Supportive information

Electronic Paper Display Design Based on a Tristable [2]Catenane

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Abstract

The supportive information has been organized as below:
Section 1 describes the calculation method to obtain geometries and energies and detailed results.
Section 2 describes the calculation method to obtain UV-vis spectrum and detailed results.
Section 3 describes the calculation method to obtain binding energy between CBPQT4+ ring with donor groups and obtained geometries.
Section 4 lists those complex structures

Section 1. Geometries and energies

We use the B3LYP flavor of Kohn-Sham density functional theory (DFT), which combines the B3 nonlocal hybrid GGA exchange-functional (generalized gradient approximation) with the Lee-Yang-Parr local and nonlocal correlation functional. The exchange functional combines exact Hartree-Fock (HF) exchange with the local exchange functional of Slater and uses the Becke nonlocal gradient correction with the Vosko-Wilk-Nusair exchange functional.

All ab initio cluster calculations were carried out with the Jaguar programs. The small components such as TTF, DNP etc has been optimized at 6-31G*. The vibration frequencies have been also calculated at same level. Then we re-optimized those components under the solvent module with dielectric constant 36.5 and probe radius 2.18 responding to the CH3CN solvent, which is generally used in experiments involved with Rotaxane molecules. We used the 6-31G**++ basis set to calculate the single point energy of target molecules under solvent model.

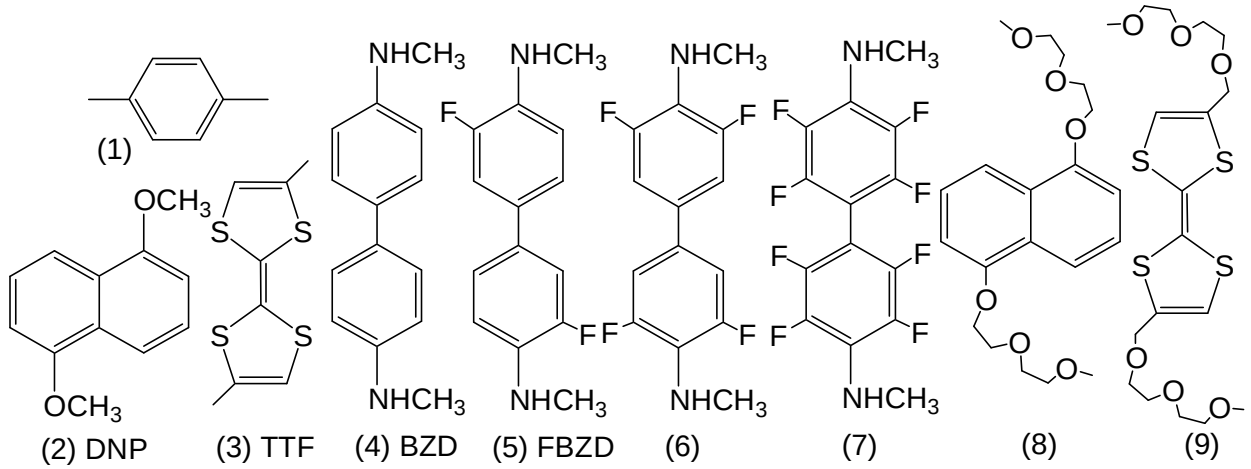


Figure S1. The candidates that have been screened in this work.

Section 2. UV-vis adsorption of complex

The total systems (donor groups + CBPQT4+) usually are consisted of hundred atoms, which is too time-consuming to perform a TD-DFT calculation. Moreover, TD-DFT still can not give accurate adsorption spectrums. We consider to develop an empirical model to predict the UV-spectrum. In rotaxane system, the maximum adsorption of complex is contributed from the charge transfer from HOMO of donor groups to LUMO of $CBPQT^{4+}$ ring. A scheme of MO shifting has been shown in Figure S2.

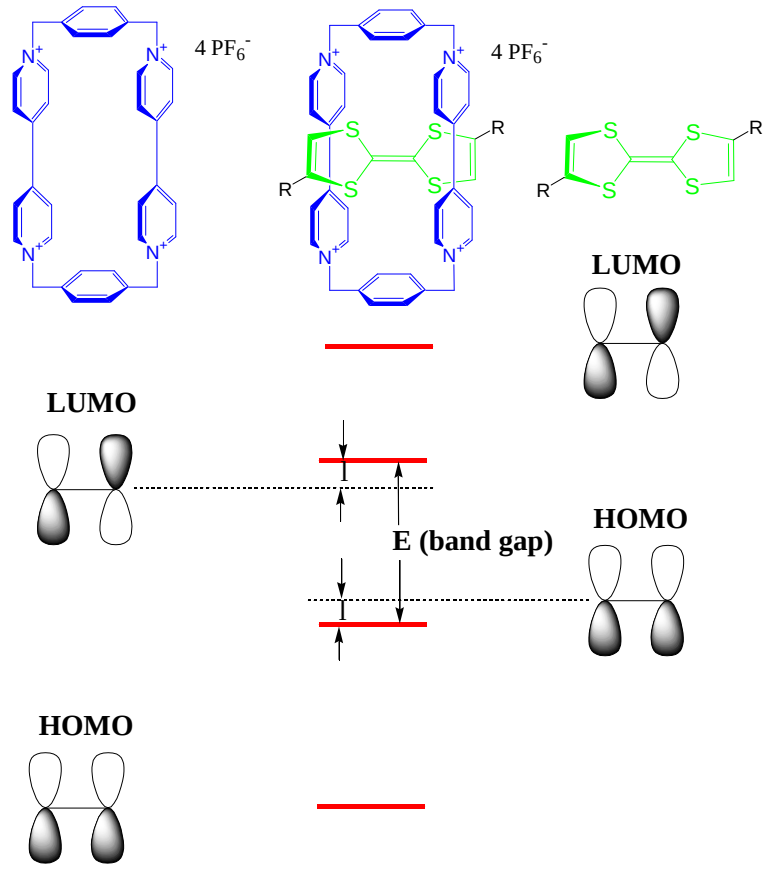


Figure S2. MO shift during the process of constructing the complex from CBPQ4+ ring and donor groups.

During the formation of the complex, we believe that the HOMO of complex mostly is contributed from the HOMO of donor groups and the LUMO of complex mostly is contributed from CBPQ4+ ring. The coupling between CBPQ4+ ring and donor groups leads to a shift of MO, which equal λ in Figure S2. Thus band gap can be written as:

$$E_{band} = E_{LUMO} - E_{HOMO} + 2l$$

It has been know that the band gap calculated from DFT usually underestimate the experimental value, around 40%. Thus we added a correct factor α to fit the experimental result, this α is expected to be around 0.6. The equation can be written as:

$$E_{band} = \frac{1}{a}(E_{LUMO} - E_{HOMO} + 2l)$$

The HOMO of donor groups were determined from B3LYP/6-31G**++ with solvent mode based on optimized structures at B3LYP/6-31G*.

The LUMO of the CBPQT4+ is determined by B3LYP/6-31G**++ with solvent model based on CBPQT4+ with four PF6- around. The structure of CBPQT4+ has been optimized at B3LYP/6-31G*. After optimization, the four PF6- was minimized by Dreiding Force Field with QM charges along with fixed CBPQT4+ structure. The distance between P atom and the N atom

Table 1 shows the fitting results. We found that λ = 0.0055 eV and α = 0.6645 gives closest fitting results to experiments. The largest error is 9nm. Thus we believe all those components follow similar rule. Cause λ come from the coupling between the CBPQ4+ ring and donor group, the small value we got, 0.0055 eV, suggests that the coupling between donor group and $CBPQT^{4+}$ is very weak and the effect can be ignored. The fitting result for α is 0.6645, which is close to 0.6 as in another empirical factor correct for DFT calculation for band gap.

Table S1. UV-vis spectrum from the fitting model and predict the unknown composites.

	(1)	DNP	TTF	BZD	FBZD	(5)	(6)
HOMO(Hartree)	-0.23501	-0.2099	-0.18016	-0.1893	-0.1949	-0.20575	-0.2190
HOMO(eV)	-6.40	-5.72	-4.91	-5.15	-5.31	-5.60	-5.96
LUMO(Hartree)	-0.1450	-0.1450	-0.1450	-0.1450	-0.1450	-0.1450	-0.1450
LUMO(eV)	-3.95	-3.95	-3.95	-3.95	-3.95	-3.95	-3.95
Band gap without correct (eV)	2.46	1.78	0.97	1.22	1.37	1.66	2.03
Band gap with correction (eV)	3.72	2.68	1.45	1.83	2.06	2.51	3.06
Calc. (nm)	333	462	853	677	601	494	405
Exp. (nm)	330	473	854	670			

Section 3. Binding energy of complex

We use B3LYP/6-31G* to optimize the structure of complex between $CBPQT^{4+}$ and donor groups. By using such optimized structure, we use BSSE to calculate the binding energy.

Tales S2. the binding energy between $CBPQT^{4+}$ and donor groups.

	DNPch3	**TTFch3**	**BZD**	**FBZD**	**TTFO3**	**DNPO3**
Ring (BSSE) (Hartree)	-1608.8536	-1608.8535	-1608.8558	-1608.8564	-1608.8536	-1608.8525
Self (BSSE) (Hartree)	-614.9784	-1902.4015	-652.6776	-851.1594	-2746.7949	-1230.3363
Complex (BSSE) (Hartree)	-2223.8404	-3511.2784	-2261.5704	-2460.0433	-4355.7613	-2839.2655
binding (kcal/mole)	5.29	14.71	23.25	17.25	70.79	48.18

Section 4. Complex structures

(1) $CBPQT^{4+}$ + $4PF_6^-$ structure

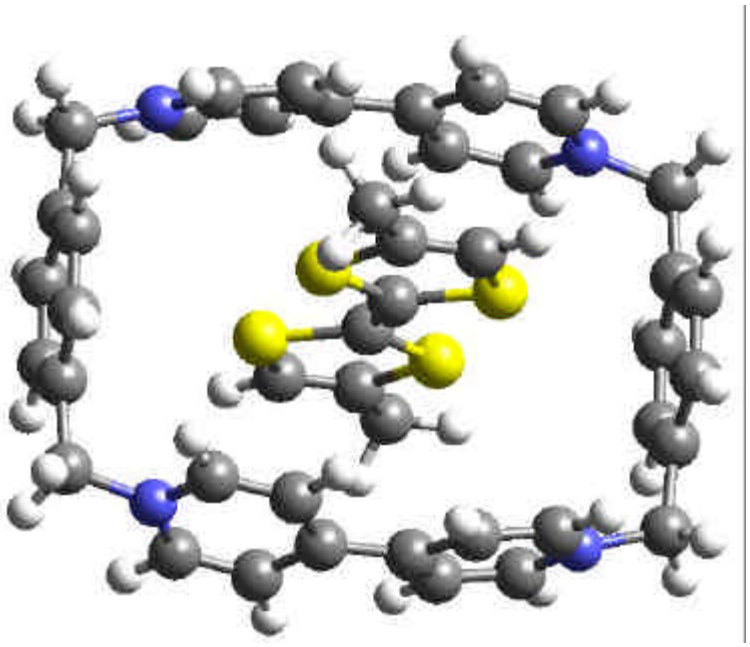
The CBPQT4+ ring was optimized at B3LYP/6-31G*. The positions of PF6- s were minimized by Dreiding force field with QM charges. The obtained structure shows that the distance between P atoms and N atoms range from 3.9-4.1 Å, which is in good agreement with experimental crystal data. Then single point energy was performed at B3LYP/6-31G**++ based on geometry obtained above with solvent model. The LUMO energy is determined at same level calculation.

Ring+PF6	x	y	z		x	y	z
N1	0.6910	-3.4611	3.3934	C51	-2.1723	2.3345	-3.3617
C2	1.0185	-4.8666	2.9439	C52	-1.7909	1.0207	-3.5627
C3	1.0894	-4.9409	1.4267	H53	-2.5556	0.2568	-3.4768
C4	2.3179	-4.8360	0.7598	H54	-3.1981	2.6121	-3.1429
C5	2.3695	-4.8008	-0.6383	H55	0.6930	3.9247	-3.8099
C6	1.1948	-4.8758	-1.3974	H56	1.4969	1.6266	-4.2010
C7	1.2372	-4.7418	-2.9120	C57	-0.8478	-1.7968	-3.9874
N8	0.8416	-3.3501	-3.3399	C58	-0.4231	-3.0944	-3.7600
C9	1.7331	-2.3367	-3.2130	H59	-1.0824	-3.9468	-3.8959
C10	1.3551	-1.0234	-3.4215	H60	-1.8680	-1.6564	-4.3288
C11	0.0256	-0.7138	-3.7689	H61	2.1065	-0.2553	-3.2646
C12	-0.4396	0.6998	-3.7926	H62	2.7461	-2.6058	-2.9270
C13	0.4560	1.7760	-3.9358	H63	2.2382	-4.9223	-3.3090
C14	0.0238	3.0752	-3.7288	H64	0.5440	-5.4256	-3.4050
N15	-1.2629	3.3380	-3.3949	C65	-0.0272	-5.0528	-0.7302
C16	-1.6612	4.7183	-2.9342	C66	-0.0798	-5.0824	0.6636

C17	-1.6155	4.8080	-1.4155	H67	-1.0397	-5.2199	1.1562
C18	-0.3969	5.0079	-0.7499	H68	-0.9482	-5.1686	-1.2972
C19	-0.3374	5.0030	0.6449	H69	3.3351	-4.7221	-1.1324
C20	-1.4957	4.8028	1.4101	H70	3.2449	-4.7864	1.3264
C21	-1.4147	4.7238	2.9275	H71	0.2394	-5.5126	3.3519
N22	-1.0567	3.3284	3.3794	H72	1.9690	-5.1328	3.4114
C23	-2.0220	2.3838	3.4665	P73	-0.6287	4.6234	-7.2466
C24	-1.7056	1.0561	3.6900	F74	0.8264	4.2135	-6.5499
C25	-0.3632	0.6586	3.8207	F75	-1.3807	3.3780	-6.4436
C26	0.0219	-0.7819	3.8229	F76	-0.3060	3.5974	-8.5149
C27	-0.9016	-1.8127	4.0317	F77	-0.9537	5.6459	-5.9737
C28	-0.5468	-3.1337	3.8039	F78	0.1147	5.8686	-8.0612
H29	-1.2416	-3.9471	3.9342	F79	-2.0790	5.0361	-7.9488
H30	-1.9091	-1.6177	4.3599	P80	2.3725	-3.6991	-7.0007
C31	1.3271	-1.1713	3.4998	F81	1.5150	-3.8981	-8.4094
C32	1.6306	-2.5025	3.2892	F82	1.2076	-2.6602	-6.4259
H33	2.6150	-2.8284	3.0060	F83	3.5403	-4.7333	-7.5772
H34	2.1149	-0.4547	3.3522	F84	3.2448	-3.5200	-5.5864
C35	0.6029	1.6818	3.8389	F85	3.1841	-2.4086	-7.6603
C36	0.2350	2.9964	3.6089	F86	1.5587	-4.9860	-6.3236
H37	0.9595	3.8027	3.5934	P87	0.2551	-3.6187	7.3818
H38	1.6524	1.4823	4.0199	F88	-1.1880	-3.0236	6.7987
H39	-2.5217	0.3445	3.7106	F89	1.0923	-2.5372	6.4374
H40	-3.0441	2.7166	3.3313	F90	0.2164	-2.5056	8.6151
H41	-2.3672	4.9707	3.4004	F91	0.2940	-4.7412	6.1526
H42	-0.6473	5.3875	3.3312	F92	-0.5711	-4.7043	8.3364
C43	-2.7222	4.6680	0.7469	F93	1.6968	-4.2117	7.9640
C44	-2.7812	4.6684	-0.6513	P94	-2.8382	4.4130	7.0063
H45	-3.7459	4.5705	-1.1417	F95	-2.1352	5.5380	8.0085
H46	-3.6428	4.5729	1.3169	F96	-1.3373	3.9917	6.4260
H47	0.6188	5.1692	1.1351	F97	-4.3373	4.8393	7.5855
H48	0.5137	5.1822	-1.3182	F98	-3.5506	3.2899	6.0019
H49	-0.9701	5.4177	-3.4087	F99	-2.7034	3.2634	8.1960
H50	-2.6634	4.9062	-3.3243	F100	-2.9731	5.5666	5.8118

(2) $TTFch_3$-$CBPQT^{4+}$ structure

Structure is optimized at B3LYP/6-31G*. B3LYP/6-31G**++ has been used to perform single point energy calculation to obtain binding energy.

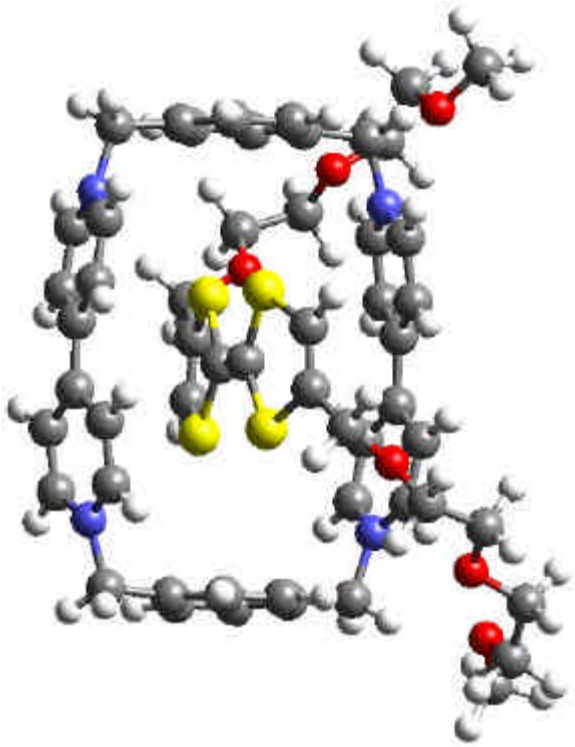


	X	y	z		x	y	z
N1	-2.280	2.703	3.382	H47	1.988	-5.175	1.211
C2	-3.220	3.806	2.929	H48	1.998	-5.172	-1.238
C3	-3.283	3.886	1.411	H49	3.122	-4.514	-3.379
C4	-4.235	3.145	0.698	H50	4.419	-3.318	-3.381
C5	-4.237	3.141	-0.698	C51	2.868	-1.217	-3.475
C6	-3.286	3.877	-1.416	C52	1.958	-0.198	-3.690
C7	-3.226	3.790	-2.934	H53	2.344	0.814	-3.709
N8	-2.283	2.691	-3.385	H54	3.926	-1.024	-3.344
C9	-2.671	1.397	-3.298	H55	0.917	-3.874	-3.610
C10	-1.783	0.360	-3.517	H56	-0.791	-2.163	-4.033
C11	-0.431	0.617	-3.819	C57	-0.086	1.974	-3.994
C12	0.582	-0.474	-3.824	C58	-1.014	2.976	-3.766
C13	0.226	-1.838	-3.845	H59	-0.764	4.025	-3.878
C14	1.174	-2.821	-3.619	H60	0.905	2.278	-4.310
N15	2.474	-2.510	-3.394	H61	-2.161	-0.647	-3.396
C16	3.454	-3.573	-2.937	H62	-3.706	1.219	-3.034
C17	3.520	-3.644	-1.419	H63	-4.202	3.563	-3.370
C18	2.660	-4.492	-0.708	H64	-2.865	4.715	-3.387
C19	2.654	-4.494	0.688	C65	-2.389	4.688	-0.704
C20	3.508	-3.648	1.408	C66	-2.387	4.692	0.692
C21	3.433	-3.584	2.927	H67	-1.693	5.344	1.217
N22	2.455	-2.519	3.386	H68	-1.697	5.338	-1.234
C23	2.854	-1.229	3.477	H69	-5.007	2.579	-1.221
C24	1.947	-0.207	3.693	H70	-5.005	2.587	1.226

C25	0.569	-0.477	3.817	H71	-2.852	4.731	3.377
C26	-0.439	0.619	3.813	H72	-4.195	3.585	3.369
C27	-0.088	1.973	3.992	S73	1.876	-0.177	0.004
C28	-1.011	2.981	3.764	C74	0.131	0.144	-0.001
H29	-0.754	4.029	3.878	S75	-0.276	1.872	-0.005
H30	0.904	2.273	4.309	C76	1.396	2.429	0.012
C31	-1.792	0.369	3.508	C77	2.390	1.527	0.018
C32	-2.675	1.412	3.292	C78	-3.083	-2.218	0.004
H33	-3.709	1.238	3.025	S79	-2.562	-0.511	-0.003
H34	-2.178	-0.634	3.382	C80	-0.817	-0.840	-0.003
C35	0.207	-1.839	3.827	S81	-0.416	-2.567	-0.010
C36	1.153	-2.825	3.599	C82	-2.089	-3.120	-0.002
H37	0.891	-3.877	3.582	H83	-2.247	-4.194	-0.001
H38	-0.812	-2.161	4.005	H84	1.553	3.503	0.015
H39	2.339	0.803	3.720	C85	3.872	1.821	0.036
H40	3.914	-1.039	3.354	C86	-4.558	-2.506	0.017
H41	4.397	-3.339	3.378	H87	4.164	2.320	0.967
H42	3.093	-4.527	3.361	H88	4.472	0.911	-0.056
C43	4.434	-2.870	0.698	H89	4.148	2.487	-0.788
C44	4.440	-2.868	-0.698	H90	-5.043	-2.089	0.907
H45	5.186	-2.274	-1.221	H91	-5.060	-2.085	-0.863
H46	5.176	-2.278	1.229	H92	-4.730	-3.585	0.016

(3) Structure of $TTFO_3$-$CBPQT^{4+}$

Structure is optimized at B3LYP/6-31G*. B3LYP/6-31G**++ has been used to perform single point energy calculation to obtain binding energy.

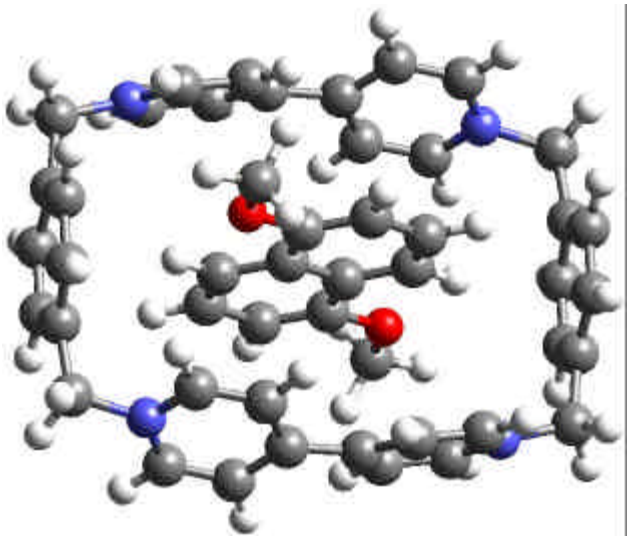


O1	2.150	2.445	3.348	C65	-5.304	1.815	1.857
C2	2.780	2.923	4.551	C66	-5.121	2.116	0.519
C3	3.708	1.879	5.130	C67	-4.167	3.075	0.116
O4	2.990	0.771	5.670	C68	-3.798	3.283	-1.306
C5	3.851	-0.030	6.500	C69	-4.148	2.346	-2.302
C6	3.068	-1.049	7.296	C70	-3.636	2.443	-3.580
O7	2.502	-2.031	6.427	N71	-2.792	3.444	-3.930
C8	2.236	-3.263	7.105	C72	-2.078	3.387	-5.265
C9	4.888	-2.315	-6.060	C73	-0.849	2.499	-5.181
O10	3.662	-2.794	-5.497	C74	-0.941	1.121	-5.428
C11	3.021	-3.749	-6.342	C75	0.161	0.286	-5.240
C12	2.081	-4.620	-5.539	C76	1.385	0.815	-4.806
O13	0.954	-3.872	-5.044	C77	2.561	-0.097	-4.510
C14	-0.057	-4.750	-4.553	N78	2.507	-0.620	-3.095
C15	-1.370	-4.033	-4.334	C79	2.980	0.145	-2.084
O16	-1.287	-3.133	-3.214	C80	2.789	-0.208	-0.763
C17	-2.574	-2.721	-2.784	C81	2.080	-1.379	-0.433
C18	-2.413	-1.731	-1.662	C82	1.653	-1.642	0.973
C19	-2.825	-1.881	-0.393	C83	2.171	-0.934	2.071
S20	-2.505	-0.585	0.763	C84	1.599	-1.044	3.333
C21	-1.533	0.374	-0.374	H85	1.971	-0.479	4.189

S22	-1.587	-0.206	-2.044	H86	3.008	-0.253	1.978
C23	-0.752	1.422	0.018	C87	0.611	-2.547	1.251
S24	0.178	2.415	-1.126	C88	0.072	-2.625	2.520
C25	1.147	3.193	0.128	H89	-0.752	-3.287	2.756
C26	0.856	2.948	1.416	H90	0.165	-3.160	0.478
S27	-0.511	1.856	1.716	C91	1.694	-2.195	-1.510
C28	1.565	3.511	2.618	C92	1.907	-1.801	-2.825
H29	2.014	3.208	5.286	H93	1.589	-2.419	-3.667
H30	3.383	3.814	4.322	H94	1.186	-3.140	-1.367
H31	4.425	1.544	4.365	H95	3.154	0.472	-0.005
H32	4.286	2.368	5.928	H96	3.493	1.056	-2.368
H33	4.379	0.623	7.208	H97	3.510	0.435	-4.606
H34	4.602	-0.539	5.879	H98	2.608	-0.985	-5.148
H35	3.769	-1.526	7.994	C99	1.500	2.202	-4.650
H36	2.283	-0.560	7.892	C100	0.396	3.036	-4.833
H37	1.515	-3.130	7.922	H101	0.519	4.110	-4.716
H38	3.160	-3.691	7.513	H102	2.461	2.647	-4.398
H39	4.723	-1.810	-7.022	H103	0.068	-0.780	-5.433
H40	5.597	-3.138	-6.208	H104	-1.874	0.690	-5.784
H41	3.771	-4.413	-6.795	H105	-2.806	3.022	-5.993
H42	2.484	-3.245	-7.159	H106	-1.828	4.416	-5.529
H43	1.719	-5.422	-6.196	C107	-2.504	4.414	-3.027
H44	2.621	-5.083	-4.701	C108	-2.993	4.363	-1.733
H45	0.267	-5.236	-3.618	H109	-2.735	5.182	-1.073
H46	-0.242	-5.547	-5.287	H110	-1.871	5.223	-3.370
H47	-1.659	-3.478	-5.238	H111	-3.870	1.717	-4.349
H48	-2.139	-4.795	-4.140	H112	-4.792	1.502	-2.092
H49	-3.171	-3.575	-2.431	C113	-3.513	3.767	1.157
H50	-3.134	-2.260	-3.616	C114	-3.733	3.431	2.479
H51	-3.364	-2.748	-0.026	H115	-3.220	3.931	3.291
H52	1.936	3.862	-0.201	H116	-2.790	4.549	0.960
H53	2.326	4.231	2.281	H117	-5.741	1.587	-0.196
H54	0.851	4.069	3.247	H118	-6.018	1.068	2.185
H55	1.826	-3.957	6.366	H119	-5.624	1.522	4.416
H56	5.318	-1.607	-5.346	H120	-4.557	2.845	4.889
N57	0.533	-1.853	3.531	C121	-2.256	1.396	4.953
C58	-0.208	-1.824	4.846	C122	-1.196	0.498	5.083
C59	-1.380	-0.862	4.798	H123	-0.223	0.857	5.408
C60	-2.664	-1.311	4.463	H124	-2.093	2.444	5.197
C61	-3.722	-0.411	4.325	H125	-4.710	-0.790	4.075
C62	-3.520	0.959	4.530	H126	-2.853	-2.373	4.320
C63	-4.634	1.956	4.260	H127	0.543	-1.572	5.600
N64	-4.590	2.439	2.825	H128	-0.540	-2.848	5.032

(4) Structure DNP-CBPQT^{4+}

Structure is optimized at B3LYP/6-31G*. B3LYP/6-31G**++ has been used to perform single point energy calculation to obtain binding energy.

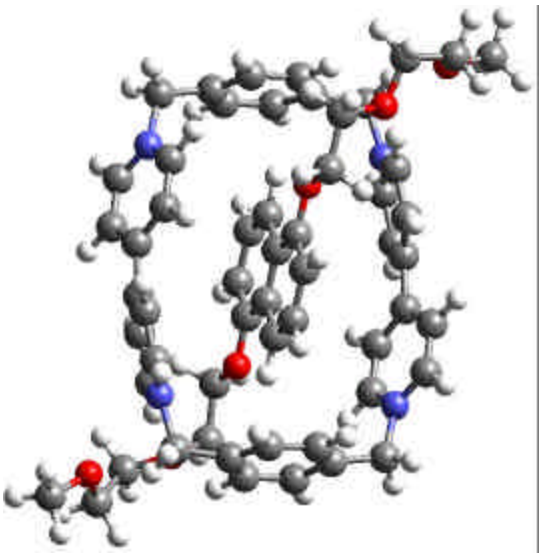


	x	y	z		x	y	z
N1	0.392	-3.484	3.329	H50	-1.298	5.351	-3.396
C2	0.521	-4.951	2.929	C51	-1.358	2.691	-3.171
C3	0.507	-5.123	1.418	C52	-1.269	1.327	-3.383
C4	1.704	-5.112	0.687	H53	-2.152	0.730	-3.193
C5	1.685	-5.121	-0.709	H54	-2.277	3.160	-2.844
C6	0.470	-5.140	-1.408	H55	1.697	3.674	-3.933
C7	0.443	-4.983	-2.921	H56	1.982	1.263	-4.362
N8	0.338	-3.516	-3.329	C57	-0.983	-1.624	-3.954
C9	1.424	-2.716	-3.227	C58	-0.841	-2.987	-3.729
C10	1.336	-1.351	-3.440	H59	-1.669	-3.676	-3.853
C11	0.104	-0.753	-3.758	H60	-1.953	-1.266	-4.281
C12	-0.048	0.737	-3.755	H61	2.233	-0.760	-3.297
C13	1.023	1.615	-3.997	H62	2.354	-3.193	-2.945
C14	0.881	2.979	-3.770	H63	1.352	-5.365	-3.392
N15	-0.285	3.501	-3.324	H64	-0.410	-5.489	-3.376
C16	-0.391	4.969	-2.921	C65	-0.718	-5.284	-0.677
C17	-0.422	5.134	-1.409	C66	-0.700	-5.276	0.719
C18	0.767	5.265	-0.675	H67	-1.637	-5.387	1.260
C19	0.744	5.269	0.721	H68	-1.669	-5.402	-1.191
C20	-0.468	5.141	1.417	H69	2.630	-5.124	-1.248
C21	-0.487	4.981	2.930	H70	2.662	-5.108	1.202
N22	-0.365	3.516	3.338	H71	-0.307	-5.473	3.413
C23	-1.426	2.690	3.184	H72	1.452	-5.309	3.376
C24	-1.314	1.326	3.396	C73	-3.952	1.713	0.044
C25	-0.082	0.758	3.765	C74	3.847	-1.733	-0.068
C26	0.103	-0.727	3.761	H75	-4.251	2.762	0.054
C27	-0.951	-1.625	4.005	H76	-4.355	1.227	-0.852

C28	-0.783	-2.985	3.779	H77	-4.348	1.211	0.934
H29	-1.584	-3.696	3.944	H78	4.257	-1.246	0.824
H30	-1.916	-1.290	4.372	H79	4.150	-2.781	-0.082
C31	1.335	-1.292	3.387	H80	4.234	-1.228	-0.960
C32	1.450	-2.655	3.172	O81	2.411	-1.738	-0.050
H33	2.377	-3.108	2.845	C82	1.759	-0.539	-0.031
H34	2.206	-0.675	3.199	C83	0.323	-0.619	-0.015
C35	0.974	1.654	4.010	C84	-0.430	0.593	0.005
C36	0.809	3.015	3.786	C85	-1.867	0.513	0.020
H37	1.613	3.723	3.951	O86	-2.515	1.713	0.038
H38	1.938	1.317	4.375	C87	-2.506	-0.713	0.015
H39	-2.186	0.711	3.208	C88	-1.736	-1.898	-0.004
H40	-2.351	3.145	2.856	C89	-0.359	-1.862	-0.019
H41	-1.418	5.346	3.371	H90	0.216	-2.776	-0.033
H42	0.341	5.503	3.413	H91	-2.253	-2.852	-0.006
C43	-1.662	5.140	0.683	H92	-3.587	-0.783	0.025
C44	-1.639	5.138	-0.714	C93	0.253	1.837	0.011
H45	-2.582	5.152	-1.256	C94	1.630	1.871	-0.004
H46	-2.622	5.154	1.194	C95	2.398	0.686	-0.026
H47	1.681	5.371	1.264	H96	3.480	0.756	-0.037
H48	1.721	5.364	-1.187	H97	2.148	2.825	0.002
H49	0.464	5.472	-3.376	H98	-0.321	2.752	0.026

(5) Structure of $DNPO_3$-$CBPQT^{4+}$

Structure is optimized at B3LYP/6-31G*. B3LYP/6-31G**++ has been used to perform single point energy calculation to obtain binding energy.

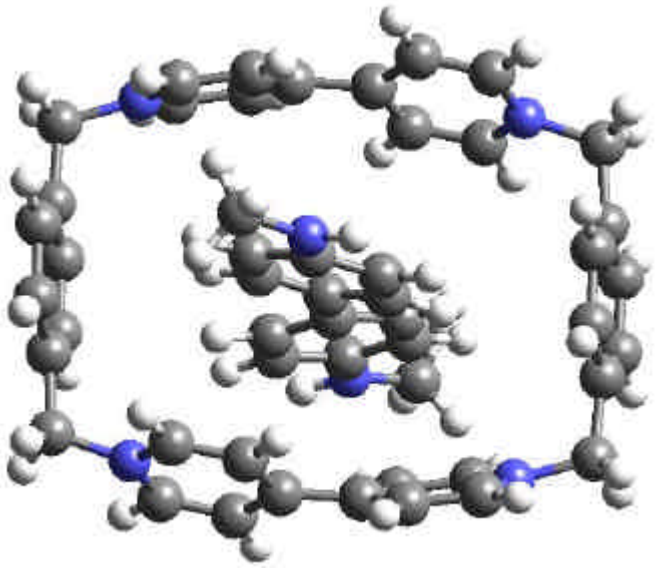


	x	y	z		x	y	z
N1	2.694	-0.732	3.940	H64	-0.234	-0.730	5.747
C2	1.995	-1.829	3.565	C65	1.133	0.828	5.153
H3	1.269	-2.229	4.266	C66	1.234	2.179	4.787
C4	2.180	-2.387	2.306	H67	2.209	2.652	4.690
H5	1.551	-3.228	2.038	C68	0.085	2.931	4.525
C6	3.078	-1.818	1.391	H69	0.188	3.971	4.225
C7	3.856	-0.735	1.850	C70	2.361	-0.063	5.270
H8	4.628	-0.284	1.236	H71	2.189	-0.883	5.972
C9	3.642	-0.214	3.118	H72	3.251	0.495	5.566
H10	4.209	0.629	3.496	C73	3.021	-3.485	6.993
C11	3.083	-2.259	-0.037	H74	3.410	-4.370	6.472
C12	2.731	-3.563	-0.433	H75	2.917	-3.715	8.061
H13	2.597	-4.362	0.288	O76	1.769	-3.066	6.436
C14	2.537	-3.860	-1.777	C77	0.782	-4.089	6.546
H15	2.248	-4.851	-2.110	H78	0.721	-4.453	7.582
N16	2.687	-2.913	-2.736	H79	1.048	-4.942	5.903
C17	3.107	-1.672	-2.389	C80	-0.576	-3.546	6.157
H18	3.223	-0.958	-3.193	H81	-1.326	-4.337	6.293
C19	3.318	-1.327	-1.065	H82	-0.849	-2.697	6.800
H20	3.596	-0.303	-0.845	O83	-0.552	-3.132	4.779
C21	2.347	-3.208	-4.200	C84	-1.838	-2.823	4.271
H22	2.198	-4.288	-4.262	H85	-2.548	-3.627	4.515
H23	3.242	-2.952	-4.773	H86	-2.228	-1.892	4.711
C24	1.129	-2.429	-4.661	C87	-1.784	-2.711	2.761
C25	-0.166	-2.953	-4.517	H88	-2.806	-2.691	2.360
H26	-0.308	-3.979	-4.184	H89	-1.265	-3.586	2.352
C27	-1.286	-2.162	-4.789	O90	-1.092	-1.508	2.370

H28	-2.278	-2.590	-4.667	C91	-0.875	-1.312	1.036
C29	-1.133	-0.826	-5.195	C92	-1.311	-2.181	0.050
C30	0.157	-0.349	-5.470	H93	-1.877	-3.072	0.294
H31	0.298	0.659	-5.849	C94	-1.014	-1.911	-1.305
C32	1.275	-1.147	-5.213	H95	-1.364	-2.608	-2.058
H33	2.265	-0.760	-5.445	C96	-0.294	-0.797	-1.679
C34	-2.328	0.109	-5.311	H97	-0.064	-0.608	-2.719
H35	-2.124	0.946	-5.984	C98	0.149	0.125	-0.694
H36	-3.231	-0.411	-5.640	C99	-0.141	-0.123	0.686
N37	-2.670	0.758	-3.974	C100	0.296	0.805	1.668
C38	-3.691	0.295	-3.208	H101	0.067	0.616	2.707
H39	-4.300	-0.495	-3.633	C102	1.000	1.929	1.292
C40	-3.924	0.803	-1.938	H103	1.337	2.635	2.044
H41	-4.750	0.395	-1.366	C104	1.301	2.196	-0.064
C42	-3.094	1.821	-1.425	H105	1.856	3.093	-0.314
C43	-2.116	2.340	-2.284	C106	0.885	1.313	-1.044
H44	-1.443	3.126	-1.962	O107	1.121	1.487	-2.377
C45	-1.908	1.791	-3.543	C108	1.795	2.688	-2.801
H46	-1.114	2.132	-4.201	H109	1.219	3.568	-2.485
C47	-3.123	2.238	0.009	H110	2.788	2.739	-2.335
C48	-3.400	1.294	1.016	C111	1.950	2.654	-4.315
H49	-3.702	0.282	0.771	H112	2.640	3.453	-4.611
C50	-3.204	1.612	2.349	H113	2.404	1.698	-4.602
H51	-3.355	0.890	3.140	O114	0.716	2.764	-5.011
N52	-2.760	2.837	2.723	C115	0.431	4.054	-5.588
C53	-2.571	3.796	1.784	H116	1.345	4.481	-6.020
H54	-2.265	4.774	2.140	H117	0.056	4.737	-4.814
C55	-2.747	3.526	0.432	C118	-0.598	3.893	-6.690
H56	-2.581	4.332	-0.275	H119	-0.780	4.886	-7.126
C57	-2.433	3.099	4.195	H120	-0.207	3.242	-7.486
H58	-2.323	4.180	4.291	O121	-1.804	3.356	-6.153
H59	-3.319	2.794	4.758	C122	-2.924	3.579	-7.020
C60	-1.189	2.350	4.637	H123	-3.093	4.653	-7.170
C61	-1.288	1.044	5.142	H124	-3.800	3.146	-6.531
H62	-2.263	0.607	5.344	H125	3.725	-2.657	6.875
C63	-0.140	0.290	5.391	H126	-2.776	3.100	-7.996

(6) Structure of BZD- CPBQT^{4+}

Structure is optimized at B3LYP/6-31G*. B3LYP/6-31G**++ has been used to perform single point energy calculation to obtain binding energy.

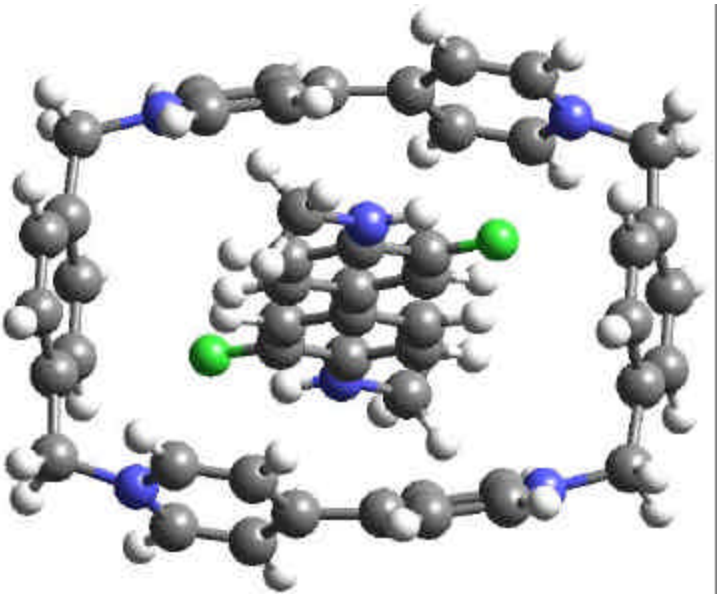


	x	y	z		x	y	z
N1	0.205	-3.512	3.343	H53	-2.115	0.854	-4.617
C2	0.340	-4.874	2.836	H54	-2.372	3.193	-4.228
C3	0.394	-4.912	1.339	H55	1.632	3.496	-3.169
C4	1.461	-4.285	0.658	H56	1.962	1.191	-3.570
C5	1.530	-4.282	-0.750	C57	-1.030	-1.557	-3.697
C6	0.537	-4.917	-1.530	C58	-0.833	-2.928	-3.446
C7	0.616	-4.852	-3.023	H59	-1.643	-3.494	-3.169
N8	0.414	-3.491	-3.517	H60	-1.974	-1.188	-3.566
C9	1.448	-2.752	-4.032	H61	2.099	-0.850	-4.625
C10	1.295	-1.369	-4.266	H62	2.358	-3.189	-4.239
C11	0.060	-0.711	-4.024	H63	1.597	-5.260	-3.292
C12	-0.074	0.714	-4.023	H64	-0.095	-5.542	-3.497
C13	1.017	1.560	-3.698	C65	-0.509	-5.587	-0.852
C14	0.821	2.931	-3.445	C66	-0.585	-5.574	0.561
N15	-0.426	3.494	-3.511	H67	-1.362	-6.055	1.022
C16	-0.627	4.854	-3.014	H68	-1.229	-6.084	-1.384
C17	-0.542	4.916	-1.521	H69	2.305	-3.799	-1.209
C18	0.506	5.585	-0.846	H70	2.198	-3.818	1.190
C19	0.586	5.572	0.567	H71	-0.468	-5.505	3.227
C20	-0.390	4.908	1.347	H72	1.255	-5.363	3.182
C21	-0.331	4.867	2.844	C73	2.033	2.236	-0.320
N22	-0.194	3.505	3.349	C74	3.185	1.563	0.116
C23	-1.250	2.844	3.927	C75	3.063	0.262	0.647
C24	-1.190	1.451	4.149	C76	1.799	-0.362	0.710
C25	-0.013	0.712	3.865	C77	0.637	0.305	0.247
C26	0.027	-0.719	3.863	C78	0.778	1.611	-0.266

C27	-1.107	-1.483	3.488	C79	-0.635	-0.308	0.249
C28	-0.992	-2.858	3.205	C80	-0.778	-1.613	-0.263
H29	-1.822	-3.358	2.862	C81	-1.796	0.360	0.715
H30	-2.019	-1.045	3.341	C82	-3.060	-0.263	0.656
C31	1.204	-1.459	4.143	C83	-3.184	-1.565	0.127
C32	1.263	-2.852	3.919	C84	-2.033	-2.239	-0.313
H33	2.124	-3.358	4.176	H85	2.103	3.187	-0.686
H34	2.031	-0.993	4.531	N86	4.343	2.244	-0.026
C35	1.119	1.476	3.486	H87	3.893	-0.233	0.980
C36	1.003	2.851	3.205	H88	1.734	-1.306	1.097
H37	1.831	3.352	2.861	H89	-0.033	2.108	-0.628
H38	2.031	1.039	3.336	H90	0.032	-2.111	-0.627
H39	-2.016	0.985	4.539	H91	-1.729	1.303	1.103
H40	-2.109	3.350	4.188	H92	-3.888	0.232	0.992
H41	-1.244	5.357	3.194	N93	-4.343	-2.246	-0.013
H42	0.479	5.498	3.233	H94	-2.104	-3.189	-0.678
C43	-1.459	4.281	0.669	C95	-5.645	-1.889	0.470
C44	-1.532	4.280	-0.739	C96	5.647	1.888	0.454
H45	-2.308	3.797	-1.196	H97	4.271	3.081	-0.515
H46	-2.195	3.814	1.203	H98	-4.272	-3.083	-0.503
H47	1.364	6.053	1.026	H99	-5.955	-0.926	0.061
H48	1.224	6.085	-1.380	H100	-6.377	-2.641	0.157
H49	0.083	5.544	-3.490	H101	-5.668	-1.839	1.562
H50	-1.607	5.262	-3.279	H102	6.378	2.640	0.140
C51	-1.461	2.755	-4.024	H103	5.673	1.838	1.546
C52	-1.309	1.373	-4.260	H104	5.958	0.925	0.044

(7) Structure of FBZD- CPBQT^{4+}

Structure is optimized at B3LYP/6-31G*. B3LYP/6-31G**++ has been used to perform single point energy calculation to obtain binding energy.



	x	y	z		x	y	z
N1	1.254274	-3.398895	3.428189	H53	-2.59934	0.419867	-3.43039
C2	1.543534	-4.810093	2.949931	H54	-3.09129	2.814544	-3.10433
C3	1.411104	-4.898817	1.435824	H55	0.808459	3.899774	-4.03386
C4	2.544901	-4.914069	0.612737	H56	1.459127	1.551353	-4.43171
C5	2.412541	-4.903225	-0.780633	C57	-0.96326	-1.75706	-4.10461
C6	1.144375	-4.871057	-1.377198	C58	-0.58322	-3.06551	-3.84201
C7	0.992729	-4.765479	-2.886344	H59	-1.2406	-3.90507	-4.0378
N8	0.63128	-3.351769	-3.312615	H60	-1.9466	-1.5906	-4.5318
C9	1.522819	-2.354968	-3.106715	H61	1.934117	-0.2805	-3.11301
C10	1.195855	-1.035295	-3.353718	H62	2.485998	-2.64235	-2.70381
C11	-0.087332	-0.694044	-3.821028	H63	1.91663	-5.02399	-3.40977
C12	-0.49027	0.740332	-3.881185	H64	0.198613	-5.41138	-3.26566
C13	0.447437	1.765617	-4.105122	C65	0.011986	-4.92956	-0.55217
C14	0.099914	3.090733	-3.898055	C66	0.143922	-4.94481	0.835244
N15	-1.144059	3.432145	-3.486471	H67	-0.75668	-4.987	1.442196
C16	-1.435965	4.8406	-3.00355	H68	-0.98572	-4.95535	-0.98132
C17	-1.32275	4.920892	-1.487254	H69	3.309168	-4.94003	-1.39529
C18	-0.064515	4.981903	-0.870243	H70	3.540899	-4.95507	1.04745
C19	0.048997	4.964072	0.518571	H71	0.837783	-5.46339	3.46749
C20	-1.092418	4.885211	1.328913	H72	2.549497	-5.06202	3.292385
C21	-0.956126	4.775708	2.839189	C73	-2.36187	-1.98003	0.15155
N22	-0.575943	3.365439	3.263456	C74	-3.46447	-1.0966	0.057595
C23	-1.450663	2.357143	3.041889	C75	-3.11498	0.268765	-0.0701
C24	-1.107553	1.041665	3.288639	C76	-1.78204	0.684181	-0.1011
C25	0.175001	0.71851	3.769088	C77	-0.6977	-0.2126	-0.00601

C26	0.591737	-0.71229	3.826122	C78	-1.04872	-1.57719	0.127126
C27	-0.330289	-1.742022	4.087387	C79	0.72237	0.213666	-0.03414
C28	0.021994	-3.066002	3.879194	C80	1.076869	1.582229	-0.10111
H29	-0.674427	-3.880382	4.043868	C81	1.80388	-0.6907	-0.00476
H30	-1.333165	-1.532101	4.443328	C82	3.13813	-0.27988	-0.03767
C31	1.900448	-1.101498	3.48994	C83	3.49134	1.087877	-0.10663
C32	2.199012	-2.438328	3.289669	C84	2.391587	1.979408	-0.13442
H33	3.180589	-2.768467	2.97087	F85	-2.64765	-3.30595	0.278873
H34	2.679744	-0.372537	3.300943	N86	-4.73318	-1.5712	0.089693
C35	1.035029	1.790744	4.065857	H87	-3.9075	1.006958	-0.1433
C36	0.636859	3.095119	3.805377	H88	-1.60215	1.748358	-0.21165
H37	1.278844	3.944114	4.011739	H89	-0.29863	-2.35174	0.213814
H38	2.016302	1.635101	4.501516	H90	0.328608	2.363413	-0.12373
H39	-1.830718	0.275328	3.037563	H91	1.620254	-1.75876	0.045887
H40	-2.412604	2.63241	2.627213	H92	3.927995	-1.02422	-0.01672
H41	-1.890274	5.015249	3.353493	N93	4.761541	1.558632	-0.14267
H42	-0.177672	5.433388	3.230562	F94	2.683937	3.308604	-0.19884
C43	-2.35316	4.899635	0.716419	C95	5.954077	0.723832	-0.14028
C44	-2.467249	4.915215	-0.678557	C96	-5.92937	-0.74364	0.033437
H45	-3.458118	4.944065	-1.125944	H97	-4.84952	-2.56764	0.20812
H46	-3.25821	4.919459	1.319482	H98	4.880768	2.559476	-0.2068
H47	1.039942	5.003065	0.961088	H99	5.980348	0.055918	-1.01027
H48	0.843114	5.041456	-1.464878	H100	6.83203	1.369497	-0.18166
H49	-0.723571	5.496245	-3.508791	H101	6.019267	0.119777	0.773226
H50	-2.437236	5.09646	-3.356734	H102	-6.8046	-1.39218	0.086507
C51	-2.100858	2.478565	-3.388282	H103	-5.97371	-0.0403	0.874369
C52	-1.806219	1.140913	-3.587068	H104	-5.98126	-0.17954	-0.90586