	2.73655400	0.35789900	-2.65810200
C	5.84417200	-1.00586700	-2.27706900
H	6.60480300	-1.86941700	-0.44221900
H	4.82175500	-0.09323000	-3.95254900
H	6.76013000	-1.19624700	-2.84073500
C	-1.26878300	0.17356900	-0.67222700
C	-2.45374500	0.36782700	0.06288000
C	-1.31863900	0.16726400	-2.07929100
C	-3.66422700	0.55966400	-0.60040500
H	-2.40665300	0.36312800	1.15141400
C	-2.53230400	0.35985100	-2.73656500
H	-0.39795800	0.00770500	-2.63972400
C	-3.70625900	0.55713600	-1.99976700
H	-4.58023700	0.71113000	-0.02580800
H	-2.56555200	0.35529900	-3.82791800
H	-4.65645100	0.70750200	-2.51732900

Cl	4.61900600	2.52784300	0.14907800
Cl	2.85037200	2.86857600	3.22902400
Cl	5.59295000	0.11855500	2.99069800
Ti	3.99146600	1.35988200	1.98034500
H	0.88696800	2.75835200	0.08474000
H	1.35320000	2.87172900	0.67724900
H	1.50323900	-2.93031300	0.65759000
H	1.14403600	-2.86345300	1.32594500

24.3. Linker-5- $\text{TiCl}_3 + 3\text{H}_2$

C	0.01267700	-0.01075600	0.02688400
N	0.01177500	-0.00900100	1.37274100
C	1.20037400	-0.00266900	1.96949500
N	2.38203800	0.05170800	1.27792600
C	2.27996900	-0.20875700	-0.06437200
N	1.11855500	-0.21453900	-0.71238900
C	1.24186800	-0.07018600	3.43878000
C	2.31711400	-0.69769000	4.09209100
C	0.19769200	0.49060600	4.19515000
C	2.36009500	-0.73984700	5.48528800
H	3.11399800	-1.16182400	3.51145900
C	0.25041100	0.45274900	5.58583400
H	-0.62874200	0.97794400	3.67848600
C	1.33228900	-0.15819600	6.23291400
H	3.20088100	-1.22467600	5.98425800
H	-0.54935900	0.91001000	6.17165200
H	1.37192400	-0.18097700	7.32417400
C	3.50257300	-0.50941300	-0.82577700
C	4.59248500	-1.13974600	-0.20037100
C	3.57833200	-0.17630200	-2.19006900
C	5.75362800	-1.41015200	-0.92396200
H	4.52873200	-1.42844000	0.84821600

C	4.74327900	-0.44147600	-2.90468900
H	2.73167900	0.31859700	-2.66349000
C	5.83329700	-1.05467100	-2.27342500
H	6.59614100	-1.89629800	-0.42914700
H	4.80873400	-0.16068800	-3.95769900
H	6.74658700	-1.25669300	-2.83742800
C	-1.27034500	0.17387300	-0.67300300
C	-2.45023400	0.40606700	0.05943900
C	-1.32400700	0.13190100	-2.07934900
C	-3.65877400	0.60235700	-0.60596600
H	-2.40081600	0.42765600	1.14768100
C	-2.53600300	0.32814000	-2.73866200
H	-0.40846800	-0.05842600	-2.63807000
C	-3.70430700	0.56506600	-2.00480900
H	-4.57054500	0.78447600	-0.03353800
H	-2.57187800	0.29575900	-3.82942000
H	-4.65302800	0.71893600	-2.52402500
Cl	4.41691500	2.57113000	0.14653300
Cl	2.93655500	2.83775300	3.38501200
Cl	5.60946500	0.12569000	2.95173300
Ti	3.96453100	1.36553600	2.01193700
H	0.72232000	2.76732100	0.45247300
H	1.48025400	2.82647100	0.39831800
H	1.03416400	-2.84100800	1.33322500
H	1.53893900	-2.94890600	0.77309800
H	1.06379700	2.13604600	-2.34404400
H	1.28306800	2.59957300	-2.90732500

24.4. Linker-5- $\text{TiCl}_3 + 4\text{H}_2$

C	0.03543900	-0.00710700	0.00853700
N	0.03435400	-0.00996200	1.35367900
C	1.22191100	-0.00687000	1.95207000

N	2.40453200	0.05979300	1.26215100
C	2.30604100	-0.19150200	-0.08138300
N	1.14439200	-0.20368900	-0.72997600
C	1.26175900	-0.09074500	3.42037100
C	2.34231100	-0.71456800	4.06869200
C	0.21001600	0.44974200	4.18116000
C	2.38235600	-0.77379400	5.46130100
H	3.14656100	-1.16183200	3.48484900
C	0.25989900	0.39511100	5.57138500
H	-0.62041100	0.93451900	3.66853700
C	1.34655000	-0.21253800	6.21353800
H	3.22712700	-1.25573300	5.95632000
H	-0.54608200	0.83650100	6.16083800
H	1.38376100	-0.24864300	7.30451700
C	3.52996500	-0.47891300	-0.84451700
C	4.62119600	-1.11203100	-0.22449400
C	3.60548300	-0.13177500	-2.20530000
C	5.78326600	-1.37211300	-0.95017100
H	4.55645700	-1.41246400	0.82062100
C	4.77116000	-0.38712300	-2.92211400
H	2.75795300	0.36536800	-2.67478300
C	5.86234100	-1.00360900	-2.29621800
H	6.62678000	-1.86117100	-0.45998400
H	4.83604300	-0.09638900	-3.97241200
H	6.77620700	-1.19827500	-2.86186400
C	-1.24752000	0.17179300	-0.69184700
C	-2.43491300	0.35546800	0.04259500
C	-1.29542400	0.17256000	-2.09916700
C	-3.64547600	0.54379700	-0.62119300
H	-2.38953200	0.34424600	1.13114700
C	-2.50950800	0.36131300	-2.75671500
H	-0.37489900	0.02411500	-2.66198900

C	-3.68547700	0.54809200	-2.02069900
H	-4.56312900	0.68676300	-0.04707700
H	-2.54078200	0.36257400	-3.84806400
H	-4.63577900	0.69562800	-2.53885400
Cl	4.42381200	2.60261800	0.14810900
Cl	2.93791300	2.82781600	3.38801800
Cl	5.63253900	0.14062100	2.93345700
Ti	3.98062100	1.37739600	2.00271200
H	0.73306100	2.76817600	0.45403800
H	1.48940400	2.83180500	0.38439500
H	1.43249300	-2.90520900	1.27619100
H	1.46017300	-2.92213100	0.51513400
H	1.12119700	2.19780700	-2.31564000
H	1.27527500	2.62180400	-2.92930300
H	1.14702200	-2.30266900	-2.23705200
H	1.10634300	-2.98656400	-2.57349100

25. Geometries of linkers-5- $\text{VCl}_x + n\text{H}_2$

25.1. Linker-5- $\text{VCl}_3 + \text{H}_2$

C	0.00350700	0.00376900	-0.00776900
N	0.00697300	0.00589700	1.33850200
C	1.19576600	-0.00025100	1.93261200
N	2.37753900	0.04041300	1.23229800
C	2.26517400	-0.24210600	-0.10694500
N	1.10075400	-0.23135800	-0.74987400
C	1.23241400	-0.05837400	3.40229400
C	2.28997100	-0.70206700	4.06688000
C	0.18962200	0.52030200	4.14785200
C	2.31386500	-0.74983100	5.46039800
H	3.08730800	-1.17108100	3.49229600
C	0.22395300	0.47862400	5.53896400

H	-0.62145300	1.02289200	3.62184700
C	1.28647300	-0.15361300	6.19753700
H	3.13917900	-1.25092300	5.96929600
H	-0.57528300	0.94803100	6.11589900
H	1.31159400	-0.18157100	7.28918200
C	3.47467300	-0.58080900	-0.87434800
C	4.55233500	-1.23907000	-0.25676600
C	3.54502500	-0.26064300	-2.24162900
C	5.69303500	-1.55520900	-0.99347700
H	4.49279000	-1.50889100	0.79687700
C	4.69112400	-0.56948000	-2.96987200
H	2.70616400	0.25438900	-2.70873100
C	5.76742600	-1.21403700	-2.34749500
H	6.52579700	-2.06577700	-0.50658600
H	4.75183300	-0.29973800	-4.02605900
H	6.66602300	-1.45181800	-2.92110700
C	-1.27576300	0.22632200	-0.70273100
C	-2.45144100	0.46387800	0.03464900
C	-1.32911500	0.21886300	-2.10974500
C	-3.65582300	0.69732300	-0.62629700
H	-2.40168100	0.46003400	1.12304600
C	-2.53665300	0.45308400	-2.76467400
H	-0.41577900	0.02592300	-2.67169300
C	-3.70112300	0.69353000	-2.02558000
H	-4.56452500	0.88263000	-0.05000700
H	-2.57260100	0.44767400	-3.85594400
H	-4.64655000	0.87670500	-2.54132400
Cl	4.40212600	2.49005000	-0.02368700
Cl	2.69916300	2.88559800	2.94401600
Cl	5.44889800	0.21940000	2.85000700
V	3.88306100	1.36957900	1.81603800
H	1.08141700	2.87867100	0.55377000

H	0.76718100	2.78088000	-0.13417900
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25.2. Linker-5-VCl₃+ 2H₂

C	0.00389500	0.00197300	0.00670600
N	0.00430800	0.00790800	1.35177900
C	1.19320600	0.01196100	1.94806000
N	2.37386000	0.08173100	1.25174700
C	2.27003000	-0.19814300	-0.08896200
N	1.10746800	-0.21721000	-0.73223000
C	1.22884600	-0.07566700	3.41682700
C	2.29078600	-0.72793900	4.06694300
C	0.18159800	0.47711100	4.17467100
C	2.31397700	-0.80841800	5.45873700
H	3.09177100	-1.17772500	3.48162000
C	0.21571000	0.40325300	5.56488600
H	-0.63376300	0.98469100	3.66012500
C	1.28207100	-0.23633800	6.20919000
H	3.14214800	-1.31607200	5.95640800
H	-0.58736800	0.85314200	6.15195200
H	1.30693100	-0.28966600	7.29987300
C	3.48788200	-0.50264700	-0.85598000
C	4.57377100	-1.15042100	-0.24324400
C	3.55647800	-0.16321100	-2.21902000
C	5.72214600	-1.43808100	-0.98041900
H	4.51361000	-1.43571000	0.80595800
C	4.70954900	-0.44307600	-2.94723200
H	2.71051600	0.34456000	-2.68133400
C	5.79459900	-1.07823500	-2.32936400
H	6.56181300	-1.94107300	-0.49752100
H	4.76940800	-0.15847900	-3.99956200
H	6.69862400	-1.29376300	-2.90329200
C	-1.27718500	0.19796200	-0.69287400

C	-2.46018800	0.41107700	0.04030000
C	-1.32547700	0.18828200	-2.09993000
C	-3.66702800	0.61839600	-0.62493900
H	-2.41421700	0.40843400	1.12891800
C	-2.53544600	0.39634900	-2.75917700
H	-0.40614300	0.01483800	-2.65838100
C	-3.70735100	0.61255900	-2.02437100
H	-4.58150500	0.78449900	-0.05192400
H	-2.56744900	0.38960200	-3.85056400
H	-4.65465400	0.77520200	-2.54354400
Cl	4.19983600	2.60833200	0.07280800
Cl	2.70689500	2.88672400	3.16639800
Cl	5.46095600	0.27337300	2.83580400
V	3.82233100	1.42755900	1.92670900
H	1.32098400	2.84157400	0.06344000
H	0.56903600	2.82734700	0.18982200
H	1.13467500	-2.85072800	1.34686800
H	1.48221100	-2.91645700	0.67219100

25.3. Linker-5-VCl₃+ 3H₂

C	0.01557300	-0.00061400	0.00269600
N	0.01383200	-0.02143100	1.34862800
C	1.19957300	-0.00562100	1.94795600
N	2.38217800	0.08198200	1.25407100
C	2.28312300	-0.18136100	-0.08915800
N	1.12211400	-0.19146900	-0.73800900
C	1.23254500	-0.09674400	3.41560000
C	2.29841500	-0.74002500	4.06709300
C	0.17843200	0.44671000	4.17156000
C	2.31971900	-0.82092500	5.45892500
H	3.10406900	-1.18213200	3.48300500
C	0.21033300	0.37185900	5.56136200

H	-0.63924800	0.94892700	3.65539900
C	1.28131500	-0.25922500	6.20713900
H	3.15333600	-1.31779800	5.95800900
H	-0.59735100	0.81473000	6.14744000
H	1.30543600	-0.31140200	7.29786100
C	3.50445800	-0.47910700	-0.85497600
C	4.58614800	-1.13750100	-0.24467400
C	3.58134200	-0.12274900	-2.21275400
C	5.73784700	-1.41747800	-0.97908600
H	4.52019900	-1.43631200	0.80073600
C	4.73854100	-0.39501600	-2.93817900
H	2.73849300	0.39119700	-2.67398400
C	5.81898400	-1.03951300	-2.32292400
H	6.57373900	-1.92869900	-0.49826500
H	4.80446300	-0.09690100	-3.98639700
H	6.72606100	-1.24873800	-2.89430000
C	-1.26721500	0.19368500	-0.69413000
C	-2.45280500	0.38072900	0.04184800
C	-1.31470100	0.20829400	-2.10127000
C	-3.66147800	0.58646300	-0.62051200
H	-2.40718200	0.35979900	1.13024500
C	-2.52655400	0.41457500	-2.75762300
H	-0.39335500	0.05428700	-2.66217900
C	-3.70110400	0.60487700	-2.01984600
H	-4.57798100	0.73253500	-0.04529400
H	-2.55800000	0.42644600	-3.84898600
H	-4.64990400	0.76617300	-2.53670000
Cl	4.36975500	2.59638600	0.06209500
Cl	2.64447400	2.88030800	3.03396200
Cl	5.43649500	0.27401400	2.89466800
V	3.86521100	1.41797600	1.86629200
H	0.71754700	2.80243000	-0.05269000

H	1.03195700	2.89255700	0.63621300
H	1.19986400	-2.86807000	1.29186800
H	1.53992600	-2.91795000	0.61203600
H	4.40594200	1.89306800	6.12254400
H	4.03245500	2.06648300	5.48077700

25.4. Linker-5-VCl₃+ 4H₂

C	-0.00378500	-0.00498200	0.01131900
N	-0.00244300	-0.00022000	1.35648200
C	1.18659300	0.00005600	1.95231900
N	2.36723800	0.06679000	1.25514100
C	2.26194600	-0.20951000	-0.08628700
N	1.09895500	-0.22439200	-0.72888300
C	1.22334800	-0.08561300	3.42093600
C	2.28296400	-0.74179700	4.07110600
C	0.18152100	0.47703700	4.17896400
C	2.31017900	-0.81488700	5.46297700
H	3.07969700	-1.19902400	3.48582600
C	0.21954700	0.40963300	5.56944700
H	-0.63203500	0.98755000	3.66442200
C	1.28419000	-0.23287000	6.21349100
H	3.13875500	-1.32138800	5.96071800
H	-0.57871700	0.86762800	6.15681000
H	1.31352900	-0.27878400	7.30433700
C	3.47922700	-0.51219000	-0.85475200
C	4.56288700	-1.16755100	-0.24589000
C	3.55073600	-0.16076000	-2.21458400
C	5.71229700	-1.44957600	-0.98316800
H	4.50048900	-1.46203400	0.80060500
C	4.70506500	-0.43568500	-2.94281300
H	2.70651500	0.35255100	-2.67401700
C	5.78791900	-1.07762600	-2.32838800

H	6.55163600	-1.95461200	-0.50219600
H	4.76772100	-0.14126000	-3.99226500
H	6.69374700	-1.28700300	-2.90162100
C	-1.28514000	0.19325300	-0.68700900
C	-2.46751700	0.40586600	0.04737300
C	-1.33435900	0.18606800	-2.09408000
C	-3.67463600	0.61521400	-0.61670000
H	-2.42084900	0.40112500	1.13595900
C	-2.54461700	0.39618300	-2.75212600
H	-0.41554500	0.01288200	-2.65346800
C	-3.71586500	0.61192600	-2.01612300
H	-4.58863800	0.78085500	-0.04280300
H	-2.57737300	0.39136100	-3.84349700
H	-4.66340400	0.77613900	-2.53436800
Cl	4.20739900	2.58973600	0.08461900
Cl	2.73193400	2.85819600	3.19069100
Cl	5.45381400	0.22945700	2.83594200
V	3.82691300	1.39713700	1.93168300
H	0.57623000	2.81847900	0.22091900
H	1.32644900	2.83284200	0.08500400
H	1.13294600	-2.85974300	1.34172900
H	1.46395300	-2.92858800	0.65909600
H	7.65802700	1.28830200	-0.03546400
H	6.93360200	1.52508100	-0.01358800
H	4.60211900	1.72619800	6.17851200
H	4.20871800	1.91015800	5.55181600

26. Geometries of linkers-6-ScCl_x + nH₂

26.1. Linker-6-ScCl₃+ H₂

C	0.01177100	0.00883000	0.00087300
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C	0.01125400	0.00629700	1.39850600
C	1.18212500	-0.01179200	2.12198300
C	2.41068900	-0.02658000	1.41440900
C	2.41121400	-0.02419300	-0.01340100
C	1.18317300	-0.00675000	-0.72180800
O	-1.28815000	0.02580900	-0.45003300
B	-2.07241700	0.03367500	0.69896600
O	-1.28900500	0.02161100	1.84850700
H	1.13354800	-0.01636600	3.20810400
H	1.13538200	-0.00722800	-1.80797300
H	-3.26214400	0.04884400	0.69854600
C	6.17447100	-0.08313500	-2.03014800
C	4.97128800	-0.04168400	-2.76214700
C	3.72409800	-0.02017400	-2.14509800
C	3.68622000	-0.04098800	-0.74402400
C	4.94271300	-0.07934900	-0.01280000
C	6.24517800	-0.10241300	-0.66710700
O	7.22442400	-0.09250400	-2.94631000
B	6.64108300	-0.05720500	-4.19082900
O	5.23340600	-0.02520100	-4.09310500
H	2.83318300	0.01352200	-2.76734800
H	7.22049500	-0.05349300	-5.22924300
C	4.96876800	-0.05222100	4.16495100
C	6.17242700	-0.09341400	3.43372600
C	6.24413300	-0.10893400	2.07075800
C	4.94217200	-0.08242200	1.41552500
C	3.68515300	-0.04566500	2.14591200
C	3.72202900	-0.02807000	3.54706100
O	5.22992800	-0.03886000	5.49611300
B	6.63752200	-0.07251600	5.59479500
O	7.22172200	-0.10585600	4.35063500
H	7.21616300	-0.07162900	6.63364400

H	2.83070700	0.00517100	4.16875200
Sc	8.02705400	-0.12785500	0.70245400
Cl	9.09936000	1.94231900	0.70822500
Cl	9.09219100	-2.19748300	0.69652800
H	5.55756600	3.09122100	0.80324600
H	6.29806800	2.90886800	0.77972600

26.2. Linker-6-ScCl₃+ 2H₂

C	0.04195800	0.01267600	-0.00038500
C	0.04196600	0.01479900	1.39722800
C	1.21324300	0.01458900	2.12030600
C	2.44163700	0.01206400	1.41232500
C	2.44163000	0.00982600	-0.01549000
C	1.21323200	0.01022200	-0.72346800
O	-1.25824900	0.01359000	-0.45084800
B	-2.04213000	0.01629300	0.69842800
O	-1.25824000	0.01707800	1.84769600
H	1.16509200	0.01646900	3.20645100
H	1.16507100	0.00877100	-1.80961300
H	-3.23195800	0.01773000	0.69842500
C	6.20466900	0.00233300	-2.03301100
C	5.00071000	0.00147700	-2.76503600
C	3.75356300	0.00383000	-2.14780600
C	3.71655300	0.00714600	-0.74641500
C	4.97342800	0.00783800	-0.01546100
C	6.27550200	0.00561500	-0.67013000
O	7.25455700	-0.00039400	-2.94935300
B	6.67032000	-0.00284600	-4.19409700
O	5.26241400	-0.00171100	-4.09627300
H	2.86199200	0.00294200	-2.77001300
H	7.24956000	-0.00559000	-5.23261900
C	5.00074400	0.01331400	4.16185900
C	6.20469200	0.01228700	3.42981900

C	6.27551100	0.01089800	2.06693000
C	4.97343600	0.01043100	1.41227500
C	3.71656400	0.01192100	2.14324000
C	3.75359100	0.01320000	3.54463500
O	5.26246000	0.01454800	5.49309700
B	6.67036800	0.01432700	5.59090600
O	7.25459300	0.01296900	4.34615600
H	7.24961600	0.01518000	6.62942700
H	2.86202600	0.01408600	4.16685000
Sc	8.05570300	0.00944600	0.69833500
Cl	9.12294800	2.08174000	0.69299500
Cl	9.12696600	-2.06076100	0.70256000
H	5.56559300	3.19912400	0.67966600
H	6.30926500	3.02859800	0.67922000
H	6.31328700	-3.00335100	0.70693300
H	5.57017300	-3.17624700	0.70984200

26.3. Linker-6-ScCl₃+ 3H₂

C	-0.00795500	-0.01384500	-0.02230400
C	0.01214800	0.04705900	1.37387600
C	1.19333800	0.05023700	2.08059100
C	2.41106700	-0.00978900	1.35693700
C	2.39053100	-0.07203600	-0.06945400
C	1.15242000	-0.07371600	-0.76027800
O	-1.31418800	-0.00219200	-0.45493200
B	-2.08121500	0.06683900	0.70358100
O	-1.28112900	0.09794600	1.84119200
H	1.16095000	0.09897400	3.16623800
H	1.08875700	-0.11956000	-1.84466500
H	-3.27060400	0.09544500	0.71945600
C	6.12364400	-0.25041500	-2.13473200
C	4.91022600	-0.25846000	-2.84962900

C	3.67215800	-0.19943200	-2.21692800
C	3.65437200	-0.13311500	-0.81668800
C	4.92092000	-0.12606200	-0.10333200
C	6.21301400	-0.17676900	-0.77519000
O	7.16079600	-0.29846000	-3.06395200
B	6.55925500	-0.33785600	-4.30008000
O	5.15319700	-0.31374300	-4.18346200
H	2.77220500	-0.20612100	-2.82695300
H	7.12418500	-0.38688000	-5.34529200
C	5.00981800	0.04404600	4.06923500
C	6.20220200	-0.01163000	3.32185000
C	6.25234600	-0.05694100	1.95905000
C	4.94141400	-0.06371500	1.32271000
C	3.69592200	-0.00701500	2.07003800
C	3.75400500	0.04916000	3.46962700
O	5.29100300	0.10462600	5.39530300
B	6.69985500	0.08885900	5.47321600
O	7.26563500	0.01996200	4.22158800
H	7.29459600	0.13001700	6.50210200
H	2.87195200	0.09691800	4.10350200
Sc	8.00308100	0.00664600	0.56117500
Cl	8.72845700	2.22090900	0.45559900
Cl	9.33888600	-1.90467900	0.62599700
H	5.39356900	3.13333400	2.22629900
H	6.06095400	2.92407400	1.92225300
H	6.59674600	-3.08077600	0.73234500
H	5.85952200	-3.27571800	0.75322900
H	6.03137300	2.79899700	-1.00177700
H	5.35769200	2.98557000	-1.30673300

26.4. Linker-6-ScCl₃+ 4H₂

C	-0.02883200	0.01770600	-0.06250000
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C	-0.00784300	-0.00166400	1.33483400
C	1.17417500	-0.00722800	2.04037700
C	2.39164700	0.00683300	1.31427800
C	2.37031400	0.02689300	-0.11334500
C	1.13141400	0.03241900	-0.80289000
O	-1.33575900	0.01948900	-0.49337900
B	-2.10219800	0.00074700	0.66735500
O	-1.30108400	-0.01239800	1.80467600
H	1.14238600	-0.02243200	3.12704200
H	1.06719400	0.04786200	-1.88809900
H	-3.29189300	-0.00337500	0.68528300
C	6.10203200	0.09304500	-2.18577600
C	4.88800000	0.09134300	-2.89967000
C	3.65073700	0.06612200	-2.26491600
C	3.63362500	0.04326100	-0.86311200
C	4.90057700	0.03949600	-0.15090400
C	6.19229300	0.06036700	-0.82470700
O	7.13850900	0.11110800	-3.11618700
B	6.53612700	0.12266600	-4.35291700
O	5.13037300	0.11045100	-4.23476900
H	2.75013000	0.06691700	-2.87395400
H	7.10095200	0.14103500	-5.39913800
C	4.99413500	-0.02429700	4.02417800
C	6.18563200	-0.01253200	3.27428600
C	6.23389800	-0.00015300	1.91079500
C	4.92215800	0.01341200	1.27617300
C	3.67741400	-0.00060300	2.02603600
C	3.73704100	-0.02015300	3.42641700
O	5.27636800	-0.05067100	5.35113700
B	6.68546300	-0.05683000	5.42688400
O	7.25010700	-0.03488200	4.17298100
H	7.28121200	-0.07790200	6.45576400

H	2.85540300	-0.03286000	4.06257300
Sc	7.98351800	-0.07999300	0.51376000
Cl	9.25272800	1.87668400	0.55464400
Cl	8.76247600	-2.27791900	0.44743200
H	5.93423800	3.27827300	1.61141700
H	6.63543200	3.01309100	1.47068500
H	6.07711600	-2.98267500	1.89543200
H	5.40720900	-3.20001400	2.18790200
H	5.28172800	2.88592200	-1.13907700
H	4.62437400	3.10351600	-1.45714500
H	5.44239100	-3.15384400	-1.33040700
H	6.10491100	-2.93724400	-1.02093100

27. Geometries of linkers-6-TiCl_x + nH₂

27.1. Linker-6- TiCl₃+ H₂

C	-0.02853700	-0.04311700	0.01085100
C	-0.03610600	-0.07181500	1.41087500
C	1.12708200	-0.08980700	2.14005600
C	2.36382700	-0.07749100	1.44062100
C	2.37158400	-0.04729300	0.00678400
C	1.14244700	-0.03095400	-0.70586700
O	-1.33049500	-0.03211700	-0.44550500
B	-2.11700800	-0.05452600	0.69966400
O	-1.34291400	-0.07928600	1.85322300
H	1.07453400	-0.11458200	3.22594000
H	1.10162000	-0.00987500	-1.79233000
H	-3.30782200	-0.05268100	0.69327500
C	6.13880300	0.00439300	-2.00801200
C	4.94376500	0.02779900	-2.74472300
C	3.70645900	0.01210200	-2.14269300

C	3.64494400	-0.03159800	-0.72128700
C	4.86049400	-0.05844600	0.01053800
C	6.14698800	-0.03812700	-0.63109100
O	7.20245600	0.03503100	-2.88411700
B	6.63345000	0.07546300	-4.15371300
O	5.24611400	0.07155500	-4.09011200
H	2.81535900	0.03574000	-2.76632500
H	7.25803200	0.10903900	-5.16618500
C	4.90569800	-0.13440000	4.22075800
C	6.10833100	-0.14160100	3.49687500
C	6.13094300	-0.12366900	2.11969600
C	4.85217600	-0.09951000	1.46343100
C	3.62922300	-0.09785100	2.18223000
C	3.67536500	-0.11305500	3.60485100
O	5.19324200	-0.14621700	5.57004800
B	6.57971200	-0.15790600	5.64879700
O	7.16239100	-0.15498800	4.38445000
H	7.19346000	-0.16947500	6.66830400
H	2.77748800	-0.10612800	4.21911900
Cl	8.65720800	1.89851400	0.84561700
Cl	8.80075800	-1.91397900	0.70044800
Ti	7.62922900	-0.04890600	0.75568700
H	5.78252400	2.71469000	2.19213600
H	5.20411600	3.15543000	2.41973200

27.2. Linker-6- $\text{TiCl}_3 + 2\text{H}_2$

C	0.00187700	0.00978000	0.04689400
C	-0.00859600	-0.03822800	1.44637000
C	1.15307100	-0.05794800	2.17793700
C	2.39124700	-0.02883100	1.48154900
C	2.40198700	0.01952200	0.04824500
C	1.17434800	0.03912800	-0.66690500

O	-1.29912900	0.01990900	-0.41221600
B	-2.08801000	-0.02273900	0.73074700
O	-1.31632600	-0.05890100	1.88561300
H	1.09826300	-0.09460200	3.26337100
H	1.13579800	0.07565500	-1.75304100
H	-3.27880000	-0.02763200	0.72167100
C	6.17322200	0.09273000	-1.95796400
C	4.97981300	0.11719300	-2.69724700
C	3.74134900	0.09511600	-2.09792900
C	3.67695300	0.04702400	-0.67666000
C	4.89065400	0.02574200	0.05778600
C	6.17807500	0.04702400	-0.58126800
O	7.23881700	0.12187500	-2.83167200
B	6.67259900	0.16479600	-4.10254900
O	5.28515700	0.16256000	-4.04195200
H	2.85149800	0.11464500	-2.72348900
H	7.29945800	0.19907300	-5.11358500
C	4.92716800	-0.10268200	4.26655000
C	6.13124800	-0.06451400	3.54620700
C	6.15654400	-0.02040200	2.16966400
C	4.87934000	-0.01351500	1.51018400
C	3.65517300	-0.04597300	2.22569400
C	3.69825200	-0.09465300	3.64768900
O	5.21190800	-0.15029400	5.61565800
B	6.59815800	-0.14204900	5.69777200
O	7.18347200	-0.08963500	4.43557400
H	7.20984500	-0.17502300	6.71804000
H	2.79903500	-0.12631500	4.25920200
Cl	8.80045300	1.88374600	0.85811700
Cl	8.71686700	-1.93211400	0.78651100
Ti	7.65640100	-0.00106500	0.80672700
H	5.98039900	2.98955300	0.83688000

H	5.23568300	3.14940600	0.82541900
H	5.18035500	-3.31625400	2.53196600
H	5.69250300	-2.80725700	2.28843800

27.3. Linker-6- Ti Cl₃+ 3H₂

C	-0.00396900	0.04643500	0.05407400
C	-0.02848900	-0.01431900	1.45290500
C	1.12561100	-0.06620800	2.19479900
C	2.37046100	-0.05628900	1.50999000
C	2.39558900	0.00523300	0.07737800
C	1.17542300	0.05685900	-0.64877100
O	-1.30011000	0.08775600	-0.41676300
B	-2.10036200	0.05103900	0.71849900
O	-1.34036800	-0.01197300	1.87995500
H	1.05997500	-0.11363400	3.27921500
H	1.14777500	0.10248000	-1.73489900
H	-3.29084800	0.07113000	0.69850600
C	6.18623800	0.01439900	-1.89345300
C	5.00118200	0.08334400	-2.64259200
C	3.75695400	0.08492300	-2.05487800
C	3.67738700	0.01266100	-0.63555000
C	4.88292700	-0.05164000	0.10912800
C	6.17663500	-0.05256300	-0.51761700
O	7.26069100	0.04271100	-2.75574000
B	6.70800500	0.12691500	-4.03081300
O	5.32032600	0.15217500	-3.98297800
H	2.87408800	0.14335000	-2.68787600
H	7.34546400	0.17090200	-5.03474100
C	4.87922700	-0.20180600	4.31690400
C	6.09000800	-0.19553600	3.60741600
C	6.12833700	-0.14720200	2.23119800
C	4.85725400	-0.10494500	1.56080100

C	3.62661600	-0.10743700	2.26532900
C	3.65647100	-0.15825500	3.68740100
O	5.15071100	-0.25055500	5.66856900
B	6.53599500	-0.27178100	5.76330800
O	7.13343300	-0.23812400	4.50585000
H	7.13789500	-0.31365500	6.78897000
H	2.75159400	-0.16199200	4.29132100
Cl	8.65914400	1.87793900	0.96531000
Cl	8.79913500	-1.94950900	0.85573600
Ti	7.64112600	-0.07563000	0.88453400
H	5.68704500	2.63346200	2.55327700
H	5.17438900	3.10961700	2.85455500
H	5.12597600	-3.48045400	2.51071600
H	5.58528800	-2.90137000	2.32525400
H	5.79512700	2.77337600	-0.61548800
H	5.23313500	3.21128000	-0.88513600

27.4. Linker-6- Ti Cl₃+ 4H₂

C	-0.01684600	-0.00219800	-0.00567000
C	-0.01600500	-0.00801600	1.39469500
C	1.15150500	-0.00802800	2.11717600
C	2.38388700	-0.00183500	1.41018000
C	2.38303200	0.00414900	-0.02397000
C	1.14980100	0.00381700	-0.72952100
O	-1.32147700	-0.00379200	-0.45432000
B	-2.10114000	-0.01065100	0.69574300
O	-1.32009600	-0.01334700	1.84488600
H	1.10552000	-0.01285300	3.20363100
H	1.10253300	0.00810300	-1.81592200
H	-3.29195600	-0.01378500	0.69644800
C	6.13822800	0.02327000	-2.06155900
C	4.93952800	0.02331300	-2.79130900

C	3.70597800	0.01734500	-2.18170200
C	3.65191700	0.01068400	-0.75942300
C	4.87062700	0.01048600	-0.03462500
C	6.15310000	0.01713200	-0.68408300
O	7.19685100	0.03051700	-2.94301300
B	6.62078600	0.03481700	-4.21090400
O	5.23399100	0.03048800	-4.13900400
H	2.81135900	0.01800400	-2.80072800
H	7.24010200	0.04135500	-5.22697700
C	4.94366200	-0.00744900	4.17450500
C	6.14151300	-0.00264000	3.44334400
C	6.15479800	0.00296200	2.06582700
C	4.87149200	0.00352100	1.41789800
C	3.65363600	-0.00183200	2.14413900
C	3.70939300	-0.00719900	3.56632800
O	5.23970800	-0.01210600	5.52184100
B	6.62659700	-0.00986700	5.59214200
O	7.20117700	-0.00401000	4.32359600
H	7.24710100	-0.01261400	6.60750800
H	2.81549000	-0.01120300	4.18637100
Cl	8.71395200	1.94228700	0.69973800
Cl	8.73572900	-1.89677300	0.67721300
Ti	7.64274000	0.01650400	0.68985500
H	5.68967100	2.77937600	2.28857600
H	5.18795300	3.29015500	2.54873700
H	5.16793200	-3.29542600	2.56514900
H	5.63646300	-2.75792400	2.29701500
H	5.66306100	2.79135000	-0.90554700
H	5.15829300	3.29722400	-1.16940400
H	5.20983700	-3.28048900	-1.16487800
H	5.70589100	-2.75919700	-0.91486900

28. Geometries of linkers-6- $\text{VCl}_x + n\text{H}_2$

28.1. Linker-6- $\text{VCl}_3 + \text{H}_2$

C	0.03318600	0.02839300	-0.00020700
C	0.03335100	0.02745400	1.40035800
C	1.20000700	-0.00706400	2.12406500
C	2.43189600	-0.04205900	1.41788100
C	2.43172200	-0.04109300	-0.01836700
C	1.19967600	-0.00515400	-0.72422500
O	-1.27093000	0.06577300	-0.44929500
B	-2.05072400	0.08718400	0.70035900
O	-1.27066000	0.06419100	1.84980200
H	1.15538500	-0.00785000	3.21086700
H	1.15482000	-0.00436200	-1.81101800
H	-3.24111200	0.12112100	0.70052300
C	6.21105000	-0.13649400	-2.02128700
C	5.01860200	-0.09515700	-2.76452700
C	3.77373600	-0.06468600	-2.17494100
C	3.70053600	-0.07637300	-0.75339700
C	4.91212400	-0.11988100	-0.02266100
C	6.20568700	-0.15006300	-0.64118700
O	7.27719300	-0.15540700	-2.89151800
B	6.71617500	-0.12567000	-4.16524700
O	5.32950400	-0.08870800	-4.10912200
H	2.88914900	-0.03047200	-2.80794900
H	7.34709300	-0.13135700	-5.17434000
C	5.01937100	-0.09843600	4.16342100
C	6.21160900	-0.13992600	3.41985200
C	6.20587900	-0.15280500	2.03977700
C	4.91223600	-0.12150300	1.42158400
C	3.70087800	-0.07844900	2.15256800
C	3.77439900	-0.06746900	3.57411800

O	5.33062500	-0.09241500	5.50793800
B	6.71730000	-0.12966600	5.56369000
O	7.27797500	-0.15921600	4.28978600
H	2.88995700	-0.03321500	4.20732800
Cl	8.64740600	1.74545800	0.70281700
Cl	8.57548200	-2.14449600	0.69696600
V	7.66633600	-0.18342700	0.69932200
H	5.10493400	3.05231900	0.81828100
H	5.83132900	2.82275600	0.81090500
H	7.34848700	-0.13570100	6.57260800

28.2. Linker-6-VCl₃+ 2H₂

C	0.08110100	0.01348900	0.03656500
C	0.06969500	-0.02240600	1.43665500
C	1.23081700	-0.04090300	2.16976700
C	2.46895000	-0.02273600	1.47401000
C	2.48066700	0.01322400	0.03817600
C	1.25398900	0.03153500	-0.67757600
O	-1.21976900	0.02521500	-0.42315300
B	-2.00936700	-0.00419900	0.71962200
O	-1.23850600	-0.03373200	1.87510700
H	1.17733200	-0.06832900	3.25582500
H	1.21800500	0.05868300	-1.76436300
H	-3.20019500	-0.00395100	0.70993000
C	6.27856300	0.04613100	-1.93199000
C	5.09236400	0.07157100	-2.68531300
C	3.84184100	0.06436400	-2.10643200
C	3.75598000	0.02905600	-0.68587700
C	4.96142900	0.00857000	0.05454100
C	6.26023200	0.01553300	-0.55254500
O	7.35271700	0.06727000	-2.79179200
B	6.80259900	0.10412500	-4.07048900

O	5.41500500	0.10688400	-4.02662900
H	2.96221700	0.08557800	-2.74687500
H	7.44271900	0.12974000	-5.07338700
C	5.03522000	-0.08835500	4.23928800
C	6.23424600	-0.06514000	3.50554300
C	6.23982700	-0.03037200	2.12581100
C	4.95007300	-0.01944300	1.49805600
C	3.73219000	-0.03925800	2.21901200
C	3.79438500	-0.07565900	3.64067700
O	5.33557500	-0.12181400	5.58585900
B	6.72216500	-0.11795100	5.65288400
O	7.29360700	-0.08308600	4.38380000
H	2.90447000	-0.09384000	4.26683500
Cl	8.58979000	2.00325600	0.82886600
Cl	8.70795900	-1.89063300	0.77622800
V	7.71110000	0.02673200	0.79621800
H	5.23844400	3.21469100	-0.83866500
H	5.86810500	2.88541900	-0.56300100
H	5.24769000	-3.41399300	0.62283100
H	5.69023500	-2.79495200	0.65366200
H	7.34541500	-0.14171400	6.66644000

28.3. Linker-6-VCl₃+ 3H₂

C	-0.01595000	0.01728000	0.00066400
C	-0.01515500	0.02637600	1.40121600
C	1.15228800	0.02244900	2.12448600
C	2.38424800	0.00792300	1.41781000
C	2.38343500	-0.00138900	-0.01841000
C	1.15067200	0.00395900	-0.72381700
O	-1.32074500	0.02512700	-0.44791100
B	-2.10032700	0.03889000	0.70201200
O	-1.31944200	0.04006200	1.85112900

H	1.10824000	0.03124200	3.21128500
H	1.10538500	-0.00134400	-1.81058800
H	-3.29115600	0.04850300	0.70262200
C	6.16321700	-0.04398400	-2.02223000
C	4.97027100	-0.04864800	-2.76496300
C	3.72525800	-0.03646300	-2.17503900
C	3.65235300	-0.01621900	-0.75362100
C	4.86437400	-0.01291500	-0.02341800
C	6.15792400	-0.02801500	-0.64225700
O	7.22924400	-0.07047500	-2.89185800
B	6.66739600	-0.08929700	-4.16583400
O	5.28037600	-0.07549900	-4.10942700
H	2.83993700	-0.04512100	-2.80790500
H	7.29816100	-0.11340800	-5.17467600
C	4.97419900	-0.00398600	4.16183500
C	6.16630000	-0.00900800	3.41774200
C	6.15941800	-0.01091300	2.03770500
C	4.86519100	-0.00367300	1.42015900
C	3.65400300	0.00252900	2.15170600
C	3.72852000	0.00065400	3.57320100
O	5.28584800	-0.01344700	5.50617800
B	6.67294100	-0.02661600	5.56116900
O	7.23331700	-0.02432300	4.28641200
H	7.30485600	-0.03771200	6.56952000
H	2.84390600	0.00025500	4.20711800
Cl	8.65871800	1.81513800	0.68443100
Cl	8.43664800	-2.08278400	0.70958600
V	7.61557300	-0.08012300	0.69730800
H	5.12784100	3.19601800	0.68319400
H	5.83986900	2.92517500	0.68469700
H	5.68997900	-2.82518700	2.30009500
H	5.10246200	-3.18256600	2.62834700

H	5.68497500	-2.84393300	-0.87032600
H	5.09825700	-3.20811200	-1.19247400

28.4. Linker-6- $\text{VCl}_3 + 4\text{H}_2$

C	-0.01849600	-0.00590900	0.01185000
C	-0.01844600	-0.00347300	1.41246000
C	1.14861200	-0.00115800	2.13633500
C	2.38093200	-0.00127000	1.43020600
C	2.38088200	-0.00377000	-0.00607400
C	1.14851100	-0.00611300	-0.71211100
O	-1.32306000	-0.00786900	-0.43733300
B	-2.10330600	-0.00658100	0.71223300
O	-1.32297800	-0.00388000	1.86174200
H	1.10399200	0.00068300	3.22314200
H	1.10381600	-0.00804500	-1.79891500
H	-3.29416400	-0.00766300	0.71227800
C	6.16205200	-0.00390100	-2.00802000
C	4.96976400	-0.00627700	-2.75129100
C	3.72439800	-0.00635000	-2.16211600
C	3.65007500	-0.00391300	-0.74070100
C	4.86148200	-0.00155100	-0.00982400
C	6.15560200	-0.00146300	-0.62800200
O	7.22869800	-0.00450300	-2.87682000
B	6.66776900	-0.00725900	-4.15161300
O	5.28067100	-0.00838400	-4.09571800
H	2.83959600	-0.00824700	-2.79575500
H	7.29938300	-0.00849500	-5.16014300
C	4.97004400	0.00591000	4.17522100
C	6.16227700	0.00572500	3.43185600
C	6.15570500	0.00329200	2.05183700
C	4.86153300	0.00098500	1.43377200
C	3.65017700	0.00116200	2.16473600

C	3.72462200	0.00372500	3.58614600
O	5.28105900	0.00857900	5.51962600
B	6.66815900	0.00998100	5.57541100
O	7.22899300	0.00826100	4.30056800
H	7.29985800	0.01235700	6.58388500
H	2.83987100	0.00402800	4.21986200
Cl	8.53282200	1.96083700	0.70816500
Cl	8.53675500	-1.95426600	0.71528200
V	7.61349900	0.00235100	0.71186400
H	5.17058000	3.24274400	2.59528100
H	5.71464800	2.80189800	2.29488900
H	5.72235600	-2.79497800	2.30320000
H	5.18067600	-3.23816500	2.60446400
H	5.16913900	3.23535500	-1.18763200
H	5.71229900	2.79563900	-0.88396000
H	5.71989900	-2.80035600	-0.87369000
H	5.17939500	-3.24402800	-1.17634800

28. H₂ adsorption at three different binding sites in Linker-2

28.1 Linker-2-1H₂ at C₃N₃

C	-0.00716600	0.03544300	0.00083900
N	-0.00774300	0.04204100	1.34039800
C	1.22351400	0.03359600	1.86797100
N	2.37401900	0.02083300	1.19497000
C	2.24976500	0.01710900	-0.14768400
N	1.06488200	0.02264100	-0.79119100
H	1.29272300	0.03841000	2.96161500
H	-0.98494600	0.04184200	-0.49391300
C	3.48616100	0.01354800	-0.96256800
C	3.41075400	0.01427600	-2.36753100
C	4.74754800	0.01187600	-0.33925300

C	4.57581500	0.01336000	-3.12970200
H	2.42902800	0.01590100	-2.84097800
C	5.90735900	0.01095600	-1.10937500
H	4.79554200	0.01162400	0.74961600
C	5.84476400	0.01171400	-2.51707900
H	4.50895700	0.01409000	-4.22017400
H	6.88310900	0.00978200	-0.61794000
B	7.13428300	0.01096900	-3.36678100
O	8.42760400	0.00938400	-2.85726200
O	7.17650800	0.01179100	-4.75620200
C	9.25890800	0.00926300	-3.96255700
C	8.52016100	0.01068500	-5.08385000
H	10.33225000	0.00811100	-3.79782500
H	8.79238100	0.01108100	-6.13508600
H	1.71812200	2.91403800	0.67303900
H	1.28866900	2.92475800	0.04420000

28.2 Linker-2-1H₂ at C₆H₄

C	-0.00012200	0.00030500	0.00008800
N	-0.00004800	0.00073900	1.33989100
C	1.23151600	0.00067800	1.86744400
N	2.38189600	0.00057100	1.19408000
C	2.25686000	0.00073100	-0.14870100
N	1.07175500	0.00019400	-0.79229600
H	1.30096700	0.00076100	2.96108200
H	-0.97809500	0.00001000	-0.49432000
C	3.49339200	0.00254700	-0.96422200
C	3.41751200	0.00667400	-2.36903700
C	4.75487400	0.00644000	-0.34111900
C	4.58235400	0.01588500	-3.13154400
H	2.43571400	0.00582300	-2.84220200
C	5.91452500	0.01576600	-1.11168500

H	4.80321100	0.00553400	0.74768200
C	5.85139700	0.02126000	-2.51938200
H	4.51510700	0.02195700	-4.22188800
H	6.89031600	0.02205800	-0.62054300
B	7.14060600	0.03950700	-3.36945500
O	8.43368600	0.04956000	-2.86011100
O	7.18207100	0.04968800	-4.75860800
C	9.26464600	0.06698300	-3.96558000
C	8.52554900	0.06693900	-5.08666500
H	10.33795400	0.07747800	-3.80103600
H	8.79730100	0.07782300	-6.13795500
H	4.70011700	2.69572200	-1.63514600
H	4.60851000	3.45175500	-1.67433500

28.3 Linker-2-1H₂ at BO₂C₂

C	0.02116900	0.05957500	-0.00872500
N	0.02299000	0.07661100	1.33101200
C	1.25505800	0.05199100	1.85692900
N	2.40405100	0.01414600	1.18245700
C	2.27747000	0.00016500	-0.16034600
N	1.09139700	0.02219500	-0.80229000
H	1.32609000	0.06415100	2.95043000
H	-0.95723800	0.07820000	-0.50199300
C	3.51222600	-0.04188000	-0.97713300
C	3.43436100	-0.05806700	-2.38194400
C	4.77443400	-0.06592300	-0.35578700
C	4.59777200	-0.09760200	-3.14563300
H	2.45214600	-0.03902000	-2.85403800
C	5.93238300	-0.10539100	-1.12773400
H	4.82453600	-0.05296900	0.73293000
C	5.86723400	-0.12204600	-2.53502200
H	4.52908100	-0.10951600	-4.23593500

H	6.90877100	-0.12345200	-0.63787500
B	7.15449100	-0.16178400	-3.38650000
O	8.44836200	-0.18674600	-2.87882600
O	7.19377400	-0.18091600	-4.77591200
C	9.27693800	-0.21243500	-3.98533100
C	8.53626900	-0.20898200	-5.10533100
H	10.35046300	-0.23116300	-3.82308000
H	8.80717200	-0.22399700	-6.15676900
H	7.58667000	2.64119500	-4.11285300
H	8.00248600	2.63459400	-3.47500600