Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Hydrogen Sorption Efficiency of Titanium Decorated Calix[4]pyrroles

Sandeep Kumar, Rohit Y. Sathe, and T. J. Dhilip Kumar*
Department of Chemistry
Indian Institute of Technology Ropar
Rupnagar 140001, India
*Email- dhilip@iitrpr.ac.in

Figure S1: Optimized geometries: (a) MeCXP, (b) MeCXP-Ti_4, (c) MeCXP-Ti_4-$4H_2$, (d) MeCXP-Ti_4-$8H_2$, (e) MeCXP-Ti_4-$12H_2$ and (f) MeCXP-Ti_4-$16H_2$ systems.

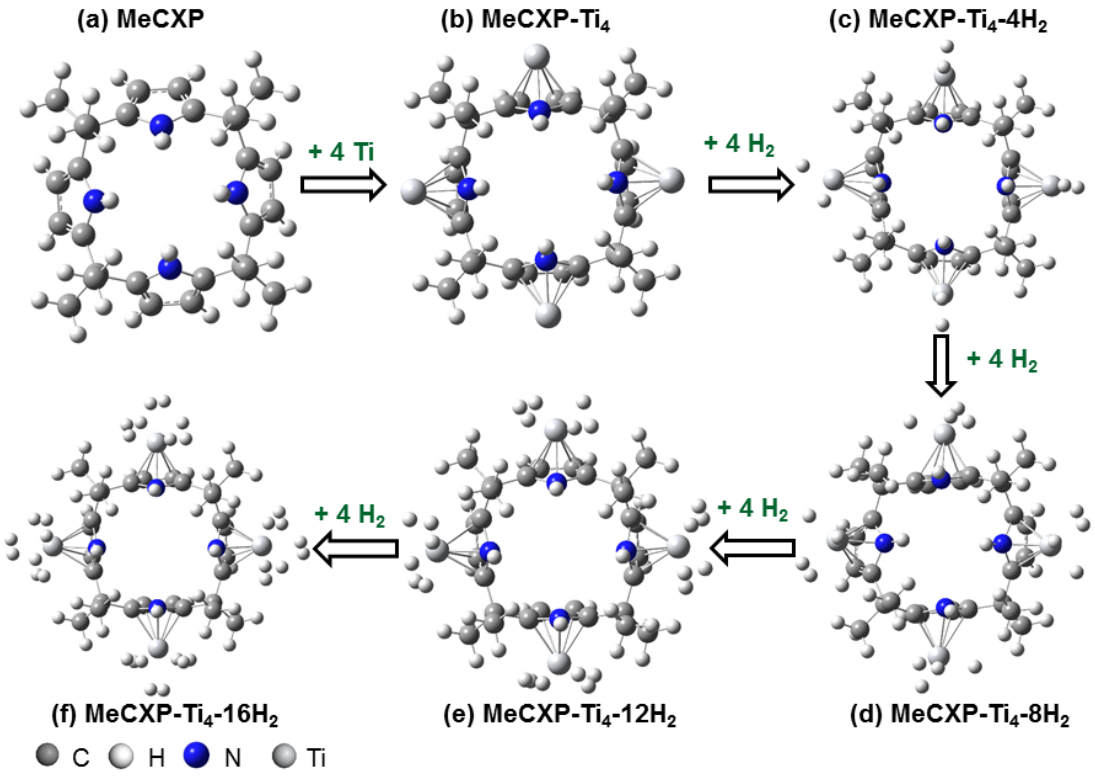

Figure S2: Two pyrrole rings of each CXP bonded with Ti metal as a sandwich type structure with 3 physisorbed H_2 molecule on sandwiched Ti.

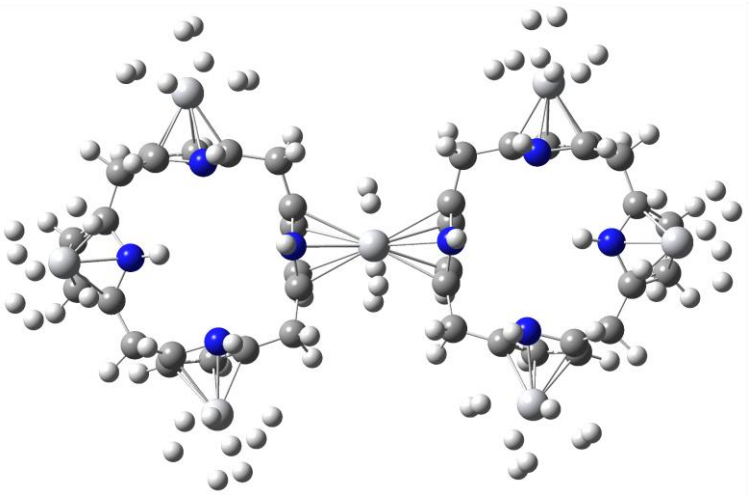

Figure S3: Top and bottom views of charge generation of electrostatic potential map of MeCXP, MeCXP-Ti_4 and MeCX-Ti_4-nH_2 systems (n = 4, 8, 12 and 16). The units used in *e/Å*^{3}

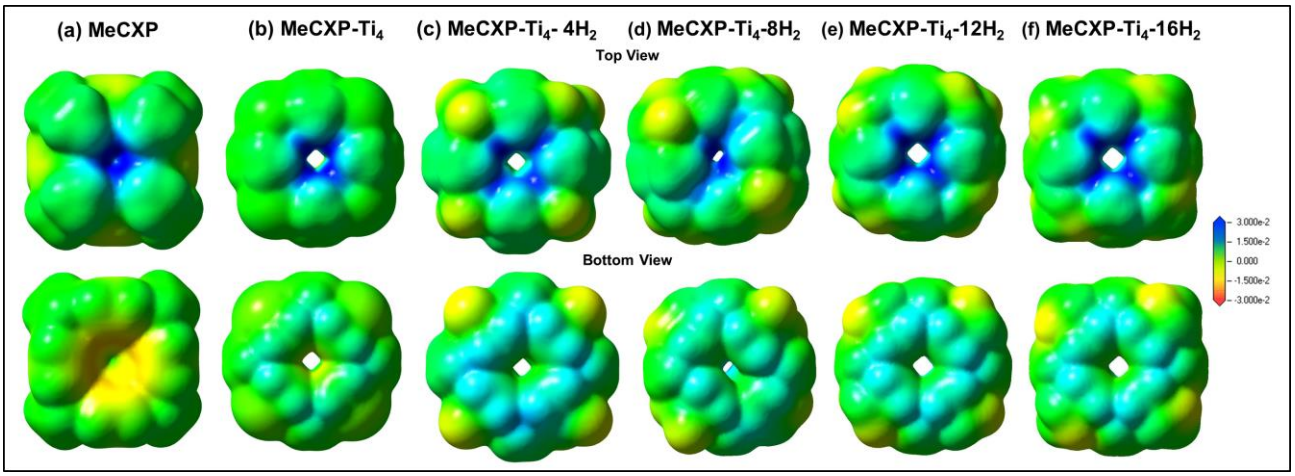

Figure S4: Hirshfeld Charges of Ti, chemisorbed hydrogen (Hc) and physisorbed hydrogen (Hp) of MeCXP-Ti_4-nH_2 system (where n = 4, 8, 12 and 16).

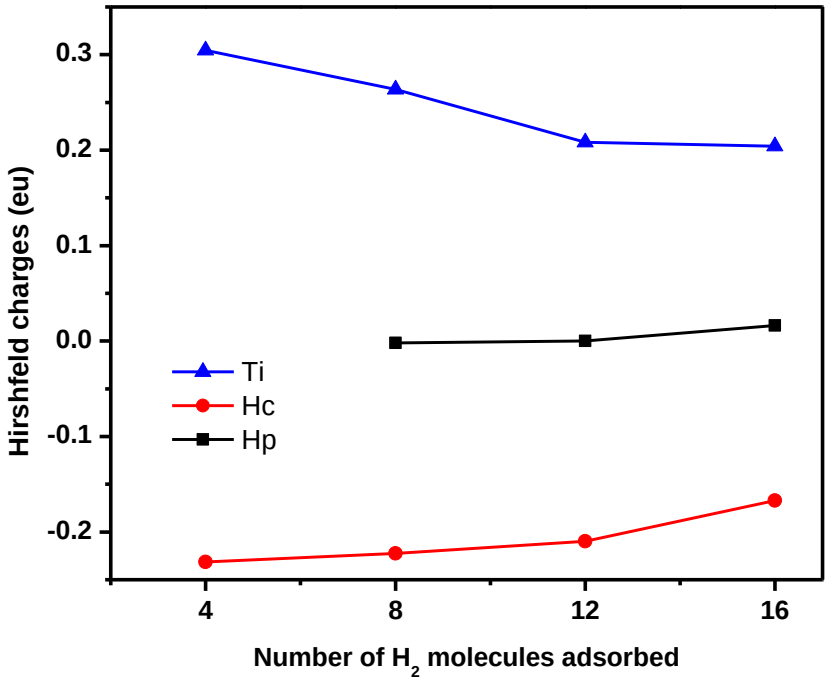

Figure S5: Snap-shots of MD simulation of H_2 trapped on MeCXPTi$_4$-16H_2 at the temperatures of (a) 200 K, (b) 273 K, (c) 373K, and (d) 473 K.

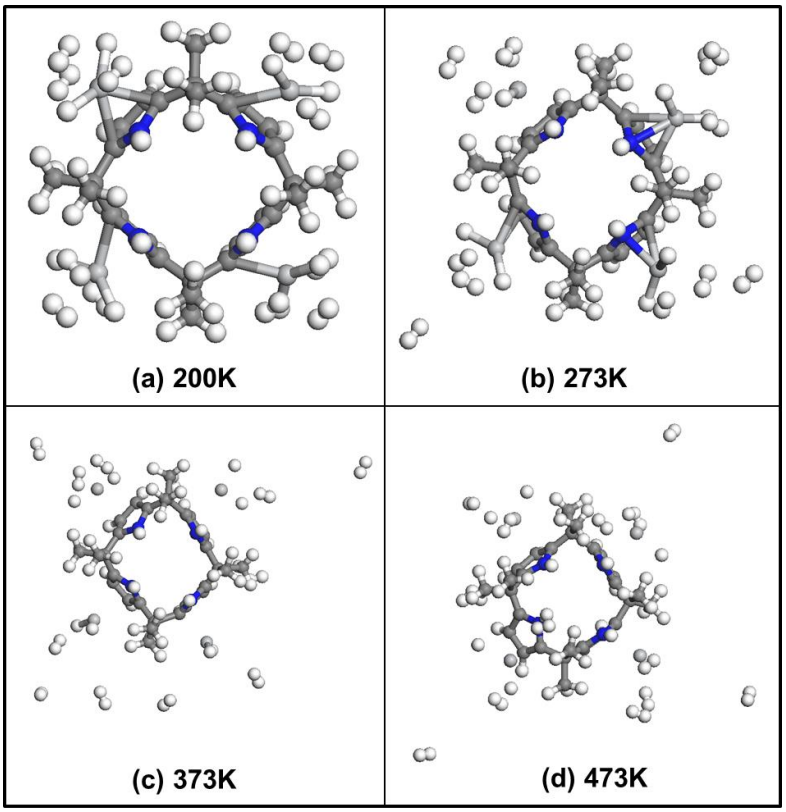

Table S1: The bond distance between Ti metal and center of pyrrole ring of MeCXP ring (Ti-Pc), Ti and chemisorbed hydrogen (Ti-Hc), Ti and physisorbed hydrogen (Ti-Hp) chemisorbed hydrogen (Hc-Hc) and physisorbed hydrogen distance (Hp-Hp). These are average bond distances measured in angstrom (Å).

System	Ti-R_c	Ti-H_c	Ti-H_p	H_c-H_c	H_p-H_p
MeCXP-Ti$_4$	1.898	-	-	-	-
MeCXP-Ti$_4$-4H_2	1.892	1.764	-	3.044	-
MeCXP-Ti$_4$-8H_2	1.923	1.750	1.884	2.900	0.818
MeCXP-Ti$_4$-12H_2	1.943	1.754	1.893	3.090	0.810
MeCXP-Ti$_4$-16H_2	1.943	1.748	1.931	3.256	0.806

Table S2: Calculated hardness (η), electrophilicity (ω), HOMO-LUMO energy gap (E_g) and average adsorption energy (E_{ad}), sequential desorption energy (E_{de}) of all hydrogen trapped MeCXP-Ti_4 systems. All these calculated energies provided in eV. The hydrogen wt % is also given.

System	η	ω	E_g	E_{ad}	E_{de}	H wt %
MeCXP-Ti_4	1.57	1.90	1.92	-	-	-
MeCXP-Ti_4-$4H_2$	4.23	1.28	2.31	1.91	1.91	7.06
MeCXP-Ti_4-$8H_2$	4.56	1.16	2.92	1.12	0.33	8.24
MeCXP-Ti_4-$12H_2$	4.73	0.97	2.89	0.84	0.28	9.39
MeCXP-Ti_4-$16H_2$	5.26	0.58	3.33	0.68	0.18	10.51

Table S3: Calculated Adsorption energy of CXP-Ti_4-nH_2 (n = 4, 8, 12 and 16 H_2)

S. No.	System	M06/6-311++G(d,p)	M06/6-311G(d,p)
		Adsorption Energy (eV)	Adsorption Energy (eV)
1	CXP-Ti_4-$4H_2$	1.71	1.87
2	CXP-Ti_4-$8H_2$	1.16	1.12
3	CXP-Ti_4-$12H_2$	0.98	0.87
4	CXP-Ti_4-$16H_2$	0.83	0.71

Table S4: Values of various bond moments for CXP their Ti decorated derivatives and H_2 adsorbed derivatives done by M06/6-311G(d,p) method

1. CXP

Dipole moment (Debye):
X= 0.0000 Y= -0.0000 Z= -4.5969 Total= 4.5969

Quadrupole moment (Debye-Ang):
XX= -144.2246 YY= -144.2246 ZZ= -128.9228
XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Traceless Quadrupole moment (Debye-Ang):
XX= -5.1006 YY= -5.1006 ZZ= 10.2012

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Octapole moment (Debye-Ang^2):

XXX= -0.0000	YYY= 0.0000	ZZZ= -29.9432	XYY= -0.0000
XXY= 0.0000	XXZ=19.6424	XZZ= -0.0000	YZZ= 0.0000
YYZ= 19.6424	XYZ= 0.0000		

Hexadecapole moment (Debye-Ang^3):

XXXX= -5212.1144	YYYY= -5212.1144	ZZZZ= -623.5241	XXXY= 0.0000
XXXZ= 0.0000	YYYX= -0.0000	YYYZ= 0.0000	ZZZX= -0.0000
ZZZY= 0.0000	XXYY= -1479.5437	XXZZ= -871.2691	YYZZ= -871.2691
XXYZ= -0.0000	YYXZ= -0.0000	ZZXY= -0.0000	

2. CXP-Ti_4

Dipole moment (Debye):

X= -0.0002	Y= -1.2864	Z= 0.4568	Total= 1.3651

Quadrupole moment (Debye-Ang):

XX= -238.6247	YY= -235.6141	ZZ= -211.0611
XY= 0.0001	XZ= 0.0002	YZ= -1.1697

Traceless Quadrupole moment (Debye-Ang):

XX= -10.1914	YY= -7.1808	ZZ= 17.3722
XY= 0.0001	XZ= 0.0002	YZ= -1.1697

Octapole moment (Debye-Ang^2):

XXX= -0.0094	YYY= -47.8239	ZZZ= 29.6013	XYY= 0.0017
XXY= -3.2849	XXZ=60.2457	XZZ= -0.0006	YZZ= 3.4005
YYZ= -2.3641	XYZ= 0.0055		

Hexadecapole moment (Debye-Ang^3):

XXXX= -11393.4657	YYYY= -10183.0729	ZZZZ= -1407.6024	XXXY= -0.0660
XXXZ= 0.0100	YYYX= 0.0418	YYYZ= -3.1993	ZZZX= 0.0035
ZZZY= -12.1136	XXYY= -3440.3796	XXZZ= -1949.4263	YYZZ=-1889.308
XXYZ= -2.4789	YYXZ= 0.0002	ZZXY= 0.0117	

3. CXP-Ti_4-$4H_2$

Dipole moment (Debye):

X= -1.1044	Y= -0.1555	Z= 0.8288	Total= 1.3895

Quadrupole moment (Debye-Ang):

XX= -259.1665	YY= -247.2177	ZZ= -232.6586
XY= -8.5422	XZ= -6.8752	YZ= 8.6472

Traceless Quadrupole moment (Debye-Ang):

XX= -12.8189	YY=-0.8701	ZZ= 13.6890

XY= -8.5422 XZ= -6.8752 YZ= 8.6472

Octapole moment (Debye-Ang^2):

XXX= -0.7348	YYY= 10.5589	ZZZ= 29.3243	XYY= -10.5381
XXY= -5.6995	XXZ= 138.4682	XZZ= -21.9685	YZZ= 11.4912
YYZ= -94.7326	XYZ= 4.3268		

Hexadecapole moment (Debye-Ang^3):

XXXX=-12806.0334	YYYY= -8515.9963	ZZZZ= -2415.9578	XXXY= -380.2534
XXXZ= -11.1839	YYYX= -15.6216	YYYZ= 309.7274	ZZZX= -65.3171
ZZZY= 71.0855	XXYY= -2822.6700	XXZZ= -2285.4728	YYZZ= -1722.3287
XXYZ= 46.2790	YYXZ= -154.2383	ZZXY= 46.9036	

4. CXP-Ti_4-8H_2

Dipole moment (Debye):

X= 0.6957	Y= -0.1282	Z= 6.7497	Total= 6.7866

Quadrupole moment (Debye-Ang):

XX= -257.4327	YY= -272.7159	ZZ= -234.2889
XY= 0.2999	XZ= -6.1497	YZ= 3.4647

Traceless Quadrupole moment (Debye-Ang):

XX= -2.6202	YY= -17.9034	ZZ= 20.5236
XY= 0.2999	XZ= -6.1497	YZ= 3.4647

Octapole moment (Debye-Ang^2):

XXX= -8.2054	YYY= 8.5168	ZZZ= 71.9940	XYY= 21.4817
XXY= -5.7060	XXZ= 192.9223	XZZ= 6.9364	YZZ= -2.6576
YYZ= 65.3203	XYZ= 14.3493		

Hexadecapole moment (Debye-Ang^3):

XXXX= -12891.0612	YYYY= -12419.2490	ZZZZ= -1638.8083	XXXY= -371.9640
XXXZ= -252.1116	YYYX= 207.6648	YYYZ= 33.5899	ZZZX= 27.6507
ZZZY= 32.5996	XXYY= -3454.5025	XXZZ= -2444.7878	YYZZ= -2203.4797
XXYZ= -10.9551	YYXZ= -57.5560	ZZXY= 57.9134	

5. CXP-Ti_4-12H_2

Dipole moment (Debye):

X= 0.0006	Y= -0.0002	Z= 3.6625	Total= 3.6625

Quadrupole moment (Debye-Ang):

XX= -287.8316	YY= -283.6309	ZZ= -227.0349
XY= -2.2813	XZ= -0.0060	YZ= -0.0004

Traceless Quadrupole moment (Debye-Ang):

XX= -21.6658 YY= -17.4651 ZZ= 39.1309
XY= -2.2813 XZ= -0.0060 YZ= -0.0004

Octapole moment (Debye-Ang^2):
XXX= -0.0114 YYY= -0.0064 ZZZ= 47.7425 XYY= -0.0006
XXY= 0.0008 XXZ= 124.4033 XZZ= 0.0128 YZZ= -0.0038
YYZ= 38.8859 XYZ= 18.1135

Hexadecapole moment (Debye-Ang^3):
XXXX= -14362.7575 YYYY= -13775.8665 ZZZZ= -1462.5859 XXXY= -574.5058
XXXZ= -0.2183 YYYX= 347.7983 YYYZ= -0.0489 ZZZX= -0.0874
ZZZY= -0.0226 XXYY= -4130.0134 XXZZ= -2325.6492 YYZZ= -2230.0497
XXYZ= -0.0470 YYXZ= -0.0324 ZZXY= 72.2428

6. CXP-Ti_4-16H_2

Dipole moment (Debye):
X= 0.0001 Y= -0.0010 Z= 2.0301 Total= 2.0301

Quadrupole moment (Debye-Ang):
XX= -279.5020 YY= -273.7935 ZZ= -233.5579
XY= -3.0027 XZ= 0.0008 YZ= 0.0001

Traceless Quadrupole moment (Debye-Ang):
XX= -17.2175 YY= -11.5091 ZZ= 28.7266
XY= -3.0027 XZ= 0.0008 YZ= 0.0001

Octapole moment (Debye-Ang^2):
XXX= 0.0008 YYY= -0.0384 ZZZ= 40.7359 XYY= 0.0059
XXY= -0.0012 XXZ= 61.2227 XZZ= -0.0015 YZZ= -0.0020
YYZ= 17.5744 XYZ= 15.9098

Hexadecapole moment (Debye-Ang^3):
XXXX= -14149.5349 YYYY= -13392.7514 ZZZZ= -1514.4888 XXXY= -495.0648
XXXZ= 0.0543 YYYX= 238.1200 YYYZ= 0.0924 ZZZX= 0.0352
ZZZY= 0.0736 XXYY= -4538.7632 XXZZ= -2429.9725 YYZZ= -2389.3300
XXYZ= 0.0363 YYXZ= 0.0152 ZZXY= 77.2319

Table S5: Values of various bond moments for MeCXP, their Ti decorated derivatives and H_2 adsorbed derivatives done by M06/6-311G(d,p) method

1. MeCXP

Dipole moment (Debye):
X= -0.0001 Y= -0.0002 Z= 4.3522 Total= 4.3522

Quadrupole moment (Debye-Ang):

XX= -194.4501	YY= -194.4498	ZZ= -188.0941
XY= -0.0000	XZ= -0.0003	YZ= -0.0006

Traceless Quadrupole moment (Debye-Ang):

XX= -2.1188	YY= -2.1184	ZZ= 4.2372
XY= -0.0000	XZ= -0.0003	YZ= -0.0006

Octapole moment (Debye-Ang^2):

XXX= 0.0013	YYY= 0.0028	ZZ= 8.6033	XYY= -0.0002
XXY= -0.0005	XXZ= -11.0259	XZZ= -0.0017	YZZ= -0.0033
YYZ= -11.0237	XYZ= -0.0000		

Hexadecapole moment (Debye-Ang^3):

XXXX= -8524.1792	YYYY= -8524.1230	ZZZZ= -1531.3808	XXXY= 0.6606
XXXZ= 0.0035	YYYX= -0.6605	YYYZ= -0.0105	ZZZX= 0.0131
ZZZY= 0.0107	XXYY= -2646.6232	XXZZ= -1569.2244	YYZZ= -1569.2098
XXYZ= 0.0016	YYXZ= 0.0034	ZZXY= -0.0000	

2. MeCXP-Ti$_4$

Dipole moment (Debye):

X= 0.0000	Y= 0.0000	Z= 0.8719	Total= 0.8719

Quadrupole moment (Debye-Ang):

XX= -297.6349	YY= -297.6349	ZZ= -261.5842
XY= -0.0000	XZ= 0.0000	YZ= 0.0000

Traceless Quadrupole moment (Debye-Ang):

XX= -12.0169	YY= -12.0169	ZZ= 24.0339
XY= -0.0000	XZ= 0.0000	YZ= 0.0000

Octapole moment (Debye-Ang^2):

XXX= 0.0000	YYY= -0.0000	ZZZ= -36.4561	XYY= -0.0000
XXY= -0.0000	XXZ= -8.0049	XZZ= 0.0000	YZZ= -0.0000
YYZ= -8.0049	XYZ= 0.0000		

Hexadecapole moment (Debye-Ang^3):

XXXX= -14549.6130	YYYY= -14549.6130	ZZZZ= -1978.8157	XXXY= -133.1421
XXXZ= -0.0000	YYYX= 133.1421	YYYZ= 0.0000	ZZZX= 0.0000
ZZZY= -0.0000	XXYY= -5093.2676	XXZZ= -2678.3119	YYZZ= -2678.3119
XXYZ= -0.0000	YYXZ= -0.0000	ZZXY= 0.0000	

3. MeCXP-Ti$_4$-4H$_2$

Dipole moment (Debye):

X= 0.2247	Y= -1.6814	Z= -1.3261	Total= 2.1531

Quadrupole moment (Debye-Ang):

XX= -306.8157	YY= -315.1425	ZZ= -281.7151
XY= -10.5856	XZ= -0.4741	YZ= -1.1095

Traceless Quadrupole moment (Debye-Ang):

XX= -5.5913	YY= -13.9181	ZZ= 19.5093
XY= -10.5856	XZ= -0.4741	YZ= -1.1095

Octapole moment (Debye-Ang^2):

XXX= 30.1673	YYY= -4.6966	ZZZ= -30.5148	XYY= -20.9295
XXY= -70.7483	XXZ= -108.8778	XZZ= 0.4297	YZZ= -1.6637
YYZ= 64.9225	XYZ= 7.4933		

Hexadecapole moment (Debye-Ang^3):

XXXX= -16553.8321	YYYY= -14404.0742	ZZZZ= -2589.8508	XXXY= -435.7983
XXXZ= -11.6418	YYYX= 37.9646	YYYZ= -3.2678	ZZZX= -0.2189
ZZZY= -8.4571	XXYY= -4257.9903	XXZZ= -2918.1760	YYZZ= -2725.0872
XXYZ= -29.0822	YYXZ= -8.8633	ZZXY= -48.2502	

4. MeCXP-Ti$_4$-8H$_2$

Dipole moment (Debye):

X= -0.0002	Y= 0.0007	Z= -1.7054	Total= 1.7054

Quadrupole moment (Debye-Ang):

XX= -320.4694	YY= -314.8280	ZZ= -292.2902
XY= 17.5417	XZ= -0.0004	YZ= -0.0019

Traceless Quadrupole moment (Debye-Ang):

XX= -11.2736	YY= -5.6321	ZZ= 16.9057
XY= 17.5417	XZ= -0.0004	YZ= -0.0019

Octapole moment (Debye-Ang^2):

XXX= 0.0352	YYY= -0.0520	ZZZ= -64.4105	XYY= -0.0251
XXY= 0.0157	XXZ= -149.2398	XZZ= -0.0035	YZZ= 0.0571
YYZ= 153.5288	XYZ= 37.1706		

Hexadecapole moment (Debye-Ang^3):

XXXX= -16196.6213	YYYY= -15016.6060	ZZZZ= -2774.6516	XXXY= 674.3334
XXXZ= -0.1377	YYYX= 167.6453	YYYZ= -0.8696	ZZZX= -0.2048
ZZZY= -0.8413	XXYY= -4579.3503	XXZZ= -3086.2002	YYZZ= -2873.3535
XXYZ= -0.1765	YYXZ= -0.0115	ZZXY= -61.4306	

5. MeCXP-Ti$_4$-12H$_2$

Dipole moment (Debye):

X= -0.0008 Y= -0.0003 Z= 0.2629 Total= 0.2629

Quadrupole moment (Debye-Ang):
XX=-344.6023 YY= -343.9927 ZZ= -270.2626
XY= 0.4999 XZ= -0.0021 YZ= -0.0053

Traceless Quadrupole moment (Debye-Ang):
XX= -24.9831 YY= -24.3735 ZZ= 49.3566
XY= 0.4999 XZ= -0.0021 YZ= -0.0053

Octapole moment (Debye-Ang^2):
XXX= -0.0128 YYY= -0.0018 ZZZ= -22.0333 XYY= -0.0009
XXY= -0.0151 XXZ=-38.7216 XZZ= -0.0136 YZZ= 0.0032
YYZ= 4.7249 XYZ= -9.4738

Hexadecapole moment (Debye-Ang^3):
XXXX= -18282.3734 YYYY= -17634.7578 ZZZZ= -2095.1723 XXXY= -311.8937
XXXZ= -0.4300 YYYX= 387.2895 YYYZ= -0.5812 ZZZX= -0.3297
ZZZY= -0.4401 XXYY= -5375.2532 XXZZ= -2954.2058 YYZZ= -2936.7565
XXYZ= -0.1848 YYXZ= -0.0786 ZZXY= -40.6368

6. MeCXP-Ti_4-$16H_2$

Dipole moment (Debye):
X= 0.0001 Y= -0.0012 Z= 0.9985 Total= 0.9985

Quadrupole moment (Debye-Ang):
XX= -331.7086 YY= -331.5747 ZZ= -280.0331
XY= 0.7431 XZ= -0.0031 YZ= 0.0010

Traceless Quadrupole moment (Debye-Ang):
XX= -17.2698 YY= -17.1359 ZZ= 34.4057
XY= 0.7431 XZ= -0.0031 YZ= 0.0010

Octapole moment (Debye-Ang^2):
XXX= -0.0032 YYY= -0.0244 ZZZ= -15.9962 XYY= 0.0180
XXY= -0.0073 XXZ= -3.7748 XZZ= -0.0114 YZZ= -0.0091
YYZ= 10.0210 XYZ= -0.4685

Hexadecapole moment (Debye-Ang^3):
XXXX= -17758.1527 YYYY= -17390.6180 ZZZZ= -2149.5902 XXXY= 121.9744
XXXZ= -0.0364 YYYX= -47.1500 YYYZ= -0.0057 ZZZX= -0.0415
ZZZY= 0.0253 XXYY= -5610.9206 XXZZ= -3140.0770 YYZZ= -3117.8279
XXYZ= 0.0008 YYXZ= 0.0060 ZZXY= -25.3649

Vibrational frequency analysis Calix[4]pyrrole

Table S6: Vibrational frequencies (cm^{-1}) of optimized CXP

60.1702	61.8778	70.1631
76.0532	90.1524	94.7451
132.7054	162.1021	190.8379
204.3564	229.2333	231.8142
247.9959	266.0129	304.1151
340.4090	342.9810	363.3509
382.1197	383.0799	392.5316
411.2103	579.8779	595.1156
610.0505	631.6164	632.7529
636.6041	637.8744	640.3148
662.9521	704.2910	707.5425
718.7235	732.1247	745.7985
758.2148	761.3710	775.3559
775.7596	802.5227	805.1677
811.7902	820.6002	845.8335
845.8466	855.9748	867.4907
876.8547	878.7777	889.4562
895.6970	896.7704	911.3098
985.4865	988.5857	991.8250
996.8188	1004.8645	1008.4810
1012.5523	1014.3151	1043.2447
1043.6698	1049.9898	1051.0172
1141.2025	1146.9372	1148.8883
1152.1120	1200.3759	1203.8672
1207.8438	1208.3294	1272.4969
1279.4394	1280.4938	1288.9620
1290.9624	1293.4724	1298.7798
1306.4175	1330.4175	1336.2286
1341.3510	1341.6207	1426.5047
1426.6978	1428.1518	1429.3393
1434.4099	1437.1416	1444.2531
1449.3376	1489.5674	1494.3620
1496.8530	1498.2486	1530.7282
1530.8239	1549.3093	1549.4977
1636.2967	1638.6968	1645.6797
1647.0777	2977.8064	2978.4022
2978.5622	2979.7326	3049.9394
3050.2432	3077.2543	3077.2697
3077.2704	3077.3190	3118.4429
3127.5238	3145.5311	3145.5903
3161.0945	3161.1313	3197.2376
3197.2805	3212.6049	3212.6418

Table S7: Vibrational frequencies (cm^{-1}) of optimized CXP-Ti_4

44.4292	48.5781	54.8432

57.4095	65.9715	78.7799
91.8575	142.9723	149.9269
151.5535	155.6202	159.3005
160.5606	165.4867	188.3176
199.9924	203.9502	252.7538
272.0427	278.9774	285.8624
302.6814	312.6110	318.0247
318.7349	336.0928	344.6901
352.2434	362.3225	368.1769
380.2108	397.2609	454.2938
461.6346	467.8945	474.1622
518.1895	520.2033	523.5774
545.3778	548.1100	567.2160
568.3586	574.8689	590.2259
612.6900	631.6325	661.9667
666.7383	700.2352	720.2301
736.9498	739.9211	754.0385
787.0150	788.1594	802.1144
813.7732	839.4145	852.0507
852.9381	860.5688	864.4291
865.4469	870.5003	881.9999
887.5439	888.6235	896.9257
899.3852	899.8335	903.0979
905.3377	906.7722	1039.0401
1043.2246	1049.7755	1053.3969
1073.2986	1085.8788	1086.8054
1097.9160	1136.4399	1146.1924
1153.9926	1177.2476	1183.3470
1192.4865	1199.6876	1211.8219
1262.6134	1263.8062	1264.4041
1266.2268	1267.9993	1274.5308
1288.3504	1313.0475	1325.5270
1330.7485	1332.0314	1335.7452
1372.9748	1378.5037	1397.4414
1398.8719	1405.8447	1409.5742
1411.3288	1418.0577	1475.5743
1478.1257	1484.7933	1485.3179
1534.9285	1536.9999	1537.0697
1537.7788	2999.1322	2999.1581
3002.0095	3002.0352	3050.0747
3050.2713	3056.2233	3056.4702
3189.9860	3192.5096	3201.7704
3201.7729	3207.4282	3209.7797
3219.4634	3219.4869	3444.9777
3496.4218	3507.0158	3562.5023

Table S8: Vibrational frequencies (cm^{-1}) of optimized CXP-Ti_4-4H_2

36.4343	40.3888	53.6009
59.4972	67.3847	68.3751
102.2262	106.3425	123.0790

133.0243	140.9230	144.9274
148.1983	162.5310	172.9916
183.4461	192.3760	198.6196
203.5866	219.2136	227.9244
234.8773	262.8246	276.4664
281.9224	302.4235	314.2169
316.0276	326.1484	333.5641
335.6590	345.2375	347.3546
350.4417	363.1485	366.9896
374.1551	386.6037	401.6674
417.8577	442.7663	446.8825
448.7683	454.5719	470.2584
490.8068	496.8553	514.4503
517.2532	529.9102	573.2139
580.1240	587.7110	592.3952
598.1505	600.6774	613.8789
618.4087	649.6509	668.4268
671.6456	674.5810	676.1199
677.5567	692.1326	697.5423
731.2562	733.6043	753.2424
758.8019	775.9976	810.9766
819.4848	821.0984	823.2265
857.8038	864.9246	877.8496
880.1470	886.7999	892.3226
904.9575	906.5778	917.3423
918.7071	922.2636	926.4249
928.4723	956.3264	959.2230
1023.7346	1047.0907	1050.3926
1064.3748	1066.3732	1087.7426
1116.8419	1123.7254	1151.7311
1155.0539	1168.3822	1169.9853
1178.0626	1180.0396	1199.3852
1205.1483	1247.2951	1248.9180
1253.3623	1260.1641	1290.8029
1297.8731	1303.5761	1308.0661
1314.6151	1323.0983	1324.7276
1332.7030	1353.6415	1367.8451
1379.7933	1388.9927	1403.3832
1428.2646	1429.6394	1433.5141
1441.9071	1481.6347	1483.7795
1487.4211	1522.2231	1525.7477
1530.0497	1592.9434	1601.7114
1620.5300	1625.9307	1632.2231
1648.2484	1664.4582	1665.2189
1672.6883	2991.2290	3003.1171
3025.1169	3035.9391	3065.3178
3076.6423	3084.9122	3086.6212
3195.4953	3199.9121	3200.6043
3208.0407	3215.2344	3216.6089
3232.0628	3232.8520	3532.2727
3584.5487	3591.9155	3597.2199

Table S9: Vibrational frequencies (cm^{-1}) of optimized CXP-Ti_4-8H_2

23.1531	37.1027	44.0113
47.6217	53.8603	57.5993
74.1136	106.4332	122.0382
136.9161	140.6957	142.9829
151.2917	157.2594	161.0895
185.4507	204.1529	208.8196
237.2591	243.1580	244.0003
246.6647	261.5057	267.8782
271.9970	277.1842	292.3102
297.8517	303.4462	318.8950
327.1159	331.2820	336.7114
343.0006	356.5810	364.9778
371.4083	378.7907	390.5279
396.0899	399.9087	405.5766
415.7327	428.5827	433.5997
437.7070	442.9051	445.6458
446.8127	453.7435	469.0949
482.9850	496.9627	503.2698
536.2246	542.8591	543.8102
570.0073	590.0573	595.2381
598.6419	604.6087	616.9662
623.4258	631.6098	642.2836
644.5485	662.6115	668.0485
681.4356	690.8658	696.6578
707.8754	719.0986	735.6238
745.1548	751.3619	762.6032
766.7468	800.2358	808.3364
815.4629	836.5206	848.5646
859.4580	874.5310	886.5067
890.9693	894.6761	896.9716
898.8019	902.0808	904.9062
907.0781	911.6993	913.3896
915.0619	916.2087	931.9892
940.8079	947.0392	948.5049
951.9826	954.7601	962.8847
976.6728	1028.0698	1042.4830
1050.2506	1057.1243	1090.5340
1098.6919	1104.3450	1121.6643
1165.8316	1172.1662	1177.5198
1180.7114	1195.2637	1204.6317
1216.5122	1232.9408	1262.6350
1267.3485	1268.5264	1270.9034
1305.7461	1313.4604	1316.7547
1330.2389	1333.9273	1346.5390
1348.3145	1353.8036	1372.3335
1378.9481	1386.3454	1395.7548
1409.9655	1410.9600	1415.9074
1417.4753	1479.9060	1495.7902

1498.2970	1503.7849	1515.9239
1520.7345	1524.7079	1524.9409
1525.4261	1533.8696	1540.9892
1586.6524	1587.2414	1589.6763
1596.8830	1600.2364	1621.6935
1625.1132	1630.4936	1641.1938
3019.8547	3023.1772	3026.4468
3029.9621	3071.7102	3079.7772
3079.8454	3083.7821	3203.2060
3206.6379	3206.6521	3208.8849
3224.3610	3230.2987	3230.5704
3235.6526	3239.3601	3263.8799
3265.8973	3271.4104	3531.2857
3537.6362	3592.1336	3595.2773

Table S10: Vibrational frequencies (cm^{-1}) of optimized CXP-Ti_4-12H_2

14.7545	48.8475	51.8979
58.5871	58.8914	59.5955
74.2062	133.1927	134.6786
136.3337	149.4329	150.7213
159.1919	162.9394	167.6307
179.7797	188.2873	196.2777
229.9473	234.5714	238.4237
275.0001	279.1564	296.0263
298.1560	304.9404	328.3323
328.6562	332.1161	336.0925
341.4391	343.9214	354.9683
355.2844	370.1971	372.8749
377.9924	381.6037	382.9510
384.5171	389.0612	392.9652
397.0228	400.5551	401.4907
404.9864	408.9945	416.3033
426.0521	433.6222	436.4727
440.9039	440.9249	444.6670
455.0270	455.1317	455.4290
456.8306	518.2946	520.8711
535.1508	535.8679	581.5999
586.6465	586.7721	595.3754
601.1882	602.9624	603.4113
606.6704	615.6101	619.6653
622.4345	631.7181	637.3734
642.1485	647.1009	661.0162
668.1497	696.8428	698.6483
730.7806	733.7544	748.1725
753.2115	762.3518	798.0457
799.8863	803.3721	805.8211
845.8092	857.1178	862.9282
871.2646	875.6384	878.5510
879.8306	883.8913	895.4872
896.0987	899.0991	899.4061

913.6396	916.0699	918.2773
918.7599	923.0181	923.8100
926.9768	928.9768	932.8919
935.8666	942.4118	944.1680
953.8251	954.6812	973.3286
973.6438	984.0138	984.1720
985.8240	986.2813	1041.9087
1045.7955	1046.9663	1051.6437
1106.5930	1109.3613	1114.5802
1118.0294	1163.0478	1166.8632
1183.4013	1185.8483	1207.3998
1223.1940	1230.1332	1246.6987
1271.9481	1272.7756	1276.4833
1277.1119	1306.8319	1314.9323
1321.3227	1337.8221	1340.0584
1355.1284	1358.4723	1364.4639
1387.3916	1396.8636	1402.1933
1404.0180	1409.8705	1410.4287
1412.6759	1417.4324	1515.1394
1515.5977	1516.2741	1516.9477
1520.8026	1520.9275	1525.0997
1525.1110	1529.5387	1529.6960
1546.5274	1546.5409	1564.4214
1564.4384	1564.8964	1565.1109
1579.3666	1579.5704	1591.3574
1591.7638	1594.3261	1595.3846
1596.1831	1600.5170	3024.1259
3024.1391	3026.2852	3026.3071
3076.3006	3076.3129	3079.5978
3079.6133	3210.0854	3210.0912
3217.4816	3217.4846	3231.6322
3231.6492	3233.3274	3233.3456
3236.4421	3236.5268	3256.6278
3256.7777	3307.4875	3307.7716
3318.6076	3319.1007	3527.3628
3527.5289	3631.8925	3634.4590

Table S11: Vibrational frequencies (cm^{-1}) of optimized CXP-Ti_4-16H_2

9.3592	51.8697	52.0917
53.2923	54.4163	61.0874
72.3343	129.9170	131.4494
135.0777	151.0901	153.5469
155.9239	163.3043	165.7141
177.7124	189.9435	195.4325
216.7813	220.6849	228.0504
249.6896	252.7442	252.8429
256.0030	271.8726	283.5240
290.1026	290.6321	308.0240
319.5428	321.5902	328.9946
334.1102	336.5687	338.1515

340.4824	351.0743	365.5425
372.5779	375.2939	380.7052
383.8320	388.4687	392.4090
397.6087	403.2538	403.9157
407.4718	413.0740	426.2773
426.5305	433.8359	450.9633
506.2461	507.9620	526.7624
531.5701	532.8639	534.5953
551.5666	552.1096	557.7682
558.9855	566.3269	568.9441
572.7902	577.1068	581.6794
583.6125	584.8066	585.2857
593.6579	596.0634	597.2387
599.3320	614.8582	617.9129
619.3533	622.8373	630.0623
637.5368	642.4588	645.3973
662.6143	696.2723	699.2179
725.9994	730.2199	735.8789
743.8218	748.8993	756.2727
762.6968	799.1912	800.3902
809.0035	811.1889	843.0752
844.3640	849.2020	863.1447
865.0411	881.0137	882.9116
884.3460	893.3464	893.8412
905.4608	906.8105	913.9702
917.7702	918.1805	918.6124
921.2599	922.0702	922.5067
924.5871	928.0915	928.6384
932.5760	933.4778	941.1993
941.4505	955.1354	956.4825
957.8044	958.9594	968.9971
969.7454	977.6862	978.5584
981.8403	982.3355	995.4428
995.5218	1043.6732	1045.8118
1047.4371	1050.2670	1051.5125
1051.7759	1107.0930	1108.2865
1116.3879	1117.6464	1163.3904
1165.9355	1188.1964	1189.7611
1210.4598	1226.7135	1232.4956
1252.3695	1270.2991	1271.3632
1276.9141	1277.7110	1305.2957
1313.1484	1323.8413	1337.3548
1345.5279	1358.1729	1361.2432
1367.3886	1389.4689	1398.1738
1402.3972	1404.6219	1408.3402
1408.4021	1409.6633	1410.0096
1413.4795	1417.1462	1443.4557
1443.4797	1508.8720	1508.9445
1511.6365	1511.7491	1521.9926
1522.1942	1523.5430	1523.8440
1526.8423	1526.8664	1531.2700

1531.4356	1545.4605	1545.5163
1546.4648	1546.7482	1555.1228
1555.5792	1563.4045	1564.5560
1578.2598	1578.4731	1586.4522
1586.6269	3022.5655	3022.5784
3028.5793	3028.5996	3076.5216
3076.5359	3081.6884	3081.7080
3201.0380	3201.1247	3208.3195
3208.3315	3215.4260	3215.4321
3231.2256	3231.3361	3233.1668
3233.1774	3236.2050	3236.2229
3322.2337	3322.2469	3327.3249
3328.1834	3407.3451	3407.4471
3431.5363	3431.5867	3520.8008
3521.1115	3640.4729	3641.5354

Table S12: Vibrational frequencies (cm^{-1}) of optimized MeCXP

46.2889	54.3502	66.3259
76.2576	82.6564	99.0314
118.0142	120.5941	124.6645
130.3128	146.8409	179.3577
185.5132	220.7616	238.1196
250.3591	254.4706	258.3266
271.0066	277.0315	281.8228
288.9073	296.7388	300.1411
313.1164	313.4194	329.0315
330.0185	339.2000	350.7938
353.7710	367.4166	371.0494
373.6449	375.6842	380.7577
391.6007	395.3278	401.5173
413.7439	424.7568	453.1755
474.2028	506.8874	512.5532
513.2338	530.1330	533.8001
548.8242	554.6311	584.9270
600.0116	645.5263	648.4419
653.6279	656.3171	695.0508
699.4621	711.4128	719.1985
725.1220	732.8779	736.8045
746.1861	755.2028	786.6329
796.0522	818.6895	841.6231
852.4514	853.9470	867.7605
892.1859	896.4224	900.1795
902.6451	906.6972	936.3902
941.5644	945.3778	946.7809
950.5328	962.6389	964.9524
969.5421	973.4211	988.7826
992.2350	994.9765	1008.9871
1016.6730	1019.4583	1021.6735

1051.7640	1067.4146	1068.7851
1070.9654	1080.5500	1115.4013
1129.2039	1131.9868	1141.3564
1150.6865	1157.4739	1160.7376
1162.7305	1166.7443	1168.3168
1172.1249	1178.9187	1237.6203
1241.3538	1245.7073	1246.9161
1249.2441	1265.8565	1273.9692
1283.9750	1287.7515	1291.1438
1294.7986	1300.1062	1363.7537
1369.5207	1371.8054	1376.2376
1385.3070	1389.9844	1394.0637
1395.7520	1397.6897	1402.8800
1414.7765	1427.5377	1441.2317
1448.5836	1451.2262	1452.2262
1453.4780	1458.1212	1461.1663
1462.0721	1464.2821	1466.2074
1468.2852	1468.5568	1474.0619
1477.6379	1479.5232	1480.8838
1484.0524	1492.8007	1495.3137
1502.7657	1505.4838	1507.4418
1514.0741	1517.8329	1604.5873
1611.4515	1614.0386	1619.3801
2193.9282	2940.4454	2947.1568
2957.3979	2961.2034	2974.6595
3001.7440	3006.6285	3016.9611
3025.9166	3028.5903	3033.7373
3046.9176	3047.3353	3064.5577
3090.9603	3093.6188	3096.9377
3103.3671	3105.0545	3125.3160
3134.0854	3138.1144	3140.0545
3149.9346	3155.6737	3161.9622
3166.8344	3171.0852	3178.4162
3190.2006	3208.7753	3239.9598
3253.4264	3346.9113	3535.0496

Table S13: Vibrational frequencies (cm^{-1}) of optimized MeCXP-Ti_4

29.7827	34.4715	56.7384
59.9088	64.9997	76.7184
80.6993	106.8979	114.5001
120.6318	136.1726	140.9703
141.8233	152.6497	167.2617
170.4350	173.8382	179.6901
220.8195	227.7476	232.2893
233.7818	239.7526	244.1005
248.8858	252.4368	256.0883
258.7169	265.3136	267.8400
269.8893	271.7537	278.5970
291.9865	295.2054	298.8090
299.6834	308.5716	309.4371

318.1542	330.0362	351.1903
359.3973	366.4060	373.7193
373.8413	385.9069	389.7012
390.5005	404.0498	404.0891
430.2447	434.1783	476.7534
484.0998	488.4793	498.3587
512.0990	516.9191	518.5672
518.7607	530.7669	534.9477
558.8904	559.7077	564.6338
577.3464	579.8626	613.9057
626.5204	652.6443	656.9219
659.8722	663.2941	690.8768
693.1622	702.4616	706.4559
790.8906	796.5909	804.8952
813.2628	854.1666	855.7642
858.7037	860.4655	862.9453
868.1927	881.9013	884.8545
892.2586	898.4589	906.4295
910.8947	930.3686	931.6932
939.3852	941.1595	950.0262
950.1337	954.3095	954.3710
987.4501	990.6206	991.4407
994.3776	1041.2649	1041.6765
1050.8160	1054.1036	1060.8555
1072.1647	1079.8618	1095.4121
1113.2608	1122.4275	1124.6446
1127.2116	1128.9634	1131.0643
1139.7902	1152.3359	1168.4232
1187.6617	1192.0245	1214.0081
1216.2788	1225.9484	1226.4828
1230.3232	1235.7538	1237.6894
1242.2207	1244.5130	1301.8056
1301.8910	1314.6697	1315.2528
1339.9798	1340.9193	1358.2415
1358.5328	1363.6113	1367.3350
1374.9746	1376.7875	1380.3375
1381.9927	1386.0614	1387.3191
1441.8665	1442.0186	1442.5346
1442.6515	1448.2140	1448.9618
1458.6151	1458.7507	1459.0587
1459.3211	1462.5209	1465.3116
1467.4168	1473.3377	1481.3663
1484.3061	1485.0733	1485.4956
1488.4744	1488.5627	1522.3972
1522.5650	1536.1214	1536.1293
2951.6066	2951.7438	2960.7522
2960.7888	3014.3523	3014.3737
3014.8875	3014.8994	3016.8691
3016.9195	3074.2080	3074.2627
3096.3535	3096.3620	3100.6405
3100.6807	3105.2690	3105.2922

3107.4940	3107.5518	3116.2211
3116.2437	3129.8505	3129.8937
3141.7864	3141.7950	3185.8928
3185.9264	3203.0590	3203.0803
3243.4379	3243.4608	3335.3608
3342.1149	3429.5395	3429.8012

Table S14: Vibrational frequencies (cm^{-1}) of optimized MeCXP-Ti_4-$4H_2$

12.0883	41.1070	51.8147
59.5465	59.9255	68.4283
82.1714	99.5172	112.0707
120.2353	137.3355	142.3929
142.5150	146.4892	147.7543
153.4394	159.1439	161.5711
194.6079	201.0085	219.8574
221.2088	226.2314	229.4215
236.8609	240.2161	251.2717
263.9238	270.3271	271.4279
272.2465	276.3060	283.5853
287.4541	291.3090	294.1987
298.5342	301.8489	306.3407
310.6020	314.7862	317.8824
327.1605	330.1482	331.4997
336.7086	348.4481	355.3931
356.6808	358.3598	360.2991
366.6588	368.5563	370.0284
382.3096	386.0568	392.8191
401.7342	413.8538	417.6806
421.8728	426.3087	439.3756
443.9870	459.3692	468.6473
475.6444	475.9131	484.4212
493.3649	502.2348	515.0265
524.6621	533.7965	537.8555
551.5610	555.4374	574.6300
603.8329	610.1686	617.6818
625.1060	632.8783	647.9934
653.1396	656.2606	657.5516
669.7977	677.2591	679.7353
686.3308	693.3939	696.8800
710.3883	817.6876	821.0181
821.6579	825.6387	869.1668
870.7665	872.2356	879.9134
881.0694	893.8924	898.4747
905.3026	921.3862	924.7448
929.3302	930.2896	936.6966
939.0419	940.2514	941.6599
947.5715	950.7651	952.1915
954.1680	1003.5768	1006.6541
1008.6882	1012.3772	1045.6877
1050.5017	1064.3490	1067.4414

1069.1907	1083.9638	1087.0575
1106.9940	1114.9189	1122.3888
1131.9655	1136.4871	1137.6958
1140.9964	1148.1781	1162.3789
1171.3421	1189.5991	1195.1808
1212.4512	1218.8806	1223.9350
1224.5492	1229.2752	1237.4170
1239.4494	1248.1512	1250.9820
1306.3401	1307.8608	1321.3781
1323.4762	1343.7020	1345.2632
1360.9595	1361.4551	1374.4545
1376.0243	1377.1185	1379.1226
1395.0694	1396.4059	1397.7773
1398.7483	1445.1786	1446.2439
1449.2393	1450.4895	1451.5823
1452.8281	1456.0553	1457.3281
1465.2950	1465.7034	1466.7282
1467.8915	1475.3525	1475.6952
1477.7133	1478.7295	1482.5832
1484.0283	1487.9503	1488.4099
1520.2022	1521.4085	1529.7439
1530.3074	1604.5529	1613.0343
1617.0393	1622.7973	1628.9887
1643.0881	1644.8056	1653.0482
3010.6937	3011.6819	3012.4899
3013.0717	3016.5113	3017.3175
3017.8867	3018.5129	3087.6994
3088.7139	3090.0469	3090.9583
3098.0694	3099.9541	3100.7184
3102.9640	3107.2999	3108.0510
3110.2973	3110.6392	3111.7723
3111.9131	3113.6849	3114.2891
3197.0740	3197.6100	3204.0058
3209.1965	3220.0309	3220.8595
3225.5613	3232.9272	3557.9232
3559.2200	3583.7519	3585.9322

Table S15: Vibrational frequencies (cm^{-1}) of optimized MeCXP-Ti_4-8H_2

14.4616	45.8849	53.7138
59.9259	63.7836	83.1699
93.8454	96.6833	111.2685
116.5738	122.0943	133.2932
144.3448	149.1401	162.6343
165.1600	167.2950	171.2875
171.7830	181.5485	193.4038
210.2387	223.8468	225.1562
233.8665	242.8118	254.3136
254.9341	257.3931	262.5601
266.0552	268.1615	284.3024
286.9720	289.2905	291.5075

296.7308	297.8390	307.0454
313.3062	315.7298	315.8190
320.2908	322.0777	329.9831
332.2688	340.3256	346.2014
352.5852	356.1074	362.6270
366.4918	372.1826	375.2153
381.7309	391.3153	393.2630
398.6596	406.2239	410.7509
416.7687	417.7169	420.3400
432.8692	433.7521	442.1506
448.0865	449.1899	453.0123
468.4507	469.7979	500.7162
505.9598	515.1876	520.2180
528.1915	531.5417	537.7779
541.1592	555.8431	563.4566
578.2866	589.8512	597.8213
606.8838	612.2001	616.9874
617.5744	624.2691	628.6913
644.7622	647.3276	656.9322
657.8712	673.4683	676.2201
685.6963	691.7488	717.4677
721.1428	727.4750	731.5208
764.3363	764.3802	800.0861
801.4854	837.7841	838.7152
873.4880	873.7304	876.6397
881.4406	886.1428	887.6652
891.8477	898.4736	901.5875
902.7143	910.9903	913.2259
931.7220	932.0094	939.9234
940.0807	947.8033	947.9367
954.3959	954.4245	959.4093
959.8080	979.2149	979.4345
998.0839	998.7985	1004.8660
1005.7003	1011.7674	1012.3021
1038.9156	1040.6717	1062.9005
1063.0636	1069.5095	1072.1137
1097.3514	1105.8451	1117.6813
1123.2650	1135.1294	1142.8824
1145.2153	1148.1717	1158.1589
1168.3635	1180.4949	1190.9615
1208.4043	1216.7083	1226.9631
1228.5619	1231.2336	1233.1731
1246.3113	1249.9329	1263.6139
1264.2728	1311.3858	1311.5014
1336.8547	1337.7741	1352.6539
1353.2254	1363.2164	1363.8831
1369.8391	1370.5565	1380.4626
1381.8833	1383.1526	1386.1376
1396.9539	1397.2195	1447.5487
1447.6427	1451.3771	1451.4828
1457.2432	1457.3348	1459.4212

1459.5551	1467.9472	1467.9954
1474.0008	1474.1184	1480.7748
1481.0763	1484.0245	1485.0357
1486.9965	1487.5590	1495.1541
1495.3931	1517.7038	1517.9029
1520.8513	1520.9048	1538.9114
1539.0002	1586.4372	1587.5284
1596.7164	1596.7763	1615.2204
1615.7460	1619.0000	1619.8939
1641.9637	1644.4124	3005.4653
3005.4807	3013.3259	3013.5360
3023.3914	3023.4147	3029.3683
3029.3816	3077.9392	3077.9508
3088.6311	3088.9303	3104.4402
3104.4512	3107.0443	3107.0649
3108.0587	3108.0979	3111.2770
3111.3184	3122.8256	3122.9934
3129.0063	3129.0467	3135.2829
3135.6516	3199.8893	3199.9123
3224.5603	3224.6890	3229.7244
3229.7475	3246.8059	3246.8232
3279.8765	3280.3835	3554.6323
3554.7208	3565.4244	3582.5496

Table S16: Vibrational frequencies (cm^{-1}) of optimized MeCXP-Ti_4-12H_2

25.5383	37.5626	59.9660
69.6371	72.5644	78.2300
87.4222	119.4367	119.6307
124.1492	132.9734	142.7010
144.2131	154.0876	159.4027
175.4311	178.4250	184.4185
197.2435	200.8685	202.9237
216.3440	237.1056	238.9405
246.5158	254.2072	263.0002
264.2216	270.7690	276.5756
283.2084	283.9368	285.8758
292.1243	293.6365	295.1697
303.9289	305.2077	312.7323
312.8715	318.9574	319.8370
327.5074	337.0623	341.3157
342.0647	348.5151	348.8388
350.1619	355.1979	366.7942
367.1004	368.2758	373.3906
377.9541	382.2773	383.1278
386.6922	392.6244	392.8308
400.7970	401.9851	405.5822
409.1446	409.1816	416.1218
424.1335	425.5351	426.6736
427.3530	434.3990	437.1951
451.8387	453.9689	460.3770

460.9246	465.3208	468.9981
488.7172	511.9071	515.8644
518.5512	531.7681	537.8945
541.9193	552.3691	569.2320
575.5369	580.8306	583.7434
598.7238	600.6611	603.6469
604.0004	617.5024	620.1568
620.6600	622.6668	649.1510
650.3226	653.6788	660.6283
680.4818	689.9042	689.9267
697.6337	705.5934	705.7907
706.9784	723.0276	808.5086
812.5465	820.5021	826.8824
859.9650	860.0766	878.6869
879.1589	885.1021	886.9497
893.3031	894.1514	904.7269
907.2331	908.2644	909.6875
914.5201	915.0333	918.3043
923.9643	933.8738	934.3250
936.2956	936.4168	939.5803
940.2204	944.1008	945.0817
952.7803	953.2385	957.3393
957.6582	966.3713	966.4196
985.6919	985.7254	986.6010
986.6758	1002.2642	1004.7683
1009.5114	1012.1783	1033.2885
1033.5821	1053.6351	1053.8921
1063.8908	1067.6756	1082.1333
1094.5705	1098.9789	1115.5962
1125.9750	1140.1200	1144.0789
1144.5606	1155.9627	1158.3994
1161.3588	1175.8269	1189.9975
1212.8140	1213.0288	1222.1804
1224.5393	1234.4672	1235.1527
1248.2829	1252.4366	1255.0335
1257.2729	1258.6814	1343.9026
1344.4071	1346.2291	1346.4476
1354.7381	1359.7782	1360.5666
1363.9162	1372.8566	1376.8419
1378.7442	1384.5600	1387.8839
1389.4210	1392.8905	1395.9055
1449.8383	1449.9407	1450.8431
1451.2203	1458.5758	1459.1391
1464.5297	1464.7296	1473.9829
1474.4268	1479.5627	1480.6563
1488.2463	1489.1620	1495.3964
1498.8485	1501.1853	1502.4412
1504.9705	1509.3179	1514.1676
1517.9673	1519.4413	1521.3813
1527.6651	1527.7828	1531.6070
1531.6403	1555.3803	1555.4626

1560.9539	1560.9724	1588.2658
1588.6380	1590.3909	1590.6176
1600.1031	1602.0961	1613.2916
1613.4452	3001.8821	3002.0218
3003.8030	3004.2628	3032.2421
3032.2572	3035.3744	3035.3872
3085.7423	3085.7677	3089.5277
3089.6116	3112.0932	3112.1059
3113.9857	3113.9956	3123.4876
3123.5005	3128.7919	3128.8199
3133.2880	3133.3523	3136.2092
3136.2630	3192.6361	3192.7315
3201.8641	3201.9985	3214.0301
3214.1607	3219.8343	3219.9992
3237.9311	3238.0476	3243.5336
3243.6346	3347.8384	3347.8896
3351.8649	3352.2819	3629.9700
3630.2028	3630.7476	3631.5030

Table S17: Vibrational frequencies (cm^{-1}) of optimized MeCXP-Ti_4-$16H_2$

16.7783	35.2319	58.7448
70.8613	75.3797	80.0150
92.0278	113.3864	115.3154
117.6588	125.3184	133.3962
140.4916	155.6974	162.5961
179.4789	180.3128	187.2738
190.2962	193.5837	201.4437
213.4823	227.0733	237.7490
238.2601	239.2426	249.6603
254.6908	258.2068	259.8205
263.1885	265.6368	274.1832
274.3077	278.1828	279.9416
283.9653	288.4806	290.3579
293.9717	297.8626	301.2523
305.7398	307.1892	313.7088
316.6270	327.0291	331.4068
331.8793	340.4230	353.3309
354.4241	355.3846	357.9546
362.7989	363.5590	366.9254
368.3303	380.1922	382.3908
383.8438	392.0268	394.4450
394.5713	399.4199	406.2339
410.2893	413.5832	419.5841
423.6687	447.2421	449.4473
452.1113	455.4816	495.7133
511.8643	512.8079	517.5169
521.6442	525.0601	532.3096
538.4387	540.5953	542.2938
544.6128	556.5488	564.2015
568.1428	570.0754	577.6431

588.8051	588.8974	590.9245
592.1714	598.1014	599.6986
602.7717	603.3205	616.4452
620.2315	623.9820	626.7415
632.1998	633.1302	642.0829
643.0128	671.8340	679.8853
680.6509	684.0451	697.7473
702.2064	703.2036	714.1955
721.3140	722.2123	735.0292
735.0773	777.8626	779.3107
825.5865	826.9805	838.5113
839.0183	844.5159	846.1414
875.3174	875.6992	878.8759
879.1357	890.9062	892.6411
894.7851	900.4187	906.7456
915.3784	917.2119	918.0694
923.2585	925.6286	933.8502
935.4847	937.5451	938.3796
939.6419	941.7766	946.5203
947.7130	950.6339	951.9180
954.7063	955.0676	960.1597
961.4692	990.2464	990.3872
991.9154	992.2052	994.2949
995.4941	997.6487	997.9772
1003.0511	1003.3405	1009.1796
1010.5533	1022.9829	1023.1499
1029.8532	1030.1430	1052.1077
1058.0618	1064.0779	1075.5039
1084.5557	1096.9642	1105.4782
1121.6387	1123.0933	1142.2138
1143.0333	1146.6251	1157.6206
1160.7830	1161.0875	1175.5387
1190.0890	1213.2997	1218.9655
1222.1993	1228.2711	1231.6814
1236.8548	1248.4196	1257.0150
1257.6466	1258.8906	1259.9182
1344.1168	1344.1868	1349.0217
1349.7590	1355.9591	1359.1114
1359.3774	1365.4595	1371.0626
1375.8298	1376.0230	1384.0964
1384.4193	1386.7778	1387.0741
1389.1448	1418.0334	1418.0644
1428.0871	1428.2361	1449.0332
1449.1244	1450.6845	1450.9652
1456.2102	1456.3461	1457.2889
1457.7211	1459.6597	1459.7679
1469.2715	1469.3667	1472.9238
1474.8293	1476.6459	1478.9979
1487.0463	1487.4838	1490.4131
1494.1783	1498.9885	1501.5746
1504.4034	1506.1265	1514.8999

1519.4948	1521.9799	1525.0199
1554.6932	1555.2443	1556.9031
1558.4430	1561.2072	1561.3315
1570.5565	1570.7258	1591.6240
1591.8860	1600.5332	1600.7423
3010.9819	3011.2527	3012.2519
3012.7758	3033.4340	3033.4459
3036.2120	3036.2273	3094.3843
3094.3860	3096.0356	3096.1285
3112.1589	3112.1656	3115.7694
3115.7751	3124.7955	3124.8214
3132.1804	3132.2522	3140.3427
3140.4264	3141.5750	3141.6374
3155.9710	3156.1794	3175.3866
3175.5704	3212.4779	3212.7436
3218.4335	3218.7666	3242.6267
3243.2825	3244.8653	3245.4576
3364.5630	3364.6288	3374.4674
3374.7569	3408.9782	3409.1585
3424.0624	3424.1855	3625.0305
3625.2065	3635.0638	3635.2514

Coordinates of optimized geometries of Ti decorated Octmethylcalix[4]pyrrole (MeCXP), calix[4]pyrrole (CXP) and their H_2 Trapped analogues

Table S18: Optimized Structure of CXP system ($C_{20}H_{20}N_4$)

C	0.71267000	3.71374400	0.90271600
C	1.13692100	2.92800100	-0.14403000
C	-1.13692100	2.92800100	-0.14403000
C	-0.71267000	3.71374400	0.90271600
C	-2.51929900	2.51929900	-0.57765300
C	-2.92800100	1.13692100	-0.14403000
C	-3.71374400	0.71267000	0.90271600
C	-3.71374400	-0.71267000	0.90271600
C	-2.92800100	-1.13692100	-0.14403000
C	-2.51929900	-2.51929900	-0.57765300
C	-1.13692100	-2.92800100	-0.14403000
C	-0.71267000	-3.71374400	0.90271600
C	0.71267000	-3.71374400	0.90271600
C	1.13692100	-2.92800100	-0.14403000
C	2.51929900	2.51929900	-0.57765300
C	2.92800100	1.13692100	-0.14403000
C	3.71374400	0.71267000	0.90271600
C	3.71374400	-0.71267000	0.90271600
C	2.92800100	-1.13692100	-0.14403000
C	2.51929900	-2.51929900	-0.57765300
H	-1.35822600	4.22080400	1.60365800
H	1.35822600	4.22080400	1.60365800

H	-4.22080400	1.35822600	1.60365800
H	-4.22080400	-1.35822600	1.60365800
H	-1.35822600	-4.22080400	1.60365800
H	1.35822600	-4.22080400	1.60365800
H	4.22080400	1.35822600	1.60365800
H	4.22080400	-1.35822600	1.60365800
H	-2.61475600	-2.61475600	-1.66957600
H	-3.23087700	-3.23087700	-0.15480800
H	3.23087700	-3.23087700	-0.15480800
H	2.61475600	-2.61475600	-1.66957600
H	3.23087700	3.23087700	-0.15480800
H	2.61475600	2.61475600	-1.66957600
H	-3.23087700	3.23087700	-0.15480800
H	-2.61475600	2.61475600	-1.66957600
N	0.00000000	2.45613000	-0.77141200
H	0.00000000	1.91874900	-1.62136800
N	-2.45613000	0.00000000	-0.77141200
H	-1.91874900	0.00000000	-1.62136800
N	2.45613000	0.00000000	-0.77141200
N	0.00000000	-2.45613000	-0.77141200
H	0.00000000	-1.91874900	-1.62136800
H	1.91874900	0.00000000	-1.62136800

Table S19: Optimized Structure of CXP-Ti_4 system ($C_{20}H_{20}N_4Ti_4$)

C	0.68578600	2.65363400	1.47674500
C	1.18027000	2.83746600	0.15071200
C	-1.18085300	2.83728600	0.15064800
C	-0.68641000	2.65354400	1.47670900
C	-2.54795800	2.54063400	-0.38453600
C	-3.07358000	1.16961000	-0.11758100
C	-3.67445500	0.68673700	1.08185300
C	-3.67382000	-0.68584600	1.08668600
C	-3.07347600	-1.17443700	-0.10974200
C	-2.55124200	-2.54465800	-0.38076300
C	-1.17573900	-2.84244800	0.13543000
C	-0.68546900	-2.68274900	1.46788300
C	0.68614200	-2.68270000	1.46783500
C	1.17633800	-2.84233700	0.13532200
C	2.54745900	2.54108600	-0.38439500
C	3.07332800	1.17014100	-0.11750600
C	3.67428400	0.68730600	1.08190200
C	3.67393600	-0.68527700	1.08663800
C	3.07370300	-1.17390900	-0.10982800
C	2.55174800	-2.54421200	-0.38094700
H	-1.32073300	2.66039700	2.35387400
H	1.32006100	2.66059600	2.35394400
H	-4.19183200	1.32394000	1.78807600
H	-4.19200900	-1.31841400	1.79655700
H	-1.32116100	-2.71278000	2.34401900
H	1.32190000	-2.71265400	2.34392400

H	4.19151700	1.32456700	1.78817900
H	4.19224400	-1.31778800	1.79647300
H	-2.57673100	-2.75884400	-1.45972600
H	-3.25590600	-3.25549100	0.06987200
H	3.25659400	-3.25494300	0.06956700
H	2.57719800	-2.75829000	-1.45993200
H	3.26162200	3.25156500	0.05239800
H	2.56032600	2.75584900	-1.46378100
H	-3.26228300	3.25101200	0.05215700
H	-2.56078300	2.75531900	-1.46393700
N	-0.00026200	2.74943500	-0.68788500
H	-0.00022300	2.52143800	-1.67336000
N	-2.54010600	-0.00576700	-0.77635800
H	-1.68530900	-0.02091600	-1.32224100
N	2.54010600	-0.00530100	-0.77636800
N	0.00024200	-2.58473800	-0.69539300
H	0.00021700	-3.02856000	-1.61707400
H	1.68535600	-0.02059800	-1.32231800
Ti	-0.00043800	4.58678100	0.20565000
Ti	-4.56023400	-0.00324100	-1.05483900
Ti	0.00043900	-4.57819300	0.20614400
Ti	4.56023900	-0.00234900	-1.05482100

Table S20: Optimized Structure of CXP-Ti_4-4H_2 system ($C_{20}H_{20}N_4Ti_4$-H_8)

C	-1.56552000	2.66842200	1.46796900
C	-1.14954400	2.97780400	0.13376400
C	-2.96054700	1.40489800	0.11339300
C	-2.61006600	1.76092300	1.45750100
C	-3.72319700	0.19382600	-0.37058700
C	-3.15021400	-1.16197700	-0.03884900
C	-3.07336500	-1.79349000	1.24488500
C	-2.12140500	-2.79614200	1.24148000
C	-1.49994100	-2.90137900	-0.04652000
C	-0.17214900	-3.53204700	-0.38263100
C	1.04624400	-2.79011800	0.09810100
C	1.59905500	-2.70392800	1.35918800
C	2.79366000	-1.91388800	1.28262600
C	2.98790300	-1.45610300	-0.10311700
C	0.14348700	3.60325900	-0.33520600
C	1.43715300	2.89081800	-0.02228900
C	2.05309100	2.69503300	1.25680700
C	2.99161000	1.67880000	1.19747800
C	3.06394800	1.13367900	-0.12246900
C	3.65801600	-0.18062100	-0.56558400
H	-3.18988300	1.47327700	2.32216900
H	-1.20926600	3.19381700	2.34185200
H	-3.77790200	-1.60815500	2.04258500
H	-1.96848700	-3.51164500	2.03626500
H	1.20824800	-3.20007600	2.23505400
H	3.42548900	-1.63113500	2.11107600

H	1.91087800	3.36080800	2.09549300
H	3.68980400	1.43138000	1.98344300
H	-0.09347500	-3.70117900	-1.45946300
H	-0.16344800	-4.52766300	0.06373700
H	4.68706700	-0.20174500	-0.19844100
H	3.74525500	-0.19127100	-1.65688100
H	0.21238100	4.59102500	0.12691200
H	0.07977000	3.79786800	-1.40959400
H	-4.72146400	0.23164100	0.07221300
H	-3.88592100	0.27697400	-1.44884300
N	-1.87522000	1.99611000	-0.65296300
H	-1.91768000	2.05964000	-1.66332700
N	-2.00334600	-1.72251200	-0.72854800
H	-1.84606500	-1.56748500	-1.71615900
N	1.92716000	1.75274700	-0.77832300
N	1.77364900	-1.93643100	-0.73684600
H	1.71014600	-2.03687400	-1.74050200
H	1.78057300	1.67302900	-1.77650600
Ti	-3.23132500	3.53847000	-0.09841500
Ti	-3.53882300	-3.18527500	-0.71376300
Ti	3.43023500	-3.50724500	0.02292000
Ti	3.48348200	3.19850300	-0.65289900
H	4.55969000	4.16399100	0.35304000
H	3.50531700	3.30911100	-2.41525500
H	-4.03435800	4.44126100	1.18119300
H	-3.50818600	3.89397500	-1.80305000
H	-4.62607200	-4.19557300	0.23023300
H	-3.56400200	-3.18322900	-2.47594900
H	2.64644700	-4.44670400	-1.24472000
H	4.94159800	-4.16904300	0.62201500

Table S21: Optimized Structure of CXP-Ti_4-8H_2 system ($C_{20}H_{20}N_4Ti_4$-H_{16})

C	3.51234600	-1.20411000	1.08935000
C	2.87836800	-1.63454600	-0.11879600
C	3.18530600	0.70965900	-0.12775300
C	3.69775500	0.16229000	1.07921100
C	2.92150000	2.14017000	-0.45665500
C	1.65924300	2.70405400	0.12027600
C	1.24755700	2.70062200	1.49234800
C	-0.11930800	2.84727300	1.59242800
C	-0.69068600	2.94947000	0.29602600
C	-2.12100900	2.85516400	-0.12397600
C	-2.76501900	1.54091900	0.14874400
C	-3.66000000	1.16898200	1.12184800
C	-4.01154700	-0.19453700	0.96889100
C	-3.23349500	-0.72769000	-0.11263100
C	2.12796800	-2.90599600	-0.34373800
C	0.72654500	-2.92193800	0.17903200
C	0.24066400	-2.65072400	1.48706800
C	-1.12881300	-2.48933000	1.45563700

C	-1.62883800	-2.65751600	0.12397600
C	-2.91600800	-2.14405900	-0.45228800
H	4.26809500	0.73657800	1.79649800
H	3.91387900	-1.89428000	1.82081600
H	1.94740300	2.71427300	2.31842800
H	-0.68324500	2.99268100	2.50357100
H	-4.11568800	1.86796900	1.81191100
H	-4.63496300	-0.77605700	1.63222400
H	0.85814500	-2.69195600	2.37363000
H	-1.77353300	-2.37749700	2.31817800
H	-2.21854500	3.10198300	-1.18972500
H	-2.68497800	3.62698000	0.41181500
H	-3.75288400	-2.75071500	-0.08935900
H	-2.90884000	-2.30352100	-1.53980300
H	2.69266100	-3.70534700	0.15148100
H	2.11995200	-3.17397600	-1.40845800
H	3.77552200	2.71206500	-0.07555500
H	2.93063000	2.30199000	-1.54301200
N	2.49514400	-0.39098800	-0.75024200
H	2.07473900	-0.34362000	-1.67112000
N	0.39879500	2.61615000	-0.59698600
H	0.34750900	2.81261000	-1.59504700
N	-0.41464100	-2.67866400	-0.67445300
N	-2.48591300	0.39040500	-0.62607800
H	-1.66374300	0.31292100	-1.21038300
H	-0.42899400	-2.98384800	-1.64568400
Ti	4.53784800	-0.64436600	-1.03962900
Ti	0.64488400	4.57710000	0.08396000
Ti	-4.55928600	0.51538600	-1.11261100
Ti	-0.63152800	-4.53865500	0.25451600
H	0.38367900	-5.29981300	1.44476500
H	-0.68237700	-5.35526000	-1.32648300
H	5.86102100	0.32928000	-0.46932000
H	4.33682200	-0.70796300	-2.80805100
H	-0.29477100	5.48482500	1.23194900
H	0.67123400	5.18616900	-1.58648800
H	-4.09782100	1.84935100	-2.13802000
H	-5.49894300	-0.69994200	-1.99492800
H	-5.63610400	1.95823100	-0.61169300
H	-5.97052800	1.35435800	-0.15035600
H	-2.12242300	-4.97144100	1.34546800
H	-1.47493600	-5.10963100	1.84126200
H	5.47590300	-2.18821200	-0.45640300
H	5.88526100	-1.56438700	-0.09840700
H	2.20114000	5.14828800	1.00661900
H	1.58867000	5.35141200	1.52283700

Table S22: Optimized Structure of CXP-Ti_4-12H_2 system ($C_{20}H_{20}N_4Ti_4$-H_{24})

C	3.59990600	-0.48689900	1.25091000
C	3.06459400	-1.00210200	0.04450300

C	2.93753900	1.33599800	0.04055800
C	3.52989100	0.90185900	1.24308300
C	2.39970900	2.67910200	-0.32126300
C	1.01360000	2.95492900	0.16287000
C	0.52119300	3.09252000	1.48373000
C	-0.86668300	3.02816400	1.48257800
C	-1.33075200	2.82986100	0.16324300
C	-2.68053300	2.39646100	-0.31302200
C	-3.06458000	1.00207000	0.04461300
C	-3.60012100	0.48683200	1.25089900
C	-3.53012000	-0.90192900	1.24302000
C	-2.93755600	-1.33600700	0.04058000
C	2.68051300	-2.39648100	-0.31314700
C	1.33073500	-2.82986300	0.16314300
C	0.86670100	-3.02815200	1.48249600
C	-0.52117600	-3.09250900	1.48368600
C	-1.01361500	-2.95493200	0.16284000
C	-2.39973100	-2.67910200	-0.32127200
H	3.96535700	1.56987000	1.97303500
H	4.09312600	-1.09512300	1.99761200
H	1.14526900	3.32852400	2.33578900
H	-1.51691400	3.20569600	2.32781000
H	-4.09346400	1.09503000	1.99754200
H	-3.96573400	-1.56996800	1.97285700
H	1.51695100	-3.20567900	2.32771300
H	-1.14523100	-3.32850200	2.33576300
H	-2.76567600	2.53568200	-1.39967900
H	-3.42895400	3.06877100	0.12298500
H	-3.07679500	-3.43122000	0.09935000
H	-2.43391100	-2.84360000	-1.40693700
H	3.42893400	-3.06880600	0.12283800
H	2.76564000	-2.53569400	-1.39980600
H	3.07677700	3.43120700	0.09937500
H	2.43389200	2.84362800	-1.40692500
N	2.56502300	0.14355600	-0.65323000
H	1.95710600	0.10501200	-1.45799100
N	-0.14340500	2.61310100	-0.61840600
H	-0.13502400	2.72208500	-1.63103100
N	0.14336700	-2.61309900	-0.61847400
N	-2.56498000	-0.14355400	-0.65317100
H	-1.95623400	-0.10495000	-1.45730400
H	0.13495600	-2.72215200	-1.63109400
Ti	4.67846200	0.22228700	-0.73245300
Ti	-0.23963400	4.70060400	-0.06559100
Ti	-4.67834300	-0.22224000	-0.73271600
Ti	0.23961400	-4.70060400	-0.06563000
H	1.32797700	-5.72440400	0.85932500
H	-0.83527200	-5.13790600	-1.39647500
H	5.92373000	1.32944200	-0.17148600
H	4.75952500	-0.85596600	-2.12918600
H	-1.32795900	5.72443100	0.85938000

H	0.83520400	5.13787500	-1.39648700
H	-4.75944600	0.85605500	-2.12941600
H	-5.92364600	-1.32946000	-0.17197300
H	-5.71759700	1.27972900	-0.25961500
H	-6.01591200	0.70229200	0.24602000
H	-1.25376200	-5.57179500	0.69939400
H	-0.67104100	-5.71950100	1.25973800
H	5.71758700	-1.27970700	-0.25919200
H	6.01591300	-0.70225300	0.24642500
H	1.25377600	5.57179700	0.69936600
H	0.67107200	5.71952300	1.25972200
H	4.31295200	1.13610800	-2.33820600
H	4.54767200	1.74518700	-1.82806400
H	-1.76611600	4.86984600	-1.15281200
H	-1.15095700	4.84015500	-1.70967400
H	-4.54744000	-1.74513100	-1.82833800
H	-4.31257100	-1.13607400	-2.33841900
H	1.15088000	-4.84017800	-1.70974500
H	1.76605800	-4.86985400	-1.15290400

Table S23: Optimized Structure of CXP-Ti_4-16H_2 system ($C_{20}H_{20}N_4Ti_4$-H_{32})

C	-3.59696000	0.28110200	1.26157700
C	-3.13976300	0.82367200	0.03542600
C	-2.84157300	-1.49770800	0.04506600
C	-3.43260100	-1.09983500	1.25952900
C	-2.21935700	-2.80395400	-0.31723800
C	-0.81949800	-2.99574900	0.16695400
C	-0.32509600	-3.07767800	1.48861200
C	1.05907400	-2.94559400	1.48894700
C	1.51022200	-2.74392700	0.16606700
C	2.83375300	-2.23932500	-0.31403800
C	3.13976200	-0.82367200	0.03543400
C	3.59699300	-0.28105800	1.26155300
C	3.43263300	1.09987900	1.25945800
C	2.84157100	1.49770400	0.04499500
C	-2.83375500	2.23931600	-0.31409000
C	-1.51022700	2.74393100	0.16600300
C	-1.05906300	2.94562600	1.48887200
C	0.32510700	3.07771300	1.48852500
C	0.81950500	2.99575900	0.16686400
C	2.21935500	2.80394100	-0.31734300
H	-3.78821000	-1.79051400	2.01082400
H	-4.10660000	0.85908400	2.02134000
H	-0.93834700	-3.32576000	2.34530300
H	1.71523900	-3.05791800	2.34012100
H	4.10665500	-0.85901100	2.02132400
H	3.78826100	1.79058800	2.01071600
H	-1.71522100	3.05797700	2.34004700
H	0.93836300	3.32581800	2.34520400
H	2.92758100	-2.37923100	-1.39981900

H	3.61848700	-2.86537000	0.12764600
H	2.84847100	3.59720000	0.10264900
H	2.24251200	2.96862200	-1.40329800
H	-3.61848900	2.86537400	0.12757700
H	-2.92758500	2.37919600	-1.39987400
H	-2.84846300	-3.59720200	0.10278900
H	-2.24252800	-2.96866600	-1.40318800
N	-2.58115100	-0.28984200	-0.66589000
H	-2.02502300	-0.21331200	-1.50423200
N	0.31634500	-2.60940600	-0.61918400
H	0.31631800	-2.76323300	-1.62634600
N	-0.31635900	2.60945900	-0.61924700
N	2.58114500	0.28981600	-0.66592100
H	2.02491100	0.21323300	-1.50418700
H	-0.31630300	2.76282100	-1.62645800
Ti	-4.69507400	-0.52100400	-0.67165300
Ti	0.53149300	-4.68976400	-0.00543800
Ti	4.69505700	0.52097500	-0.67174000
Ti	-0.53148700	4.68977400	-0.00556100
H	-1.68985800	5.50482000	1.04073000
H	0.61142500	5.07411600	-1.29360400
H	-5.74152100	-1.72508500	0.07556200
H	-4.73155400	0.62221600	-2.01556000
H	1.68984100	-5.50481100	1.04087100
H	-0.61147900	-5.07411800	-1.29342000
H	4.73151600	-0.62228800	-2.01561100
H	5.74150600	1.72510400	0.07539500
H	5.78194900	-0.94314000	-0.14294500
H	6.02516600	-0.36275200	0.38477700
H	0.91521100	5.60138500	0.83394800
H	0.33072700	5.66300200	1.40414800
H	-5.78197200	0.94311600	-0.14286400
H	-6.02517000	0.36273300	0.38487000
H	-0.91516400	-5.60139500	0.83415100
H	-0.33066300	-5.66296900	1.40433100
H	-4.25677200	-1.43077000	-2.27002000
H	-4.42979200	-2.04965600	-1.74390100
H	2.07400700	-4.71411700	-1.08425700
H	1.46267900	-4.74497100	-1.64975800
H	4.42976400	2.04959800	-1.74403000
H	4.25672200	1.43069900	-2.27012400
H	-1.46261900	4.74493300	-1.64989800
H	-2.07397300	4.71411800	-1.08442000
H	6.20913600	0.44399000	-1.91814400
H	6.44144700	1.02278700	-1.40219300
H	-0.44800600	6.48760600	-0.79188900
H	-1.02317500	6.57480400	-0.23064000
H	-6.20917700	-0.44406400	-1.91803600
H	-6.44147700	-1.02284400	-1.40206200
H	0.44798700	-6.48759100	-0.79176100
H	1.02315800	-6.57480000	-0.23051600

Table S24: Optimized Structure of MeCXP ($C_{28}H_{36}N_4$)

C	-0.36384900	-3.58704800	-1.24992500
N	0.23818100	-2.45195100	0.57862800
H	0.23292100	-2.46872100	1.73436200
C	1.05464000	-3.43901400	-1.25076500
C	1.41183300	-2.76859700	-0.10942400
C	-0.84751400	-2.98823700	-0.10826500
C	2.79301700	-2.28086900	0.28860500
C	3.01909000	-2.36045200	1.81515100
H	4.01905600	-2.00378500	2.05901700
H	2.92152700	-3.40574400	2.16455800
H	2.30139700	-1.74371300	2.38601500
C	3.84422700	-3.17139600	-0.39435100
H	3.78897000	-3.10690800	-1.48662200
H	3.69729900	-4.22162200	-0.09919800
H	4.85873600	-2.85623800	-0.09544200
C	-3.83270200	0.35531700	-1.15249100
N	-2.38760200	-0.25618600	0.39873700
H	-1.60006700	-0.20523000	1.08252800
C	-3.70469200	-1.06308900	-1.17793700
C	-2.79790800	-1.42011600	-0.19110200
C	-3.00751400	0.83910600	-0.16260700
C	-2.31126500	-2.77588700	0.29093400
C	-2.51652300	-2.88785500	1.81774300
H	-2.21922200	-3.87891800	2.16721200
H	-3.57242400	-2.71048100	2.05241200
H	-1.92541100	-2.13866100	2.37800100
C	-3.17384400	-3.85516500	-0.38114800
H	-3.13023200	-3.78564900	-1.47355500
H	-4.21472900	-3.74907900	-0.09101700
H	-2.82834300	-4.85264200	-0.08653900
C	3.82823200	-0.32785000	-1.17093600
N	2.40156000	0.22195200	0.41652200
H	1.68711500	0.13696600	1.16070500
C	3.69022700	1.09055900	-1.14588700
C	2.78896400	1.41025000	-0.15532900
C	3.01856100	-0.84897500	-0.18355000
C	2.25334200	2.75665600	0.28728300
C	2.20234500	2.82160100	1.83464500
H	1.77823600	3.78639300	2.16178200
H	3.22891900	2.73935300	2.24658100
H	1.61805200	2.02900200	2.29045400
C	3.16078200	3.87399200	-0.21832500
H	3.19095200	3.88213600	-1.31085500
H	4.18428500	3.72365300	0.15909600
H	2.79797800	4.84520200	0.12394800
C	0.35923300	3.72441100	-1.30339700
N	-0.23019100	2.39794800	0.35647500

H	-0.17964200	1.85938400	1.21822300
C	-1.05925600	3.57639100	-1.30295400
C	-1.40881200	2.75882300	-0.25704600
C	0.86053500	2.97844300	-0.25793300
C	-2.72954700	2.25369400	0.28948700
C	-2.69047000	2.30824900	1.83673900
H	-3.66607600	2.01284700	2.25967500
H	-2.44909600	3.32527800	2.18337400
H	-1.94508200	1.63018100	2.28189700
C	-3.84538900	3.17230600	-0.19520300
H	-3.88925300	3.19337600	-1.28762800
H	-3.66624600	4.19622600	0.15718700
H	-4.80957100	2.83874700	0.18278300
H	0.94155600	4.30465400	-2.00282500
H	-1.76077700	4.04176600	-1.99189400
H	-4.49219400	0.95357300	-1.78109800
H	-4.26026700	-1.74967700	-1.81134500
H	-0.96325200	-4.03263800	-2.05263000
H	1.71917900	-3.76172100	-2.05413400
H	4.19289800	1.79006700	-1.80498200
H	4.47471600	-0.90119300	-1.82465500

Table S25: Optimized Structure of MeCXP-Ti_4 ($C_{28}H_{36}N_4Ti_4$)

C	2.91180700	1.26865600	-1.49135300
N	2.18030400	1.58515000	0.62927300
H	1.82332300	1.32480800	1.53741900
C	2.10413000	2.37912400	-1.49106600
C	1.70248700	2.70356300	-0.16225500
C	3.09709300	0.78644000	-0.16262200
C	0.57050500	3.61224600	0.27138400
C	0.60201100	3.81286200	1.78539500
H	-0.19194100	4.50328700	2.09100000
H	1.56811400	4.22966200	2.09081000
H	0.45715600	2.87976500	2.34707500
C	0.78644000	4.97780500	-0.38591000
H	0.77582700	4.91470300	-1.47894900
H	1.75694600	5.38525200	-0.08465600
H	-0.01056400	5.66492200	-0.08383200
C	1.26865600	-2.91180700	-1.49135300
N	1.58515000	-2.18030400	0.62927300
H	1.32480800	-1.82332300	1.53741900
C	2.37912400	-2.10413000	-1.49106600
C	2.70356300	-1.70248700	-0.16225500
C	0.78644000	-3.09709300	-0.16262200
C	3.61224600	-0.57050500	0.27138400
C	3.81286200	-0.60201100	1.78539500
H	4.50328700	0.19194100	2.09100000
H	4.22966200	-1.56811400	2.09081000
H	2.87976500	-0.45715600	2.34707500
C	4.97780500	-0.78644000	-0.38591000

H	4.91470300	-0.77582700	-1.47894900
H	5.38525200	-1.75694600	-0.08465600
H	5.66492200	0.01056400	-0.08383200
C	-1.26865600	2.91180700	-1.49135300
N	-1.58515000	2.18030400	0.62927300
H	-1.32480800	1.82332300	1.53741900
C	-2.37912400	2.10413000	-1.49106600
C	-2.70356300	1.70248700	-0.16225500
C	-0.78644000	3.09709300	-0.16262200
C	-3.61224600	0.57050500	0.27138400
C	-3.81286200	0.60201100	1.78539500
H	-4.50328700	-0.19194100	2.09100000
H	-4.22966200	1.56811400	2.09081000
H	-2.87976500	0.45715600	2.34707500
C	-4.97780500	0.78644000	-0.38591000
H	-4.91470300	0.77582700	-1.47894900
H	-5.38525200	1.75694600	-0.08465600
H	-5.66492200	-0.01056400	-0.08383200
C	-2.91180700	-1.26865600	-1.49135300
N	-2.18030400	-1.58515000	0.62927300
H	-1.82332300	-1.32480800	1.53741900
C	-2.10413000	-2.37912400	-1.49106600
C	-1.70248700	-2.70356300	-0.16225500
C	-3.09709300	-0.78644000	-0.16262200
C	-0.57050500	-3.61224600	0.27138400
C	-0.60201100	-3.81286200	1.78539500
H	0.19194100	-4.50328700	2.09100000
H	-1.56811400	-4.22966200	2.09081000
H	-0.45715600	-2.87976500	2.34707500
C	-0.78644000	-4.97780500	-0.38591000
H	-0.77582700	-4.91470300	-1.47894900
H	-1.75694600	-5.38525200	-0.08465600
H	0.01056400	-5.66492200	-0.08383200
H	-3.46446200	-0.90747000	-2.34850100
H	-1.93057500	-3.01673900	-2.34778100
H	0.90747000	-3.46446200	-2.34850100
H	3.01673900	-1.93057500	-2.34778100
H	3.46446200	0.90747000	-2.34850100
H	1.93057500	3.01673900	-2.34778100
H	-3.01673900	1.93057500	-2.34778100
H	-0.90747000	3.46446200	-2.34850100
Ti	-2.76103200	3.79659400	0.16777600
Ti	3.79659400	2.76103200	0.16777600
Ti	2.76103200	-3.79659400	0.16777600
Ti	-3.79659400	-2.76103200	0.16777600

Table S26: Optimized Structure of MeCXP-Ti_4-$4H_2$ ($C_{28}H_{36}N_4Ti_4$-H_8)

C	1.45392100	2.59540800	-1.56148400
C	1.11257200	2.95570600	-0.21961200
C	2.93308200	1.38359300	-0.24744700

C	2.50164900	1.69043500	-1.57914200
C	3.76533700	0.19432000	0.23379300
C	3.13495300	-1.14509700	-0.13856500
C	2.94270100	-1.70708700	-1.44082100
C	1.99472900	-2.71448900	-1.40759500
C	1.48488800	-2.89240400	-0.07946400
C	0.18323900	-3.56655500	0.35522300
C	-1.02259800	-2.80123400	-0.18402600
C	-1.46742000	-2.64267300	-1.48583300
C	-2.64542400	-1.83710100	-1.48012900
C	-2.96970100	-1.44375800	-0.10938200
C	-0.16529000	3.62316500	0.29547300
C	-1.43548200	2.87369400	-0.10591100
C	-1.93237700	2.61267900	-1.42459300
C	-2.86911500	1.59271100	-1.40606400
C	-3.06609800	1.10589700	-0.07697700
C	-3.72091100	-0.19902800	0.36980200
H	3.02413400	1.37573200	-2.46935500
H	1.05059800	3.08180700	-2.43652600
H	3.57133900	-1.48590300	-2.28974200
H	1.78334100	-3.38406100	-2.22725100
H	-1.01585300	-3.09910400	-2.35301400
H	-3.21876800	-1.55995300	-2.35093200
H	-1.72244200	3.23459700	-2.28122500
H	-3.48442100	1.31145400	-2.24672500
N	1.89961600	2.01430200	0.55793700
H	1.99112600	2.10341700	1.56086300
N	2.05933600	-1.75607400	0.61977300
H	1.98713100	-1.65423300	1.62256800
N	-2.00308000	1.77219200	0.65455800
N	-1.83840300	-1.98619700	0.61253700
H	-1.86014900	-2.10504100	1.61370300
H	-1.94879600	1.73825300	1.66315100
Ti	3.21175500	3.52913900	-0.14819800
Ti	3.58040600	-3.21302000	0.37668500
Ti	-3.39424900	-3.50631700	-0.32018800
Ti	-3.53831400	3.20125700	0.30350000
H	-4.47873100	4.12611700	-0.86585700
H	-3.77055800	3.44849000	2.03856600
H	3.96785100	4.32791300	-1.52506700
H	3.63758900	3.98855200	1.50382500
H	4.56519800	-4.15033900	-0.74146000
H	3.81276300	-3.36378100	2.11871200
H	-2.91629400	-4.41788000	1.11920500
H	-4.79432900	-4.12628300	-1.18554200
C	3.97126500	0.27951800	1.75932500
C	5.14931100	0.27026800	-0.45010700
C	-0.10044100	3.77198300	1.82826500
C	-0.24388700	5.03621500	-0.32890200
C	-5.14024100	-0.24372000	-0.23963800
C	-3.84931200	-0.23426600	1.90512000

C	0.17649400	-5.00024600	-0.22395700
C	0.12854500	-3.66767200	1.89263300
H	-0.72671200	-5.51944800	0.09532000
H	0.19733700	-4.99883900	-1.31578000
H	1.05508000	-5.54201500	0.13139100
H	-0.77846400	-4.19177400	2.20012300
H	0.99402900	-4.22356900	2.25761200
H	0.14021900	-2.68565500	2.37890800
H	-5.71938500	0.61893600	0.09394700
H	-5.11733200	-0.23146800	-1.33169200
H	-5.64873600	-1.15845200	0.06962100
H	-4.35197600	-1.15309200	2.21733200
H	-2.87567500	-0.19977400	2.40666700
H	-4.43416900	0.61623000	2.26147800
H	-1.15602000	5.53787800	-0.00183600
H	0.62116100	5.62592100	-0.02265000
H	-0.25175100	5.00034400	-1.42077700
H	-0.99046600	4.28692700	2.19533300
H	-0.04404700	2.80368300	2.33810200
H	0.77874000	4.35244200	2.11741800
H	5.07044000	0.26590200	-1.53954900
H	5.65462000	1.19198500	-0.15951400
H	5.76106600	-0.58313300	-0.15208100
H	3.02736600	0.21859400	2.31265100
H	4.60461200	-0.54079100	2.10199600
H	4.44957000	1.22496600	2.02497200

Table S27: Optimized Structure of MeCXP-Ti_4-8H_2 ($C_{28}H_{36}N_4Ti_4$-H_{16})

C	-0.45693300	2.39371800	-1.70608300
C	-1.16941200	2.70181800	-0.52658600
C	1.16588600	2.80247000	-0.10325400
C	0.90829100	2.47316200	-1.47562700
C	2.45718700	2.53496100	0.66564200
C	3.07257600	1.23015900	0.22007500
C	3.86993600	0.98188700	-0.94619100
C	3.81674600	-0.36197000	-1.28938800
C	3.01390600	-1.04895800	-0.36920000
C	2.64118000	-2.50269500	-0.23438500
C	1.16946200	-2.70170000	-0.52737200
C	0.45698300	-2.39333700	-1.70680600
C	-0.90824200	-2.47283100	-1.47638300
C	-1.16586600	-2.80244600	-0.10409300
C	-2.64113700	2.50278500	-0.23369600
C	-3.01385500	1.04909600	-0.36902800
C	-3.81657400	0.36237400	-1.28951900
C	-3.86978200	-0.98158900	-0.94673300
C	-3.07257300	-1.23020100	0.21955900
C	-2.45718500	-2.53510900	0.66483300
H	1.67800200	2.42051600	-2.23413600
H	-0.92381400	2.28238600	-2.67744900

H	4.49463800	1.72355000	-1.42393000
H	4.42573100	-0.84188300	-2.04172600
H	0.92388300	-2.28174700	-2.67813300
H	-1.67796500	-2.41996300	-2.23486600
H	-4.42545300	0.84249200	-2.04181100
H	-4.49439600	-1.72312400	-1.42478500
N	-0.15679300	2.70320800	0.49952900
H	-0.35462200	3.14046400	1.39596900
N	2.45867500	-0.05472400	0.50287100
H	1.59128300	-0.17661700	1.01235800
N	-2.45874400	0.05459900	0.50280700
N	0.15680200	-2.70344900	0.49872700
H	0.35461400	-3.14089200	1.39507400
H	-1.59162000	0.17639500	1.01276600
Ti	0.04627200	4.49732300	-0.79286200
Ti	4.44386100	-0.17717600	1.05793500
Ti	-0.04633200	-4.49714100	-0.79404800
Ti	-4.44400600	0.17689900	1.05765200
H	-5.72661600	1.18752700	0.43425000
H	-4.33761200	0.12271800	2.82652800
H	0.65478200	5.34281900	-2.22519100
H	-1.34745000	5.18563600	-0.00467400
H	5.72650400	-1.18760800	0.43430300
H	4.33751200	-0.12352100	2.82682600
H	1.34719900	-5.18583900	-0.00585400
H	-0.65473400	-5.34208900	-2.22674000
C	2.19402000	2.51891000	2.16984700
C	3.47060800	3.63845700	0.34900300
C	-2.98291000	2.97895400	1.18308700
C	-3.46550500	3.30934200	-1.23559300
C	-3.47056400	-3.63856400	0.34793100
C	-2.19398800	-2.51941500	2.16903200
C	3.46562100	-3.30885800	-1.23654300
C	2.98295700	-2.97936700	1.18223300
H	3.24771300	-4.37142800	-1.10679100
H	3.22795900	-3.03417400	-2.27028900
H	4.53357600	-3.13685500	-1.06935300
H	2.68714500	-4.02447500	1.31944100
H	4.06873100	-2.91597700	1.32792800
H	2.50710800	-2.37042500	1.96198300
H	-4.45833200	-3.37682700	0.74208000
H	-3.55213900	-3.81522300	-0.73000300
H	-3.15995400	-4.58041300	0.80648600
H	-1.78172300	-3.47820700	2.50589100
H	-1.49640700	-1.72728200	2.46623200
H	-3.13179400	-2.34055500	2.70344600
H	-4.53347800	3.13753800	-1.06832300
H	-3.24736100	4.37184200	-1.10563800
H	-3.22800600	3.03483300	-2.26942400
H	-4.06870500	2.91571600	1.32869300
H	-2.50723200	2.36960200	1.96262500

H	-2.68690000	4.02394600	1.32074800
H	3.55210500	3.81544900	-0.72888200
H	3.16009900	4.58018000	0.80788200
H	4.45839400	3.37653400	0.74298600
H	1.49630500	1.72683000	2.46686700
H	3.13181400	2.33973800	2.70417700
H	1.78195700	3.47768900	2.50698800
H	5.51569700	1.36781100	1.18401200
H	5.91180800	0.91716700	0.61501600
H	-5.51575200	-1.36816200	1.18314300
H	-5.91187700	-0.91733600	0.61428400
H	1.09682500	5.14100300	0.62189000
H	0.30619500	5.32090700	0.84557300
H	-0.30657000	-5.32116500	0.84413000
H	-1.09715300	-5.14114700	0.62039300

Table S28: Optimized Structure of MeCXP-Ti_4-12H_2 ($C_{28}H_{36}N_4Ti_4$-H_{24})

C	-1.38459900	2.63361900	-1.50402500
C	-1.87749200	2.49336400	-0.18951600
C	0.40334700	3.11973300	-0.13971300
C	-0.04907300	3.01863700	-1.48175500
C	1.83885900	3.11431200	0.36441600
C	2.55496500	1.85789100	-0.09744100
C	2.89634000	1.45312500	-1.40298900
C	3.31549300	0.12787800	-1.40424800
C	3.23692200	-0.40606800	-0.08878900
C	3.17327700	-1.87228500	0.30197100
C	1.87750400	-2.49333000	-0.18964900
C	1.38476700	-2.63343700	-1.50423500
C	0.04923700	-3.01845200	-1.48216900
C	-0.40334200	-3.11968600	-0.14020200
C	-3.17333500	1.87225600	0.30185700
C	-3.23695800	0.40608300	-0.08909100
C	-3.31542200	-0.12770300	-1.40462900
C	-2.89622600	-1.45293500	-1.40350800
C	-2.55496200	-1.85786300	-0.09798100
C	-1.83890700	-3.11434400	0.36378100
H	0.53879200	3.29403600	-2.34504600
H	-1.99968200	2.57424500	-2.39191600
H	2.95326700	2.12449700	-2.24925000
H	3.73399900	-0.39895900	-2.24918900
H	1.99996200	-2.57393700	-2.39204100
H	-0.53851900	-3.29375400	-2.34556600
H	-3.73388600	0.39922700	-2.24953200
H	-2.95306600	-2.12420600	-2.24985400
N	-0.72246900	2.67342500	0.63828400
H	-0.74757900	2.65782400	1.64826100
N	2.64849400	0.66023700	0.68061000
H	2.49482900	0.62687200	1.67886200
N	-2.64851900	-0.66029700	0.68020200

N	0.72238100	-2.67350500	0.63798800
H	0.74735400	-2.65799100	1.64796900
H	-2.49509500	-0.62710400	1.67849700
Ti	-1.20423900	4.59375100	-0.18079800
Ti	4.65934800	1.21961700	0.16791700
Ti	1.20426800	-4.59372000	-0.18127400
Ti	-4.65932100	-1.21968400	0.16738900
H	-5.97999200	-0.42699200	-0.67711300
H	-4.85676300	-2.45256700	1.42426700
H	-0.34002800	5.76912600	-1.16088400
H	-2.47964900	4.98582800	0.98395700
H	5.97992400	0.42706200	-0.67686500
H	4.85693600	2.45223900	1.42502700
H	2.47954300	-4.98587700	0.98359400
H	0.34026000	-5.76897800	-1.16168100
C	1.88068000	3.20652800	1.88846400
C	2.56985300	4.32563600	-0.22353300
C	-3.28951000	2.05706300	1.81337800
C	-4.35269500	2.58473300	-0.36752900
C	-2.56984900	-4.32559400	-0.22439100
C	-1.88088100	-3.20675900	1.88780900
C	4.35274100	-2.58465400	-0.36735700
C	3.28925400	-2.05728500	1.81348000
H	4.40027100	-3.61818700	-0.01644000
H	4.25290700	-2.60156700	-1.45790800
H	5.28463800	-2.06334600	-0.13142900
H	3.17282100	-3.11711900	2.06311700
H	4.27142400	-1.73769500	2.16759500
H	2.53215000	-1.48596000	2.36864200
H	-3.59121200	-4.35836100	0.16317600
H	-2.61312300	-4.28348400	-1.31793400
H	-2.04405700	-5.24729600	0.03434400
H	-1.44325500	-4.14691100	2.23285200
H	-1.33250800	-2.38556700	2.37003600
H	-2.92054700	-3.16876500	2.22681600
H	-5.28463300	2.06342400	-0.13176800
H	-4.40023400	3.61822800	-0.01649400
H	-4.25273400	2.60178100	-1.45806700
H	-4.27171400	1.73739300	2.16732300
H	-2.53245600	1.48569700	2.36856700
H	-3.17315500	3.11687000	2.06316300
H	2.61324600	4.28365500	-1.31707700
H	2.04402000	5.24730200	0.03524100
H	3.59116800	4.35837600	0.16415900
H	1.33220900	2.38531100	2.37053700
H	2.92030900	3.16844200	2.22757400
H	1.44307000	4.14666200	2.23357600
H	5.12877500	2.82828300	-0.72007700
H	5.43137100	2.25834400	-1.22508400
H	-2.76705900	4.95340200	-1.19102400
H	-2.17418700	5.17263700	-1.71261600

H	-5.12879800	-2.82815300	-0.72094100
H	-5.43147800	-2.25809500	-1.22576500
H	2.76725000	-4.95322200	-1.19130900
H	2.17445400	-5.17239900	-1.71300800
H	0.03337200	5.33475300	1.01094800
H	-0.64218400	5.20808900	1.48354300
H	5.25982000	-0.06569900	1.38699700
H	5.04899600	0.58078800	1.87124300
H	0.64203800	-5.20833600	1.48291200
H	-0.03344900	-5.33498900	1.01022100
H	-5.25970200	0.06535400	1.38681600
H	-5.04885100	-0.58125200	1.87088900

Table S29: Optimized Structure of MeCXP-Ti_4-16H_2 ($C_{28}H_{36}N_4Ti_4$-H_{32})

C	-0.96445800	2.81975500	-1.46278400
C	-1.46305700	2.76825100	-0.14586500
C	0.88697600	3.04725900	-0.11630200
C	0.41395600	3.00688200	-1.45482600
C	2.30897600	2.81056900	0.37673900
C	2.81464600	1.45585700	-0.09065000
C	2.99499400	0.98344900	-1.40535500
C	3.19319400	-0.39340900	-1.40442600
C	3.11052800	-0.89051600	-0.07602400
C	2.82928800	-2.32278300	0.35316300
C	1.46301000	-2.76821600	-0.14602000
C	0.96437100	-2.81983700	-1.46290700
C	-0.41403600	-3.00703700	-1.45487600
C	-0.88701600	-3.04732300	-0.11632500
C	-2.82930300	2.32276400	0.35336200
C	-3.11052700	0.89053200	-0.07593400
C	-3.19298000	0.39349200	-1.40437500
C	-2.99477200	-0.98336600	-1.40534600
C	-2.81464400	-1.45586000	-0.09063700
C	-2.30899400	-2.81057600	0.37673800
H	1.03014300	3.16869900	-2.32643800
H	-1.58692300	2.84360100	-2.34721200
H	3.09803300	1.62571400	-2.26995800
H	3.45300600	-0.99160200	-2.26463300
H	1.58679200	-2.84379000	-2.34736200
H	-1.03023300	-3.16899600	-2.32645500
H	-3.45264100	0.99173400	-2.26459300
H	-3.09760100	-1.62558800	-2.27000700
N	-0.28731400	2.78082400	0.66775800
H	-0.31342500	2.80788000	1.67739400
N	2.75468200	0.26631300	0.69993600
H	2.72597800	0.28153200	1.71039300
N	-2.75483700	-0.26635200	0.70002700
N	0.28731000	-2.78072600	0.66765100
H	0.31347100	-2.80769400	1.67728700
H	-2.72615800	-0.28160400	1.71048100

Ti	-0.47371800	4.75501600	-0.18405000
Ti	4.80524500	0.48223300	0.03506500
Ti	0.47371600	-4.75498300	-0.18388600
Ti	-4.80524500	-0.48218700	0.03488800
H	-5.79908100	0.55090900	-0.99119700
H	-5.05147700	-1.73449400	1.25137200
H	0.59487400	5.64026600	-1.27152500
H	-1.73703900	5.12260100	0.98971700
H	5.79915700	-0.55068200	-0.99113800
H	5.05132900	1.73442400	1.25167900
H	1.73701800	-5.12254800	0.98991600
H	-0.59470000	-5.64028800	-1.27146100
C	2.37277400	2.89166700	1.90012900
C	3.21927900	3.89223200	-0.21243600
C	-2.88967100	2.46723700	1.87252500
C	-3.90172300	3.22440600	-0.26550800
C	-3.21930200	-3.89223800	-0.21244000
C	-2.37278400	-2.89171000	1.90012400
C	3.90166600	-3.22442400	-0.26578100
C	2.88968100	-2.46734200	1.87231400
H	3.75343500	-4.25018800	0.07875300
H	3.85714200	-3.22014900	-1.36045200
H	4.89683400	-2.87176500	0.01590300
H	2.64514300	-3.49755500	2.14889100
H	3.89353700	-2.25158100	2.24501100
H	2.18699000	-1.79686300	2.38546200
H	-4.23737500	-3.74912800	0.15733800
H	-3.23826900	-3.85792100	-1.30724100
H	-2.85558800	-4.88366100	0.06562500
H	-2.08357600	-3.88586400	2.25017800
H	-1.71382300	-2.15840500	2.38432800
H	-3.39755900	-2.70102100	2.23278500
H	-4.89687200	2.87171400	0.01620200
H	-3.75350700	4.25015700	0.07907200
H	-3.85724200	3.22018200	-1.36018100
H	-3.89353000	2.25149700	2.24522400
H	-2.18700600	1.79670000	2.38563400
H	-2.64507600	3.49742400	2.14915000
H	3.23823600	3.85792500	-1.30723700
H	2.85559200	4.88366300	0.06564000
H	4.23735400	3.74910800	0.15732800
H	1.71377400	2.15838600	2.38431100
H	3.39754100	2.70092300	2.23278600
H	2.08362300	3.88582700	2.25021300
H	5.43604800	1.99518000	-0.95389300
H	5.58734500	1.38329300	-1.47186900
H	-1.96578200	5.29706200	-1.25350500
H	-1.34437700	5.38968600	-1.77474700
H	-5.43600000	-1.99497400	-0.95429100
H	-5.58727500	-1.38302600	-1.47221000
H	1.96569100	-5.29706600	-1.25350700

H	1.34418600	-5.38969100	-1.77463700
H	0.87147100	5.23552400	1.03524500
H	0.18094200	5.20513800	1.50597500
H	5.17474800	-0.88523500	1.25854600
H	5.09964300	-0.20488700	1.74205300
H	-0.18082100	-5.20506800	1.50619200
H	-0.87140900	-5.23547700	1.03554800
H	-5.17468500	0.88489700	1.25886000
H	-5.09957600	0.20437100	1.74209700
H	0.91457000	-6.60765800	0.30091300
H	0.31251300	-6.70520600	-0.23304800
H	-6.59505100	-0.93014800	0.70714700
H	-6.75487300	-0.33891000	0.17673600
H	-0.91438700	6.60784200	0.30057400
H	-0.31233800	6.70517600	-0.23343500
H	6.59496400	0.93017200	0.70758100
H	6.75488200	0.33908100	0.17704500