Supporting Information

Cucurbit[7]uril effect on reference substances for NMR in deuterium oxide solution

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1. Effect of sodium ion on DSS or TSP forming the inclusion complex with CB[7] monitored by ^{1}H NMR

Fig. S1 Effect of sodium ion on DSS forming the inclusion complex with CB[7] monitored by ^{1}H NMR. Sodium ion concentration is (a) 1.5 mM (Fig. 2b), (b) 3.0 mM, and (c) 154 mM. The concentration of DSS and CB[7] is 1.5 mM, respectively. The H$^{1'}$, H$^{2'}$, H$^{3'}$, and Si-CH$_3$' indicate the H^1, H^2, H^3, and Si-CH$_3$ of DSS forming the inclusion complex with CB[7], respectively.
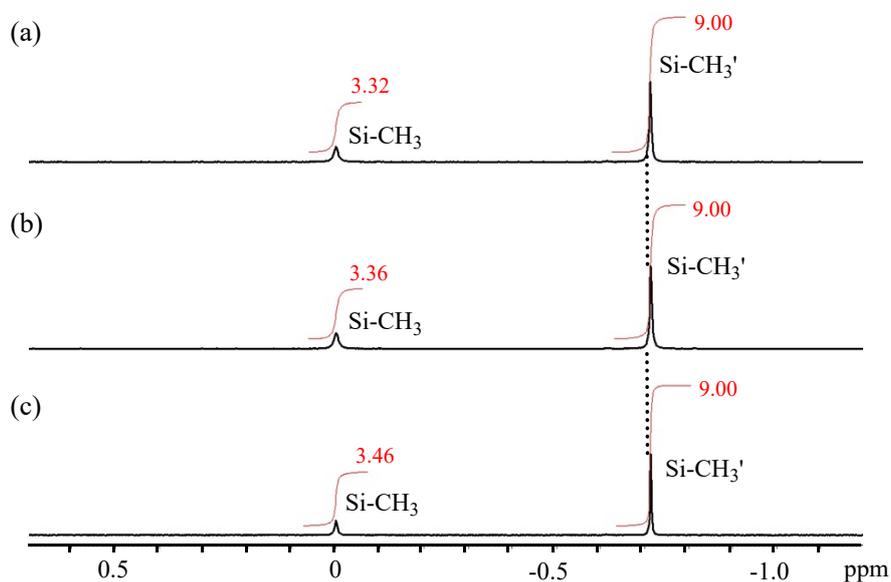

Fig. S2 Effect of sodium ion on TSP forming the inclusion complex with CB[7] monitored by ^{1}H NMR. Sodium ion concentration is (a) 1.5 mM (Fig. 3b), (b) 3.0 mM, and (c) 154 mM. The concentration of TSP and CB[7] is 1.5 mM, respectively. The Si-CH$_3$' indicate the Si-CH$_3$ of TSP forming the inclusion complex with CB[7].

2. Stoichiometric ratio of inclusion complex DSS and CB[7], and TSP and CB[7]
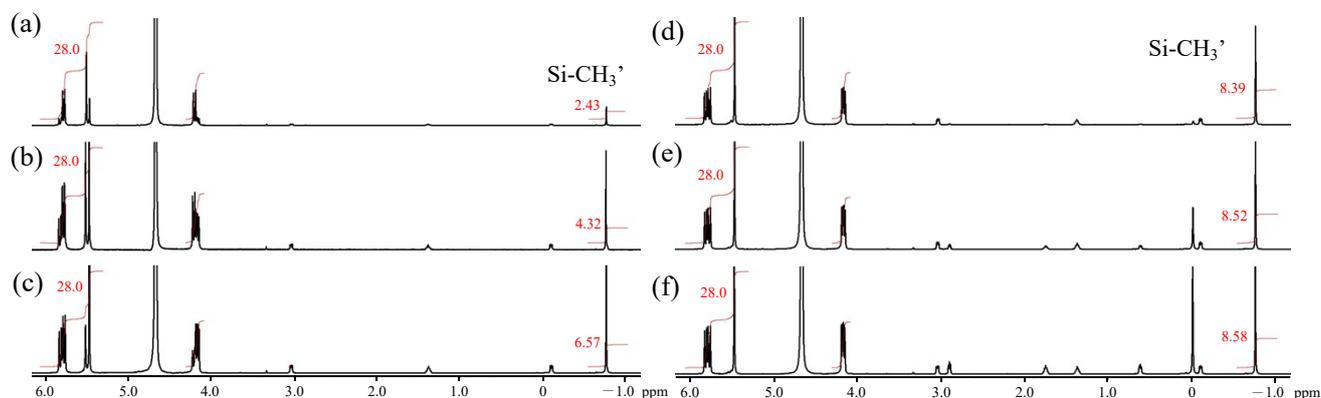
Fig. S3 Quantitative NMR spectra of DSS and CB[7] mixture D_2O solution. The CB[7] concentration is 1.5 mM (constant). The DSS concentrations are (a) 0.375, (b) 0.75, (c) 1.125, (d) 1.5, (e) 2.25, and (f) 3.0 mM. The Si-CH$_3$' indicates the Si-CH$_3$ of DSS forming the inclusion complex with CB[7].
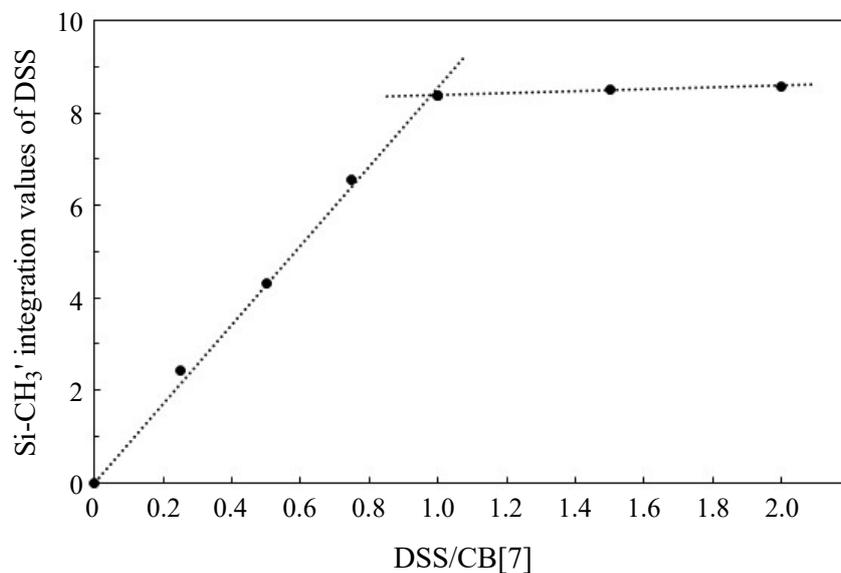
Fig. S4 Stoichiometric ratio of inclusion complex of DSS and CB[7] in D_2O solution. Stoichiometric ratio is determined with the Si-CH$_3$' integration values of DSS when the concentration of CB[7] is constant (1.5 mM) and the concentrations of DSS changed from 0 to 3.0 mM.
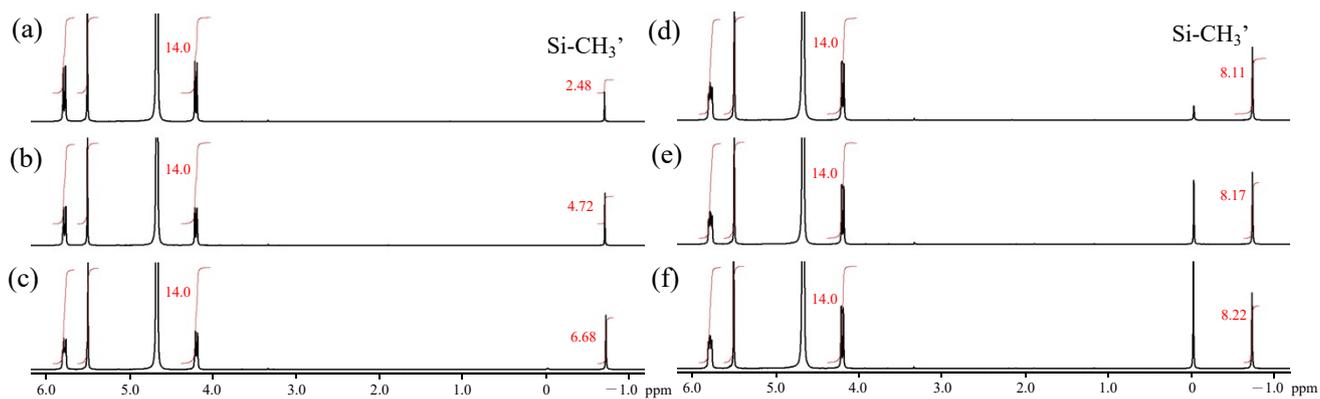
Fig. S5 Quantitative NMR spectra of TSP and CB[7] mixture D_2O solution. The CB[7] concentration is 1.5 mM (constant). The TSP concentrations are (a) 0.375, (b) 0.75, (c) 1.125, (d) 1.5, (e) 2.25, and (f) 3.0 mM. The Si-CH$_3$' indicates the Si-CH$_3$ of TSP forming the inclusion complex with CB[7].
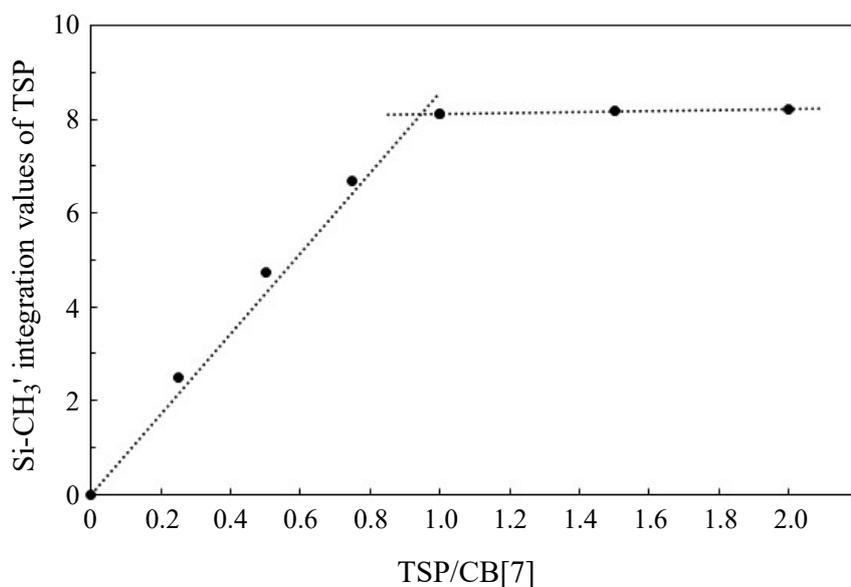
Fig. S6 Stoichiometric ratio of the inclusion complex of TSP and CB[7] in D_2O solution. Stoichiometric ratio is determined with the Si-CH$_3$' integration values of TSP when the concentration of CB[7] is constant (1.5 mM) and the concentrations of TSP change from 0 to 3.0 mM.

3. ITC of DSS and CB[7], and TSP and CB[7]
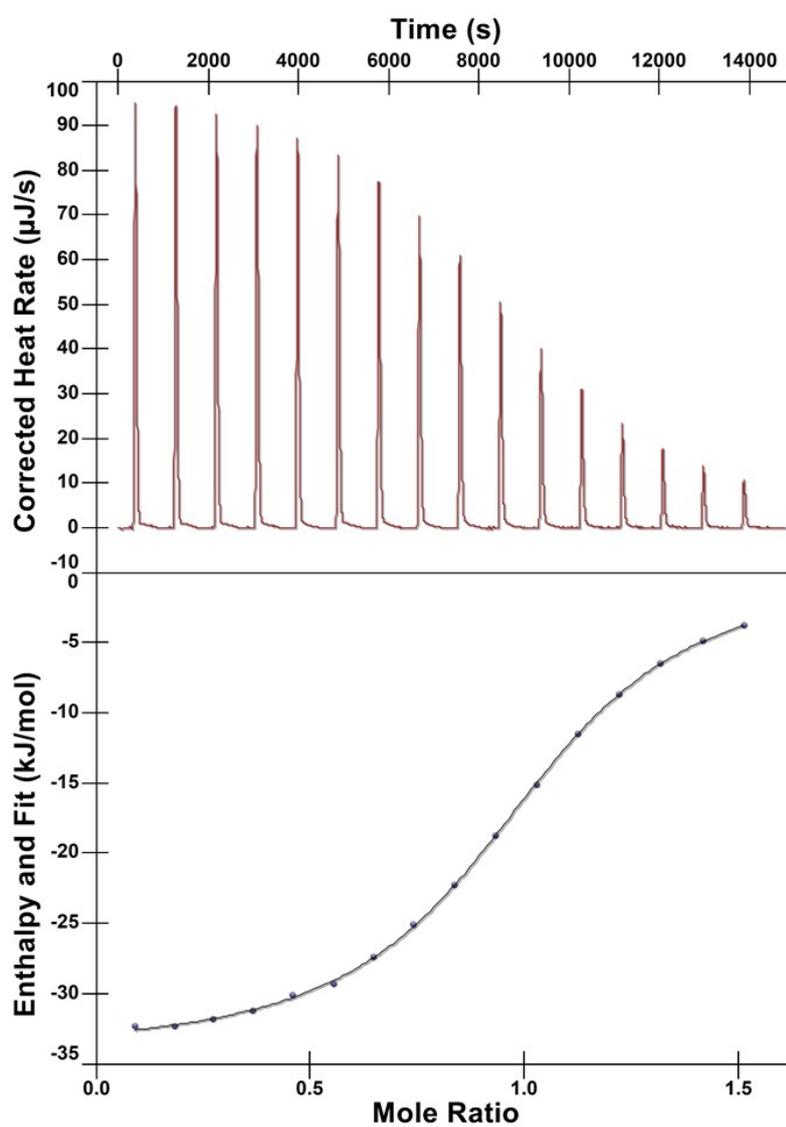
Fig. S7 ITC of DSS and CB[7] in 0.2 mol L^{-1} phosphate buffer at 303.15 K.
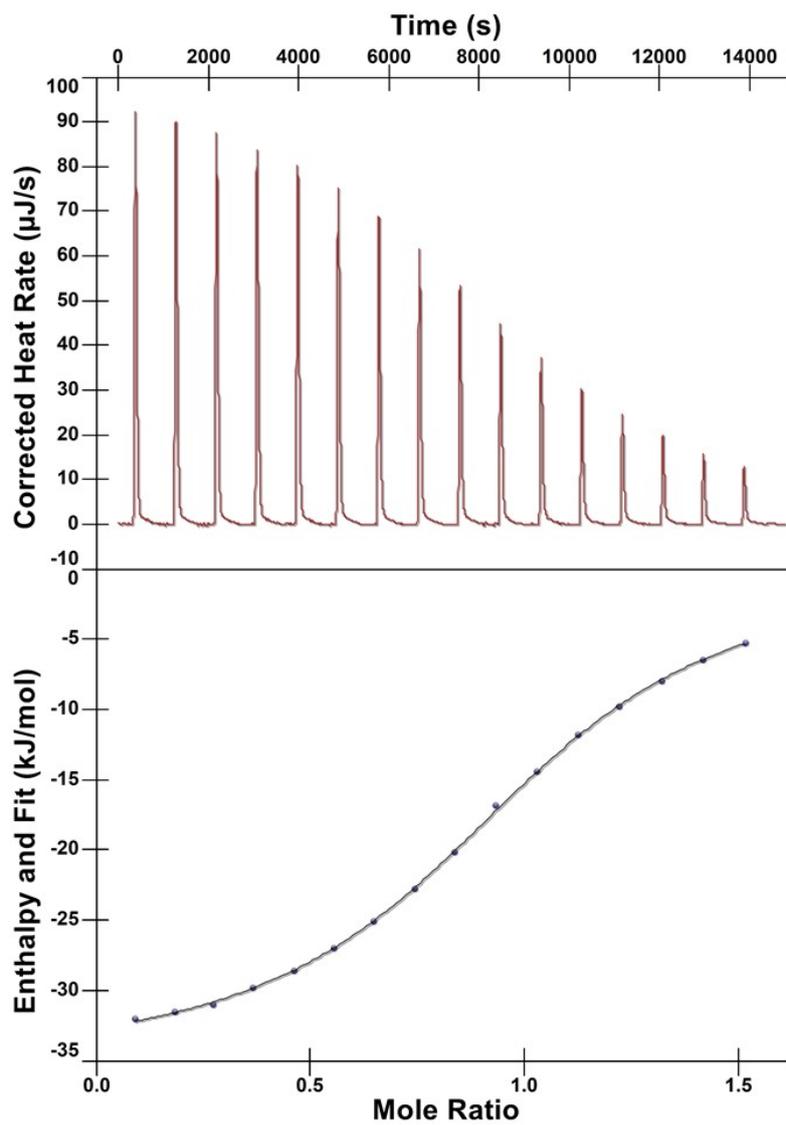
Fig. S8 ITC of TSP and CB[7] in 0.2 mol L^{-1} phosphate buffer at 303.15 K.

4. 1D ROESY between TSP and CB[7] under the inclusion complexation condition
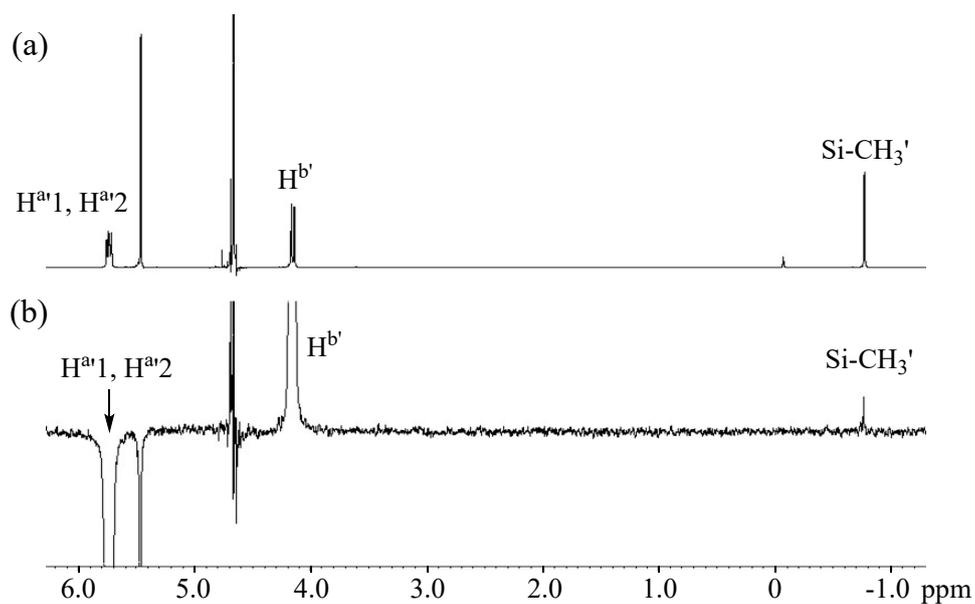
Fig S9 ROEs between TSP and CB[7] under the inclusion complexation condition (TSP = CB[7] = 3 mM). (a) ^{1}H NMR, (b) 1D ROESY irradiating at the $H^{a'}1$ and $H^{a'}2$ proton signals of CB[7]. $H^{a'}1$, $H^{a'}2$, and Si-CH$_3$'indicate that H^a1 and H^a2 of CB[7] and the Si-CH$_3$ of TSP shifted because of the inclusion complexation between TSP and CB[7], respectively.

5. Molecular modeling calculation of inclusion complex of DSS and TSP with CB[7]

Optimized structure of DSS using density functional theory (DFT) calculation

The conformational analysis of DSS was determined by using ChemBio3D Ultra ver. 14 (PerkinElmer Informatics, Inc., USA) and CONFLEX5 (CONFLEX corporation, Japan). Because CONFLEX5 cannot perform a conformational analysis of structures containing sodium atom, 4,4-dimetyl-4-silapentane-1-sulfonic acid (DSS-H), where the sodium atom of DSS is replaced by a hydrogen atom, was used as the initial structure. All of the various conformations of DSS-H obtained by CONFLEX5 were classified into six groups by clustering. Furthermore, the hydrogen atom in the sulfo group of these DSS-H was changed to a sodium atom, and these conformations were optimized with a solvent accessible surface (SAS) model at B3LYP/6-31+g(d) level by Gaussian 16 (Fig. S10 Groups A–F).

Group A	Group B	Group C

Group D	Group E	Group F
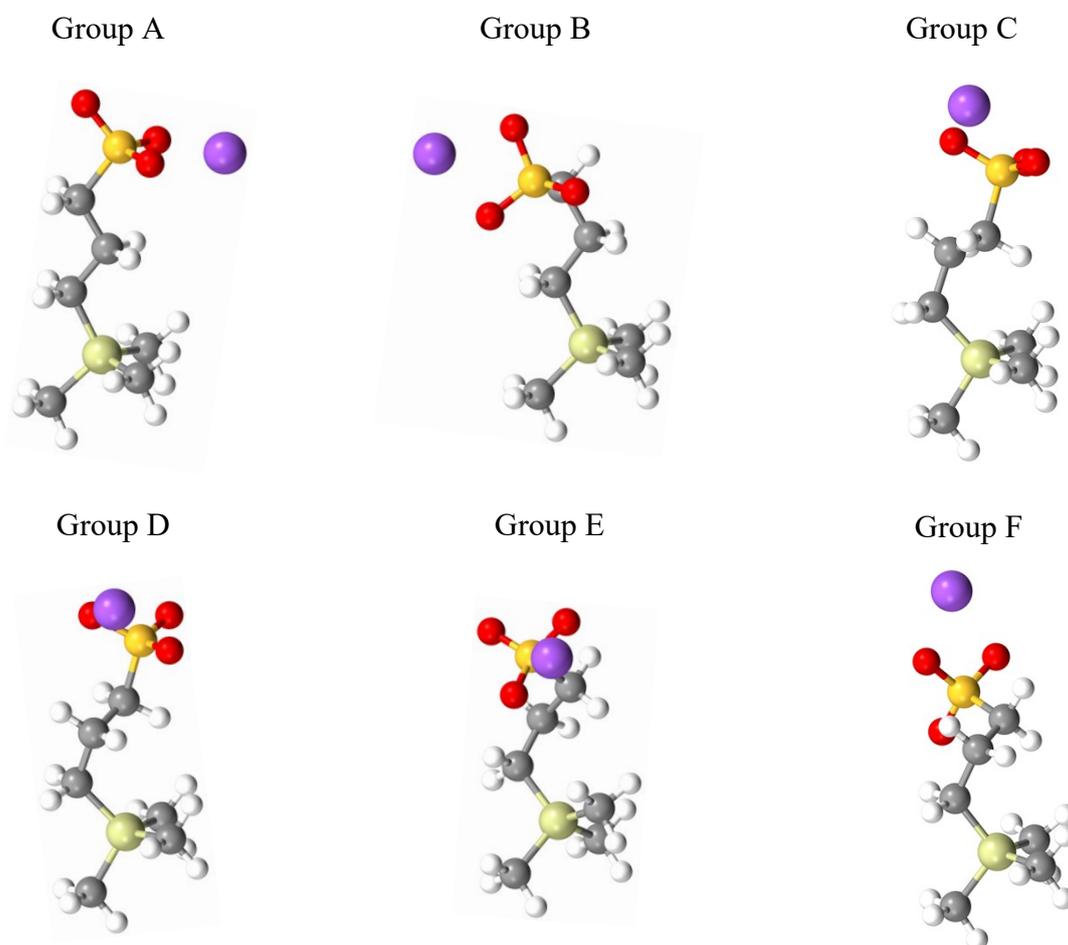
Fig. S10 Optimized structures of DSS in each group.

Table S1 Atomic coordinates and energies of DSS (Groups A–F).

DSS_Group A

$E_{DSS\_A} = -1313.4248973$ (a.u.)

C	4.626575	-1.028616	-0.000626	H	1.606597	-1.714852	-0.877607
Si	3.083360	0.072439	0.000001	H	1.606665	-1.715218	0.876881
C	1.543225	-1.052477	-0.000224	H	0.101241	0.320357	0.882549
C	0.183374	-0.325803	-0.000025	H	0.101121	0.320565	-0.882435
C	-0.990998	-1.307092	-0.000050	H	-0.982431	-1.948761	-0.887591
C	3.088375	1.166352	1.549452	H	-0.982406	-1.948822	0.887448
C	3.088021	1.167569	-1.548590	H	2.220314	1.836986	1.579806
S	-2.631232	-0.519830	-0.000002	H	3.988293	1.794057	1.584109
O	-3.619636	-1.618946	0.000047	H	3.072640	0.562649	2.466177
O	-2.681743	0.376840	1.222913	H	3.987843	1.795434	-1.582854
O	-2.681830	0.376820	-1.222916	H	3.072282	0.564575	-2.465783
H	5.544349	-0.426431	-0.000616	H	2.219856	1.838095	-1.578333
H	4.657178	-1.676384	-0.886261	Na	-3.027649	2.234591	-0.000004
H	4.657518	-1.676928	0.884599				

DSS_Group B

$E_{DSS\_B} = -1313.4226021$ (a.u.)

C	3.606485	1.998348	-0.073627	H	1.057779	0.802466	1.476486
Si	2.932386	0.225498	-0.033071	H	0.560450	0.932340	-0.197485
C	1.107954	0.288381	0.503164	H	0.441742	-1.612346	-0.341438
C	0.396228	-1.072906	0.612556	H	0.915134	-1.702913	1.348741
C	-1.072463	-1.008003	1.056496	H	-1.450762	-2.003774	1.311001
C	3.086487	-0.542946	-1.760904	H	-1.211927	-0.354063	1.923688
C	3.949355	-0.799476	1.199922	H	2.732580	-1.581521	-1.778267
S	-2.234422	-0.416789	-0.217753	H	4.130742	-0.545684	-2.099811
O	-1.976585	1.064613	-0.423000	H	2.499218	0.017628	-2.499534
O	-2.017983	-1.249406	-1.420095	H	5.011713	-0.808650	0.923075
O	-3.609297	-0.551224	0.409661	H	3.877566	-0.390620	2.216365
H	4.659822	2.018149	-0.382206	H	3.612885	-1.843460	1.238730
H	3.542533	2.474285	0.913573	Na	-4.030808	1.654009	0.264971
H	3.043422	2.623465	-0.778717				

DSS_Group C

$E_{DSS\_C} = -1313.4217914$ (a.u.)

C	-4.587034	0.585191	0.668891	H	-1.861731	1.646216	1.491359
Si	-2.914206	0.074344	-0.065099	H	-1.633585	0.013492	2.071512
C	-1.564714	0.637133	1.166528	H	-0.015070	1.320583	-0.207091
C	-0.093111	0.707876	0.699254	H	0.507225	1.205617	1.471506
C	0.523045	-0.665033	0.427210	H	0.470660	-1.314221	1.307991
C	-2.927892	-1.807563	-0.317547	H	0.041604	-1.182704	-0.407299
C	-2.665504	0.936377	-1.735821	H	-2.035101	-2.172576	-0.839210
S	2.286460	-0.614115	-0.017672	H	-3.798999	-2.104873	-0.916303
O	3.003471	0.083789	1.122155	H	-2.992487	-2.339494	0.640547
O	2.697231	-2.016609	-0.238431	H	-3.466605	0.668512	-2.436865
O	2.397010	0.278260	-1.239351	H	-2.673682	2.028886	-1.628502
H	-5.416151	0.282004	0.016567	H	-1.712828	0.657608	-2.203662
H	-4.652415	1.672589	0.803219	Na	3.756137	1.741401	-0.202299
H	-4.753245	0.120557	1.649608				

DSS_Group D

$E_{DSS\_D} = -1313.4217914$ (a.u.)

C	4.587121	-0.584573	-0.669402	H	1.633567	-0.013434	-2.071370
Si	2.914326	-0.074358	0.065095	H	1.861688	-1.646193	-1.491306
C	1.564714	-0.637117	-1.166409	H	-0.507215	-1.205662	-1.471285
C	0.093133	-0.707865	-0.699074	H	0.015126	-1.320533	0.207303
C	-0.523069	0.665034	-0.427096	H	-0.041702	1.182764	0.407419
C	2.666303	-0.936955	1.735623	H	-0.470684	1.314193	-1.307899
C	2.927504	1.807498	0.318007	H	1.713639	-0.658682	2.203787
S	-2.286492	0.614071	0.017704	H	3.467484	-0.669006	2.436546
O	-2.397115	-0.278363	1.239327	H	2.674863	-2.029431	1.627964
O	-2.697245	2.016567	0.238503	H	3.799366	2.105124	0.915505
O	-3.003500	-0.083755	-1.122212	H	2.990358	2.339693	-0.640060
H	5.416258	-0.281710	-0.016949	H	2.035317	2.171915	0.841123
H	4.753207	-0.119298	-1.649839	Na	-3.756538	-1.741245	0.202187
H	4.652601	-1.671881	-0.804419				

DSS_Group E

$E_{\text{DSS\_E}} = -1313.4200164$ (a.u.)

C	3.556929	0.990949	1.44887		H	1.858887	-1.61204	1.424095
Si	2.549373	0.257158	0.01786		H	0.633334	-0.359979	1.469213
C	1.272885	-0.932694	0.785197		H	1.022773	-2.308657	-0.885482
C	0.393899	-1.80256	-0.139219		H	-0.082087	-2.599234	0.445929
C	-0.712832	-1.077269	-0.915215		H	-0.348481	-0.211141	-1.473989
C	1.752595	1.685269	-0.947477		H	-1.196869	-1.760511	-1.620712
C	3.713969	-0.698849	-1.13825		H	1.325396	1.357006	-1.903396
S	-2.090225	-0.462691	0.110258		H	2.497873	2.458889	-1.175161
O	-2.522961	-1.579534	0.976291		H	0.949898	2.152235	-0.363834
O	-1.590377	0.759687	0.859619		H	4.492231	-0.039845	-1.544879
O	-3.135425	0.01497	-0.880184		H	4.218729	-1.518977	-0.611065
H	4.333695	1.673594	1.080428		H	3.178065	-1.135066	-1.991212
H	4.055677	0.207013	2.03344		Na	-3.088905	2.126414	-0.113003
H	2.916647	1.558946	2.136253					

DSS_Group F

$E_{\text{DSS\_F}} = -1313.4197552$ (a.u.)

C	-3.911675	-0.873913	-1.273138		H	-0.799003	-0.123553	-1.494004
Si	-2.765872	-0.075844	0.012709		H	-1.761041	1.326606	-1.713666
C	-1.303222	0.682583	-0.946289		H	0.370608	2.071459	-0.914277
C	-0.253562	1.527931	-0.193430		H	-0.757434	2.297490	0.408712
C	0.685094	0.773809	0.758985		H	1.286629	1.478767	1.341301
C	-3.718461	1.286536	0.931900		H	0.151124	0.122944	1.456753
C	-2.234756	-1.409173	1.255594		H	-3.099489	1.775719	1.695216
S	1.907652	-0.304934	-0.056868		H	-4.598994	0.874335	1.442003
O	1.183183	-1.426016	-0.693219		H	-4.070870	2.065604	0.243255
O	2.676472	0.578764	-1.021342		H	-3.103291	-1.997839	1.579955
O	2.866947	-0.720610	1.042331		H	-1.506018	-2.097312	0.810275
H	-4.798944	-1.312899	-0.798559		H	-1.780260	-0.981029	2.158013
H	-3.398093	-1.675786	-1.819323		Na	4.630155	0.261225	0.047707
H	-4.260172	-0.140953	-2.012353					

Optimized structure of TSP using DFT calculation

The conformational analysis of TSP was determined by ChemBio3D Ultra ver. 14 and CONFLEX5. Because CONFLEX5 cannot perform a conformational analysis of structures containing sodium atom, 3-(trimethylsilyl) propionic acid (TSP-H), where the sodium atom of TSP is replaced by a hydrogen atom, was used as the initial structure. All of the various different conformations of TSP-H obtained by CONFLEX5 were classified into two groups by clustering. Furthermore, the hydrogen atom in the carboxyl group of these TSP-H was changed to a sodium atom, and these conformations were optimized with a SAS model at B3LYP/6-31+g(d) level by Gaussian 16 (Fig. S11 Groups A and B).
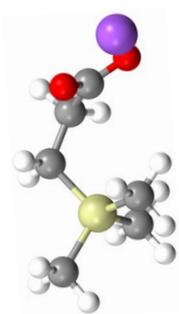
Group A   Group B
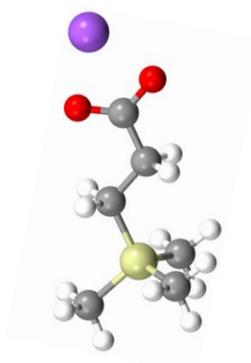
Fig. S11 Optimized structures of TSP in each group.

Table S2 Atomic coordinates and energies of TSP (Groups A and B).

TSP_Group A

$E_{\text{TSP\_A}} = -838.8544038$ (a.u.)

C	2.543071	0.813910	1.476764	H	2.786590	-1.445980	-1.879844
Si	1.781984	-0.179087	0.046776	H	3.781345	-0.037416	-1.476794
C	3.182311	-0.850759	-1.046521	H	3.862733	-1.494834	-0.474102
C	0.799354	-1.633598	0.763251	H	0.323548	-2.219436	-0.032522
C	0.693477	0.962352	-1.019091	H	0.006720	-1.287203	1.437730
C	-0.551843	1.570641	-0.341631	H	1.455259	-2.304557	1.333985
C	-1.712368	0.591195	-0.140814	H	1.342756	1.777101	-1.375658
O	-2.391345	0.674309	0.933663	H	0.369713	0.412350	-1.912264
O	-1.973938	-0.237792	-1.070172	H	-0.312698	2.024370	0.626119
H	1.770674	1.220312	2.142175	H	-0.950537	2.380991	-0.971544
H	3.139470	1.658267	1.106653	Na	-3.684492	-0.961462	0.152219
H	3.204314	0.184748	2.087118				

TSP_Group B

$E_{\text{TSP\_B}} = -838.8558762$ (a.u.)

C	2.613991	0.960662	-1.546647	H	3.067680	-2.252809	0.885043
Si	2.204022	-0.062416	0.000074	H	3.068653	-2.252190	-0.885324
C	3.268256	-1.634672	0.000187	H	4.339485	-1.394221	0.000856
C	2.614743	0.961501	1.546039	H	2.386012	0.406367	2.465288
C	0.372059	-0.565150	0.000657	H	2.045059	1.899101	1.575840
C	-0.635584	0.592603	-0.000430	H	3.680488	1.223745	1.575592
C	-2.118271	0.194016	-0.000077	H	0.183723	-1.209107	-0.870098
O	-2.968699	1.143695	0.000190	H	0.183812	-1.207381	0.872712
O	-2.441970	-1.034362	-0.000200	H	-0.490584	1.245644	0.871063
H	2.044962	1.898665	-1.576247	H	-0.490602	1.243906	-0.873236
H	2.384022	0.405374	-2.465494	Na	-4.576793	-0.389439	0.000178
H	3.679899	1.222127	-1.577269				

Most stable structure of CB[7] using DFT calculation

The conformational analysis of CB[7] was determined by ChemBio3D Ultra ver. 14 and CONFLEX5. The number of CB[7] conformations is only one, as the CB[7] structure is rigid. The obtained conformation was optimized with a SAS model at B3LYP/6-31+g(d) level by Gaussian 16 (Fig. S12).
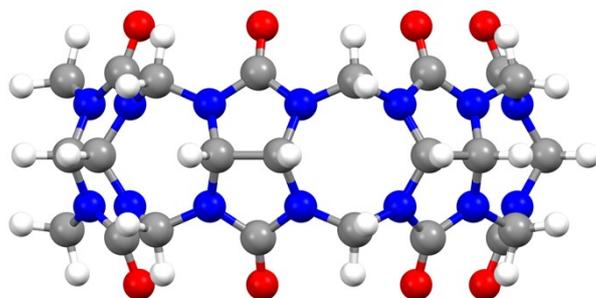
Fig. S12 Most stable structure of CB[7].

Table S3 Atomic coordinates and energy of CB[7].

$E_{CB[7]} = -4212.4243543$ (a.u.)

N	-1.231945	1.121111	-5.137575	C	0.000000	-1.821800	5.587715
C	0.000000	0.783516	-5.822607	H	0.000000	-1.866965	6.686432
H	0.000000	1.218891	-6.832410	N	1.232064	-1.220966	5.116540
N	1.231945	1.121111	-5.137575	C	-1.795316	0.000000	5.655016
C	-1.985911	0.000000	-4.810885	H	-2.859017	0.000000	5.407499
O	-3.117624	0.000000	-4.359278	H	-1.668187	0.000000	6.747384
C	1.985911	0.000000	-4.810885	C	1.795316	0.000000	5.655016
O	3.117624	0.000000	-4.359278	H	2.859017	0.000000	5.407499
N	-1.231945	-1.121111	-5.137575	H	1.668187	0.000000	6.747384
C	0.000000	-0.783516	-5.822607	N	-1.232064	1.220966	5.116540
H	0.000000	-1.218891	-6.832410	C	0.000000	1.821800	5.587715
N	1.231945	-1.121111	-5.137575	H	0.000000	1.866965	6.686432
C	-1.794785	-2.455097	-5.095303	N	1.232064	1.220966	5.116540
H	-2.858828	-2.348665	-4.873500	C	-1.985896	2.089926	4.336383
H	-1.666044	-2.927492	-6.080010	O	-3.117341	1.894174	3.928606
C	1.794785	-2.455097	-5.095303	C	1.985896	2.089926	4.336383
H	2.858828	-2.348665	-4.873500	O	3.117341	1.894174	3.928606
H	1.666044	-2.927492	-6.080010	N	-1.231878	3.241675	4.144957
N	-1.232176	-3.322916	-4.081204	C	0.000000	3.234294	4.908656
C	0.000000	-4.068578	-4.245363	H	0.000000	4.064187	5.630101
H	0.000000	-4.585442	-5.215996	N	1.231878	3.241675	4.144957
N	1.232176	-3.322916	-4.081204	C	-1.794624	4.424730	3.527207
C	-1.986152	-3.768106	-3.001775	H	-2.858600	4.232058	3.373701
O	-3.117717	-3.415138	-2.719367	H	-1.666052	5.278247	4.208664
C	1.986152	-3.768106	-3.001775	C	1.794624	4.424730	3.527207
O	3.117717	-3.415138	-2.719367	H	2.858600	4.232058	3.373701
N	-1.232052	-4.722963	-2.329945	H	1.666052	5.278247	4.208664
C	0.000000	-5.047249	-3.021307	N	-1.232041	4.765678	2.236776
H	0.000000	-6.107785	-3.311979	C	0.000000	5.508781	2.060776
N	1.232052	-4.722963	-2.329945	H	0.000000	6.395799	2.710709
C	-1.794051	-5.520351	-1.259255	N	1.232041	4.765678	2.236776
H	-1.664233	-6.585053	-1.501925	C	-1.985247	4.695893	1.070713
H	-2.858335	-5.281469	-1.204801	O	-3.115794	4.252802	0.969343
C	1.794051	-5.520351	-1.259255	C	1.985247	4.695893	1.070713
H	2.858335	-5.281469	-1.204801	O	3.115794	4.252802	0.969343
H	1.664233	-6.585053	-1.501925	N	-1.231930	5.265915	0.051186
N	-1.231930	-5.265915	0.051186	C	0.000000	5.858482	0.533159

C	0.000000	-5.858482	0.533159	H	0.000000	6.939943	0.333992
H	0.000000	-6.939943	0.333992	N	1.231930	5.265915	0.051186
N	1.231930	-5.265915	0.051186	C	-1.794051	5.520351	-1.259255
C	-1.985247	-4.695893	1.070713	H	-1.664233	6.585053	-1.501925
O	-3.115794	-4.252802	0.969343	H	-2.858335	5.281469	-1.204801
C	1.985247	-4.695893	1.070713	C	1.794051	5.520351	-1.259255
O	3.115794	-4.252802	0.969343	H	2.858335	5.281469	-1.204801
N	-1.232041	-4.765678	2.236776	H	1.664233	6.585053	-1.501925
C	0.000000	-5.508781	2.060776	N	-1.232052	4.722963	-2.329945
H	0.000000	-6.395799	2.710709	C	0.000000	5.047249	-3.021307
N	1.232041	-4.765678	2.236776	H	0.000000	6.107785	-3.311979
C	-1.794624	-4.424730	3.527207	N	1.232052	4.722963	-2.329945
H	-2.858600	-4.232058	3.373701	C	-1.986152	3.768106	-3.001775
H	-1.666052	-5.278247	4.208664	O	-3.117717	3.415138	-2.719367
C	1.794624	-4.424730	3.527207	C	1.986152	3.768106	-3.001775
H	2.858600	-4.232058	3.373701	O	3.117717	3.415138	-2.719367
H	1.666052	-5.278247	4.208664	N	-1.232176	3.322916	-4.081204
N	-1.231878	-3.241675	4.144957	C	0.000000	4.068578	-4.245363
C	0.000000	-3.234294	4.908656	H	0.000000	4.585442	-5.215996
H	0.000000	-4.064187	5.630101	N	1.232176	3.322916	-4.081204
N	1.231878	-3.241675	4.144957	C	-1.794785	2.455097	-5.095303
C	-1.985896	-2.089926	4.336383	H	-2.858828	2.348665	-4.873500
O	-3.117341	-1.894174	3.928606	H	-1.666044	2.927492	-6.080010
C	1.985896	-2.089926	4.336383	C	1.794785	2.455097	-5.095303
O	3.117341	-1.894174	3.928606	H	1.666044	2.927492	-6.080010
N	-1.232064	-1.220966	5.116540	H	2.858828	2.348665	-4.873500

Optimized structure of inclusion complex of DSS and CB[7] using DFT calculation

The initial conformers of the inclusion complex of DSS and CB[7] were constructed, in which the trimethylsilyl group of Group A–F DSS was located in the CB[7] cavity based on the inclusion complex structure estimated by NMR measurements. All conformations in water were optimized with a SAS model at B3LYP/6-31+g(d) level, the structures with the smallest energy were regarded as the optimized conformation of the inclusion complex (Fig. S13 Groups A'–F'). The stabilization energies E (kJ mol^{-1}) for the inclusion complexation were calculated using the following equation: $E = E_{\text{DSS\_complex}} - (E_{\text{DSS}} + E_{\text{CB[7]}})$, where $E_{\text{DSS\_complex}}$, E_{DSS}, and $E_{\text{CB[7]}}$ represent the total energy of the inclusion complex, DSS, and CB[7], respectively.

Group A'

2.35Å

2.33Å

$E = -60.7 \text{ kJ mol}^{-1}$

Group B'

2.36Å

2.30Å

2.33Å

2.34Å

$E = -56.7 \text{ kJ mol}^{-1}$

Group C'   2.23Å

2.23Å

$E = +30.2 \text{ kJ mol}^{-1}$

Group D'

2.37Å

2.30Å

2.32Å

2.32Å

$E = -54.3 \text{ kJ mol}^{-1}$

Group E'

Group F'

2.26Å

2.27Å

2.41Å

2.30Å

2.33Å

$E = -36.9 \text{ kJ mol}^{-1}$
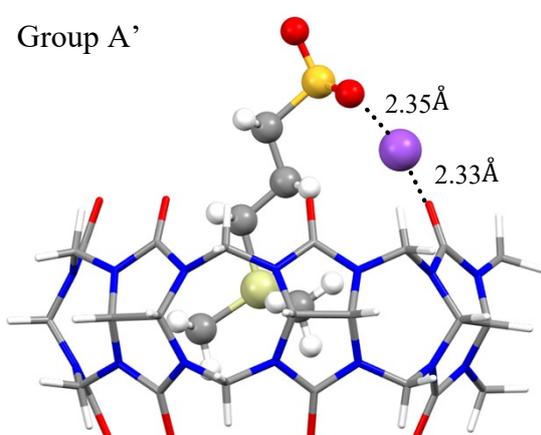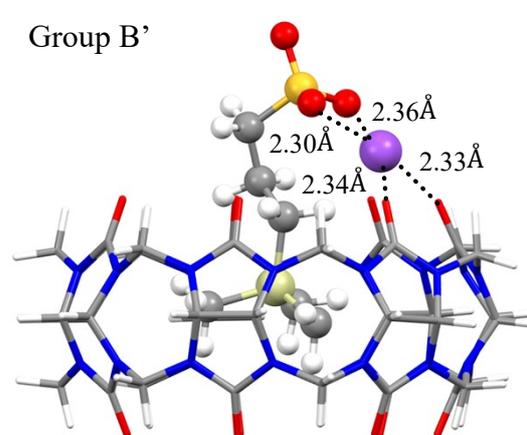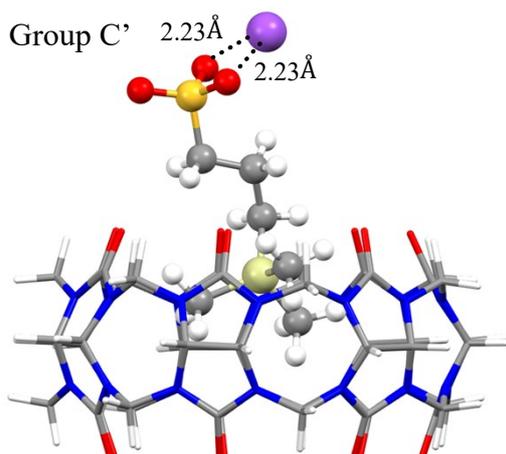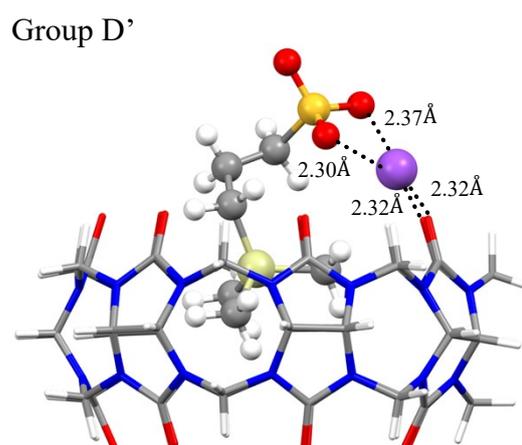
$E = -46.2 \text{ kJ mol}^{-1}$
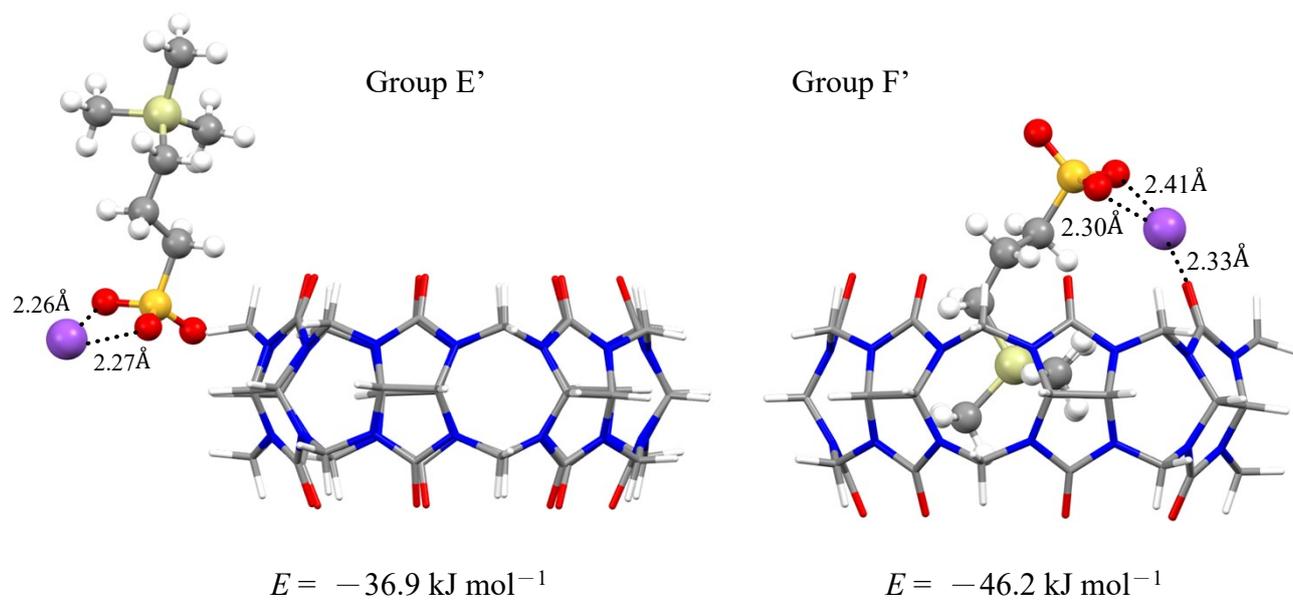
Fig S13 Optimized structures of inclusion complex of DSS and CB[7].

Table S4 Atomic coordinates and energies of inclusion complex of DSS and CB[7] (Groups A'–F').

Inclusion complex of DSS and CB[7] Group A'

$E_{\text{DSS\_complex\_A'}} = -5525.8723554$ (a.u.)

N	2.221380	4.583220	0.517679	O	1.045448	-3.983894	2.451792
C	1.955731	5.417004	-0.640550	C	0.722173	-4.725251	-2.600462
H	2.608429	6.302245	-0.624455	O	0.533718	-4.355221	-3.745567
N	2.030003	4.769427	-1.933220	N	2.147286	-4.611643	0.500947
C	1.121806	4.489857	1.368213	C	1.868668	-5.437469	-0.659819
O	1.111679	3.973109	2.469713	H	2.509159	-6.331630	-0.647810
C	0.801421	4.724351	-2.583524	N	1.950165	-4.786134	-1.950384
O	0.608952	4.358943	-3.729445	C	3.473965	-4.260805	0.951280
N	0.056609	5.130408	0.748433	H	3.396066	-3.991506	2.006983
C	0.433535	5.766497	-0.496554	H	4.136704	-5.131982	0.839144
H	0.239934	6.847705	-0.440402	C	3.189588	-4.500509	-2.638827
N	-0.155653	5.219810	-1.705744	H	2.942833	-4.352347	-3.692246
C	-1.202225	5.354564	1.429424	H	3.867032	-5.359421	-2.533527
H	-1.063339	5.056136	2.470814	N	4.084602	-3.128845	0.263056
H	-1.443989	6.426758	1.379344	C	4.747047	-3.252278	-1.035193
C	-1.502843	5.518850	-2.153544	H	5.428808	-4.113762	-1.021075
H	-1.535349	5.315983	-3.226174	N	3.886456	-3.310290	-2.190798
H	-1.711929	6.583125	-1.970539	C	4.487750	-1.994537	0.937862
N	-2.323435	4.591343	0.913847	O	4.198990	-1.693032	2.093335
C	-3.110006	5.008216	-0.234279	C	3.919172	-2.141951	-2.943541
H	-3.355281	6.077481	-0.152766	O	3.346023	-1.948090	-3.999073
N	-2.545059	4.727065	-1.535699	N	5.314598	-1.264433	0.105370
C	-3.011990	3.688674	1.721132	C	5.479284	-1.879999	-1.194833
O	-2.669934	3.306025	2.825789	H	6.548232	-1.976622	-1.429899
C	-3.279146	3.783702	-2.246763	N	4.770524	-1.249611	-2.293276
O	-3.096106	3.455398	-3.405296	C	5.974199	-0.044750	0.521035
N	-4.178878	3.335656	1.054198	H	6.995282	-0.052200	0.122235
C	-4.368143	4.078333	-0.172882	H	6.020175	-0.047461	1.610313
H	-5.317449	4.632619	-0.133829	C	5.216572	-0.031629	-2.942221
N	-4.288376	3.319000	-1.408052	H	4.784845	-0.025728	-3.945736
C	-5.190776	2.492104	1.657828	H	6.314750	-0.041606	-3.012435
H	-6.164716	2.995041	1.573750	N	5.334737	1.187324	0.110296
H	-4.925729	2.374216	2.710780	C	5.511085	1.805438	-1.187107
C	-5.378405	2.505312	-1.915944	H	6.581759	1.884847	-1.420778
H	-5.227908	2.404650	-2.993025	N	4.792646	1.191929	-2.288913
H	-6.329785	3.021922	-1.720598	C	4.518434	1.927169	0.944620
N	-5.296182	1.160857	1.095330	O	4.222739	1.625325	2.098352

C	-6.057474	0.833150	-0.095859
H	-7.062271	1.275668	-0.030952
N	-5.451432	1.167236	-1.369332
C	-4.950065	0.034603	1.833319
O	-4.452971	0.028102	2.944979
C	-5.169795	0.045528	-2.139938
O	-4.779144	0.044679	-3.293845
N	-5.317502	-1.082363	1.091552
C	-6.070846	-0.736164	-0.099376
H	-7.083175	-1.161763	-0.038302
N	-5.468180	-1.074634	-1.373371
C	-5.236773	-2.417644	1.648674
H	-4.972647	-2.308992	2.702841
H	-6.219067	-2.903029	1.559742
C	-5.415312	-2.411527	-1.924956
H	-5.261484	-2.309193	-3.001413
H	-6.374971	-2.914021	-1.733099
N	-4.238252	-3.276558	1.044470
C	-4.434768	-4.008960	-0.187442
H	-5.392603	-4.548790	-0.154882
N	-4.338793	-3.243863	-1.418163
C	-3.075562	-3.646129	1.709518
O	-2.728966	-3.272552	2.815888
C	-3.338355	-3.724452	-2.258735
O	-3.148712	-3.394813	-3.415790
N	-2.397616	-4.553106	0.897987
C	-3.191012	-4.957780	-0.250066
H	-3.452499	-6.023202	-0.168759
N	-2.622770	-4.684723	-1.551539
C	-1.287148	-5.333206	1.411636
H	-1.143574	-5.038536	2.453464
H	-1.543950	-6.401856	1.359904
C	-1.592174	-5.490645	-2.170648
H	-1.622425	-5.286528	-3.243103
H	-1.816436	-6.551863	-1.988270
N	-0.025793	-5.125637	0.730171
C	0.341907	-5.766482	-0.515187
H	0.133690	-6.844976	-0.459333
N	-0.240525	-5.211323	-1.723666
C	1.048577	-4.501211	1.350532

C	3.959203	2.102207	-2.937281
O	3.385678	1.923301	-3.995203
N	4.135164	3.070967	0.274178
C	4.802209	3.189313	-1.022290
H	5.498684	4.038816	-1.002524
N	3.945474	3.267621	-2.179547
C	3.542460	4.210036	0.966455
H	3.460264	3.938534	2.021249
H	4.219002	5.070916	0.857214
C	3.266233	4.470178	-2.621617
H	3.955471	5.318833	-2.510433
H	3.019042	4.331468	-3.676221
C	-2.079795	0.022688	-0.685819
Si	-0.428932	-0.000330	0.230352
C	-0.759895	-0.014485	2.102586
C	0.487128	-0.026931	3.008930
C	0.122291	-0.039094	4.498654
C	0.526536	-1.534401	-0.325573
C	0.554242	1.527364	-0.293658
S	1.583713	-0.044202	5.592799
O	1.077734	-0.051473	6.989126
O	2.380210	-1.266036	5.199833
O	2.378695	1.182756	5.212291
H	-1.937127	0.036079	-1.773541
H	-2.670708	0.907139	-0.422166
H	-2.682047	-0.860846	-0.445583
H	-1.376515	0.862366	2.347717
H	-1.384760	-0.888989	2.334501
H	1.089273	-0.919301	2.792766
H	1.094537	0.865583	2.808483
H	-0.457222	0.848201	4.771651
H	-0.453866	-0.932678	4.757930
H	1.475760	-1.652688	0.208440
H	0.751344	-1.480372	-1.398817
H	-0.063778	-2.442045	-0.158633
H	0.790871	1.485746	-1.364844
H	-0.025105	2.440757	-0.119847
H	1.498557	1.624291	0.253218
Na	3.580360	-0.032142	3.596803

Inclusion complex of DSS and CB[7] Group B'

$E_{\text{DSS\_complex\_B'}} = -5525.8685632$ (a.u.)

C	1.466822	-0.704145	-0.802018	H	3.914940	5.197583	1.042337
Si	0.005313	-0.112181	0.247233	C	3.147750	4.582902	-2.517069
C	0.456761	-0.301418	2.084743	H	2.939887	4.422047	-3.576999
C	-0.515843	0.334075	3.101426	H	3.808212	5.453101	-2.395779
C	-0.482298	-0.237867	4.526697	N	1.956232	4.642488	0.578118
C	-0.341455	1.689691	-0.201040	C	1.746219	5.493267	-0.581860
C	-1.504076	-1.158198	-0.192088	H	2.398438	6.377314	-0.524665
S	1.085256	-0.082316	5.465264	N	1.882002	4.856988	-1.873579
O	1.735578	1.211398	5.037290	C	0.833814	4.605589	1.409113
O	0.698207	-0.133828	6.900874	O	0.787607	4.121529	2.523735
O	1.967819	-1.228179	5.027703	C	0.674637	4.773300	-2.560021
H	1.247076	-0.627928	-1.874433	O	0.527187	4.389555	-3.706713
H	1.716955	-1.750139	-0.591192	N	-0.198319	5.256794	0.749075
H	2.364978	-0.102753	-0.612739	C	0.220597	5.844624	-0.504703
H	0.589946	-1.371410	2.296861	H	0.023820	6.926668	-0.495400
H	1.448205	0.158675	2.195900	N	-0.319070	5.254808	-1.717094
H	-0.350432	1.415540	3.144698	C	-1.490192	5.474155	1.370484
H	-1.555137	0.195702	2.773792	H	-1.380071	5.237682	2.431041
H	-1.225083	0.275389	5.144492	H	-1.761930	6.532620	1.252132
H	-0.707610	-1.309307	4.531192	C	-1.664178	5.497479	-2.200145
H	-1.094148	2.135333	0.457350	H	-1.661760	5.285759	-3.271627
H	-0.703124	1.774847	-1.233735	H	-1.920652	6.553700	-2.031270
H	0.569095	2.293850	-0.119789	N	-2.569503	4.650093	0.863328
H	-1.806943	-0.992203	-1.233766	C	-3.328971	4.953121	-0.334371
H	-1.285436	-2.225807	-0.076977	H	-3.662573	6.000976	-0.311361
H	-2.362650	-0.925616	0.446606	N	-2.686842	4.667390	-1.601070
Na	3.274878	0.072506	3.660372	C	-3.181018	3.679248	1.650114
N	0.143988	-5.149853	0.694388	O	-2.845488	3.345275	2.772187
C	0.588954	-5.736455	-0.551121	C	-3.341449	3.676967	-2.322950
H	0.436606	-6.825605	-0.528989	O	-3.090923	3.334878	-3.465355
N	0.020748	-5.180467	-1.765325	N	-4.270578	3.188309	0.938820
C	1.155725	-4.466891	1.355806	C	-4.511147	3.924800	-0.286157
O	1.090953	-3.982357	2.469514	H	-5.501255	4.402646	-0.248991
C	0.993279	-4.660841	-2.613646	N	-4.365791	3.183291	-1.523268
O	0.827916	-4.293380	-3.762847	C	-5.227948	2.282503	1.541425
N	2.279200	-4.467568	0.526224	H	-4.951943	2.177379	2.592905
C	2.097638	-5.324248	-0.633606	H	-6.232862	2.723303	1.463479
H	2.785686	-6.181010	-0.579937	C	-5.376978	2.290030	-2.050815
N	2.202242	-4.681321	-1.924425	H	-5.190255	2.189444	-3.122198
C	3.579695	-4.106729	1.049648	H	-6.368205	2.738272	-1.887026

H	3.443562	-3.841725	2.100624	N	-5.256272	0.949422	0.971611
H	4.255732	-4.971652	0.969641	C	-5.990549	0.602624	-0.229814
C	3.456990	-4.336280	-2.557600	H	-7.006720	1.021169	-0.182748
H	3.246859	-4.181282	-3.617973	N	-5.367559	0.955431	-1.489482
H	4.161066	-5.171616	-2.436772	C	-4.889732	-0.169785	1.711820
N	4.207995	-2.968090	0.397658	O	-4.393530	-0.164832	2.824663
C	4.912169	-3.056027	-0.880167	C	-5.049781	-0.158239	-2.258421
H	5.619296	-3.896630	-0.854978	O	-4.644158	-0.147357	-3.407412
N	4.089329	-3.126973	-2.064790	N	-5.228798	-1.295155	0.968490
C	4.528185	-1.817762	1.087579	C	-5.965709	-0.964325	-0.235365
O	4.183886	-1.535164	2.231824	H	-6.967936	-1.415824	-0.196820
C	4.140106	-1.961692	-2.822913	N	-5.327093	-1.285899	-1.495565
O	3.613843	-1.783692	-3.905302	C	-5.133771	-2.634146	1.518209
N	5.349428	-1.046919	0.287112	H	-6.109083	-3.130312	1.411929
C	5.608814	-1.658575	-1.001043	H	-4.886886	-2.529060	2.576895
H	6.692490	-1.721658	-1.171184	C	-5.263397	-2.619832	-2.054954
N	4.949365	-1.055139	-2.143124	H	-5.098558	-2.510099	-3.129051
C	5.934388	0.197126	0.739202	H	-6.222926	-3.126706	-1.876226
H	6.970510	0.243370	0.384042	N	-4.114230	-3.476560	0.926400
H	5.932794	0.186736	1.829624	C	-4.273730	-4.212849	-0.311812
C	5.357701	0.195259	-2.751127	H	-5.212645	-4.785133	-0.288578
H	4.986296	0.188506	-3.778461	N	-4.192167	-3.448767	-1.541980
H	6.456418	0.251884	-2.755645	C	-2.969387	-3.841420	1.623599
N	5.252668	1.400675	0.310397	O	-2.658554	-3.473870	2.742353
C	5.450364	2.034595	-0.975840	C	-3.130043	-3.842095	-2.346185
H	6.524027	2.180041	-1.159030	O	-2.914683	-3.473326	-3.487446
N	4.823384	1.385521	-2.113190	N	-2.264027	-4.740860	0.829437
C	4.356882	2.085788	1.109122	C	-2.995688	-5.120325	-0.364199
O	4.029690	1.763961	2.248433	H	-3.225052	-6.195752	-0.338943
C	3.975975	2.252855	-2.802352	N	-2.385413	-4.773786	-1.632245
O	3.476973	2.053968	-3.893770	C	-1.117220	-5.464133	1.338448
N	3.932052	3.206389	0.422364	H	-1.015260	-5.200354	2.393382
C	4.652248	3.371687	-0.840104	H	-1.300269	-6.544117	1.241155
H	5.294921	4.261329	-0.785094	C	-1.305809	-5.515291	-2.248359
N	3.845556	3.405935	-2.034930	H	-1.481666	-6.590621	-2.095910
C	3.263710	4.311432	1.098872	H	-1.323845	-5.286808	-3.316211
H	3.130357	4.019074	2.142834				

Inclusion complex of DSS and CB[7] Group C'

$E_{\text{DSS\_complex\_C'}} = -5525.8346543$ (a.u.)

C	-1.415556	-0.940239	0.039901	H	-3.111591	-6.002207	-2.259703
Si	-0.050652	-0.247711	1.163512	C	-2.195033	-5.278772	1.169701
C	-0.029597	-1.243839	2.785773	H	-1.943822	-5.136883	2.223019
C	0.520316	-0.609854	4.085282	H	-2.631767	-6.277406	1.023600
C	2.049656	-0.510836	4.153215	N	-3.532404	-4.065472	-1.607476
C	1.561304	-0.394310	0.185571	C	-4.089240	-4.377801	-0.303343
C	-0.428567	1.563881	1.513349	H	-4.559384	-5.372166	-0.324719
S	2.655308	-0.243616	5.849586	N	-3.190582	-4.281991	0.827977
O	2.162631	-1.424263	6.677352	C	-4.199952	-3.015377	-2.228790
O	4.128779	-0.126280	5.794123	O	-4.067590	-2.663649	-3.387629
O	1.949541	0.993866	6.383556	C	-3.533131	-3.248735	1.692741
H	-1.406357	-0.432850	-0.933905	O	-3.032587	-3.027128	2.781440
H	-2.412386	-0.801134	0.471445	N	-5.086006	-2.476966	-1.304048
H	-1.282145	-2.012436	-0.152075	C	-5.112508	-3.215357	-0.060795
H	-1.081239	-1.500529	2.973096	H	-6.133775	-3.570758	0.141244
H	0.466634	-2.208628	2.618824	N	-4.581391	-2.542839	1.112591
H	0.087831	0.384978	4.242644	C	-6.044075	-1.453779	-1.667725
H	0.189149	-1.237695	4.923653	H	-6.040799	-1.379970	-2.757336
H	2.534968	-1.433716	3.821071	H	-7.039275	-1.763285	-1.319040
H	2.459106	0.314797	3.563578	C	-5.275476	-1.491009	1.829460
H	2.429149	-0.218059	0.824927	H	-4.833641	-1.440966	2.827066
H	1.588380	0.331018	-0.638891	H	-6.341617	-1.752440	1.909748
H	1.661181	-1.393973	-0.254752	N	-5.757103	-0.131103	-1.155430
H	-0.585846	2.113627	0.575189	C	-6.050075	0.308697	0.191302
H	-1.337944	1.660069	2.116421	H	-7.092904	0.068886	0.446291
H	0.376167	2.068828	2.059235	N	-5.164038	-0.168175	1.239200
Na	0.836352	-0.147034	7.937215	C	-5.346561	0.906181	-1.982802
N	4.316717	2.534599	-2.547743	O	-5.150930	0.836490	-3.183286
C	5.179070	2.364096	-1.395094	C	-4.535076	0.878631	1.910608
H	6.027950	3.061208	-1.455750	O	-3.876856	0.784041	2.931672
N	4.547319	2.464709	-0.094890	N	-5.251344	2.050574	-1.199153
C	4.249488	1.392816	-3.337416	C	-5.762753	1.847737	0.143067
O	3.723933	1.305280	-4.433325	H	-6.661162	2.462793	0.300158
C	4.621616	1.276458	0.623636	N	-4.827528	2.055323	1.229247
O	4.304569	1.122867	1.789443	C	-5.043313	3.354746	-1.792036
N	4.934505	0.384076	-2.671760	H	-5.018958	3.211433	-2.874470
C	5.607765	0.857877	-1.479151	H	-5.882075	4.013658	-1.523287
H	6.694203	0.720626	-1.583767	C	-4.470914	3.362470	1.749602
N	5.159758	0.306668	-0.215243	H	-4.113449	3.223879	2.772173
C	5.182644	-0.902121	-3.287794	H	-5.374271	3.990665	1.756588

H	4.850897	-0.828547	-4.325750		N	-3.806613	4.003764	-1.413128
H	6.261258	-1.112441	-3.256278		C	-3.633585	4.782724	-0.207467
C	5.523868	-1.010488	0.272927		H	-4.481155	5.473761	-0.084898
H	5.400097	-0.997593	1.358184		N	-3.414897	4.044592	1.024958
H	6.578407	-1.199725	0.022805		C	-2.755234	4.159322	-2.306939
N	4.474542	-2.014002	-2.689443		O	-2.701487	3.711998	-3.439278
C	4.928943	-2.739170	-1.522009		C	-2.236141	4.434007	1.658113
H	5.989886	-3.005677	-1.638120		O	-1.923541	4.190701	2.809226
N	4.716471	-2.105772	-0.232735		N	-1.797416	4.960358	-1.693598
C	3.416646	-2.641727	-3.333871		C	-2.268248	5.515498	-0.437519
O	2.926028	-2.313488	-4.400016		H	-2.372794	6.607137	-0.529192
C	3.923139	-2.878137	0.609150		N	-1.504203	5.191323	0.748923
O	3.728466	-2.685752	1.796025		C	-0.709599	5.535660	-2.457493
N	3.053180	-3.743552	-2.567095		H	-0.765110	6.633179	-2.387942
C	3.979123	-3.984892	-1.475282		H	-0.841931	5.225384	-3.496300
H	4.505285	-4.938052	-1.633363		C	-0.233397	5.798730	1.095351
N	3.425478	-3.941141	-0.138680		H	-0.076500	5.619619	2.161182
C	2.138528	-4.743533	-3.078711		H	-0.289651	6.880223	0.905292
H	2.647843	-5.718851	-3.101909		N	0.607637	5.100578	-2.047061
H	1.870635	-4.443457	-4.094114		C	1.330203	5.682086	-0.930493
C	2.672607	-5.022523	0.464902		H	1.309752	6.779825	-1.001131
H	2.715852	-4.883158	1.547207		N	0.921148	5.265718	0.394365
H	3.147655	-5.977161	0.194719		C	1.443899	4.411879	-2.918553
N	0.905774	-4.878184	-2.331565		O	1.139195	3.974420	-4.014619
C	0.778169	-5.672537	-1.127564		C	1.900756	4.516361	1.038837
H	1.246457	-6.656961	-1.276913		O	1.885762	4.163619	2.204086
N	1.268263	-5.074235	0.099628		N	2.702111	4.356558	-2.333261
C	-0.325870	-4.550203	-2.886886		C	2.767274	5.078912	-1.081981
O	-0.509476	-4.014609	-3.965844		H	3.556738	5.843561	-1.131881
C	0.260913	-4.920470	1.047085		N	2.923824	4.281634	0.122299
O	0.416835	-4.632476	2.220363		C	3.852272	3.819126	-3.029036
N	-1.310545	-4.988321	-2.008824		H	3.564069	3.682854	-4.073609
C	-0.770349	-5.752438	-0.903945		H	4.674419	4.546047	-2.962228
H	-1.160757	-6.780747	-0.933176		C	4.194218	3.717950	0.541847
N	-0.952443	-5.193548	0.422461		H	4.993726	4.449875	0.350463
C	-2.711998	-4.982780	-2.371162		H	4.119457	3.526444	1.614563
H	-2.775187	-4.674541	-3.417072					

Inclusion complex of DSS and CB[7] Group D'

$E_{\text{DSS\_complex\_D'}} = -5525.860217$ (a.u.)

Atom	x	y	z	Atom	x	y	z
C	1.065227	1.487110	-0.008574	H	6.239842	2.705819	1.503595
Si	0.393752	0.119661	1.118766	C	5.356526	2.404555	-2.000890
C	0.945626	0.413117	2.914003	H	5.172077	2.346915	-3.075857
C	0.963149	-0.758307	3.922673	H	6.350099	2.839878	-1.817268
C	-0.379271	-1.399218	4.296429	N	4.278324	3.218995	1.024222
C	-1.493219	0.144647	0.958130	C	4.498628	3.987672	-0.183976
C	1.021441	-1.514102	0.404321	H	5.484459	4.474229	-0.144561
S	-1.496229	-0.416102	5.350415	N	4.346631	3.280218	-1.441944
O	-0.858086	-0.281837	6.685167	C	3.172827	3.662698	1.742227
O	-1.730478	0.890769	4.631587	O	2.847910	3.297766	2.857358
O	-2.796305	-1.194132	5.350341	C	3.344596	3.823650	-2.238045
H	0.716661	1.337834	-1.039336	O	3.113654	3.538474	-3.399776
H	2.161347	1.482884	-0.033721	N	2.532839	4.630343	0.974987
H	0.744081	2.484756	0.305543	C	3.306648	5.007608	-0.194213
H	1.970031	0.802630	2.862821	H	3.631275	6.054976	-0.106926
H	0.337538	1.237527	3.306101	N	2.689179	4.790459	-1.485576
H	1.576456	-1.576207	3.527093	C	1.403591	5.380497	1.487349
H	1.457224	-0.427163	4.846084	H	1.263671	5.071701	2.525685
H	-0.965749	-1.672584	3.416219	H	1.634967	6.455019	1.447576
H	-0.217390	-2.320877	4.864421	C	1.688448	5.658107	-2.068693
H	-1.946169	-0.735251	1.427408	H	1.723366	5.513498	-3.150669
H	-1.802997	0.154736	-0.095690	H	1.938895	6.700580	-1.824945
H	-1.896281	1.040027	1.443983	N	0.144419	5.155133	0.796308
H	0.614229	-1.680355	-0.601951	C	-0.246839	5.861581	-0.407273
H	2.114194	-1.518953	0.319784	H	-0.052636	6.937748	-0.288751
H	0.728626	-2.359307	1.032596	N	0.327388	5.389601	-1.651314
Na	-3.608648	0.124060	3.561418	C	-0.928595	4.518422	1.410789
N	-2.229617	-4.441718	0.354006	O	-0.921121	3.979040	2.500552
C	-2.068844	-5.329268	-0.788784	C	-0.630963	4.918675	-2.538637
H	-2.770476	-6.172692	-0.709887	O	-0.448789	4.601929	-3.700531
N	-2.168945	-4.717569	-2.093778	N	-2.035323	4.639960	0.566441
C	-1.108422	-4.465575	1.186260	C	-1.769164	5.520948	-0.556764
O	-1.036062	-3.969738	2.296631	H	-2.419188	6.406830	-0.501656
C	-0.957649	-4.706360	-2.777926	N	-1.852248	4.923078	-1.871716
O	-0.787304	-4.351031	-3.930260	C	-3.368117	4.331532	1.039390
N	-0.111694	-5.183554	0.541176	H	-3.283848	4.036393	2.087433
C	-0.566518	-5.764610	-0.704213	H	-3.995676	5.232170	0.958777
H	-0.431001	-6.855715	-0.678724	C	-3.094749	4.646475	-2.555353
N	0.007224	-5.220645	-1.920836	H	-2.852943	4.508460	-3.611316
C	1.148353	-5.521799	1.183942	H	-3.773716	5.503148	-2.438923

H	1.046192	-5.288448	2.245905		N	-4.032786	3.237473	0.339960
H	1.317809	-6.600610	1.057809		C	-4.667186	3.397021	-0.969533
C	1.343034	-5.533798	-2.387844		H	-5.328238	4.274688	-0.954176
H	1.364959	-5.310446	-3.456729		N	-3.787012	3.452224	-2.109777
H	1.541108	-6.603746	-2.228193		C	-4.520018	2.132127	1.007362
N	2.308694	-4.796249	0.705201		O	-4.319829	1.846681	2.185907
C	3.033287	-5.121640	-0.510785		C	-3.839052	2.297218	-2.881664
H	3.299348	-6.188847	-0.514723		O	-3.260525	2.107786	-3.935143
N	2.398688	-4.767999	-1.762261		N	-5.316879	1.412855	0.136657
C	3.024234	-3.934671	1.529949		C	-5.430809	2.046298	-1.161395
O	2.747470	-3.642905	2.680320		H	-6.491084	2.175034	-1.420173
C	3.083147	-3.773138	-2.449057		N	-4.715583	1.413360	-2.254040
O	2.833147	-3.375062	-3.573095		C	-6.000669	0.192088	0.513760
N	4.137639	-3.500175	0.821326		H	-7.013688	0.218253	0.095710
C	4.281215	-4.172988	-0.453832		H	-6.067624	0.174655	1.601905
H	5.238448	-4.713759	-0.487108		C	-5.187759	0.224281	-2.935758
N	4.135253	-3.353519	-1.643218		H	-4.751276	0.230242	-3.937213
C	5.143527	-2.642472	1.417433		H	-6.285161	0.263329	-3.010930
H	6.130997	-3.107309	1.283617		N	-5.367684	-1.041182	0.089026
H	4.911428	-2.570467	2.482146		C	-5.534210	-1.637323	-1.219475
C	5.184335	-2.501947	-2.167417		H	-6.602965	-1.701017	-1.466959
H	4.982104	-2.357529	-3.230983		N	-4.794886	-1.021510	-2.307423
H	6.152486	-3.008828	-2.038965		C	-4.557102	-1.799027	0.913461
N	5.190353	-1.286890	0.895964		O	-4.288597	-1.534852	2.082379
C	5.915562	-0.916935	-0.304463		C	-4.006719	-1.948935	-2.986997
H	6.914448	-1.377997	-0.294782		O	-3.446805	-1.773457	-4.052751
N	5.257343	-1.188455	-1.565485		N	-4.142664	-2.914929	0.210953
C	4.892504	-0.182706	1.691298		C	-4.843857	-3.030401	-1.069697
O	4.448521	-0.213474	2.824750		H	-5.553269	-3.868551	-1.029165
C	4.997487	-0.032682	-2.293069		N	-4.019015	-3.126440	-2.247169
O	4.587754	0.020372	-3.439229		C	-3.525375	-4.055403	0.877084
N	5.227652	0.960989	0.970199		H	-3.387457	-3.780629	1.925023
C	5.956251	0.647512	-0.245044		H	-4.210939	-4.914419	0.809642
H	6.977069	1.053284	-0.184525		C	-3.413711	-4.352459	-2.730982
N	5.337891	1.050007	-1.490620		H	-4.137745	-5.169076	-2.604608
C	5.229350	2.278744	1.583162		H	-3.197882	-4.211773	-3.792172
H	4.968491	2.144434	2.635163					

Inclusion complex of DSS and CB[7] Group E'

$E_{\text{DSS\_complex\_E'}} = -5525.8650615$ (a.u.)

C	8.973156	-0.021173	6.054440		H	-7.627854	0.453469	3.287422
Si	9.112867	-0.481235	4.219987		C	-7.418383	0.423208	-0.353987
C	8.183889	0.869339	3.237396		H	-7.443008	0.420443	-1.445926
C	8.300192	0.905330	1.696305		H	-8.443419	0.497343	0.040045
C	7.509989	-0.212704	1.013578		N	-6.258087	-0.875237	2.457465
C	10.938562	-0.500668	3.707114		C	-7.053106	-1.419672	1.377671
C	8.373864	-2.213206	3.977694		H	-8.120553	-1.380276	1.639531
S	7.587150	-0.169496	-0.801237		N	-6.842394	-0.838749	0.063681
O	9.046123	-0.271130	-1.182531		C	-5.330467	-1.784425	2.951415
O	6.739953	-1.287086	-1.280084		O	-4.615726	-1.625924	3.925294
O	7.090146	1.199152	-1.242831		C	-6.413519	-1.778952	-0.867658
H	9.497145	-0.749556	6.686685		O	-6.313960	-1.607667	-2.070004
H	7.925815	0.005953	6.382263		N	-5.400551	-2.925885	2.159666
H	9.408523	0.965852	6.256808		C	-6.506514	-2.879012	1.219864
H	7.121467	0.848902	3.524338		H	-7.247430	-3.651569	1.472247
H	8.567549	1.825440	3.625637		N	-6.164344	-2.962006	-0.183795
H	7.921665	1.866975	1.326985		C	-4.727756	-4.150765	2.544892
H	9.352589	0.841796	1.393512		H	-4.245254	-3.961689	3.506324
H	7.879841	-1.207802	1.276446		H	-5.474032	-4.951516	2.655139
H	6.444432	-0.169108	1.263868		C	-5.826186	-4.190957	-0.871039
H	11.065224	-0.775343	2.652145		H	-5.991253	-4.021526	-1.937267
H	11.504853	-1.226960	4.304467		H	-6.493575	-4.988549	-0.514041
H	11.406924	0.481515	3.852236		N	-3.699631	-4.593745	1.628164
H	8.809678	-2.914864	4.701255		C	-3.957502	-5.360763	0.426959
H	7.287336	-2.215278	4.132107		H	-4.634085	-6.197802	0.653486
H	8.568905	-2.619019	2.977520		N	-4.450999	-4.620532	-0.718493
Na	9.064389	1.725523	-2.234283		C	-2.353274	-4.576047	1.973381
N	2.926064	3.034555	-0.362347		O	-1.879305	-4.108873	2.994358
C	2.696247	3.786753	-1.575767		C	-3.582812	-4.678272	-1.803752
H	3.639881	4.227009	-1.928815		O	-3.816758	-4.285190	-2.932881
N	2.040984	3.082013	-2.667239		N	-1.654625	-5.228944	0.965936
C	2.126581	3.454008	0.688247		C	-2.529977	-5.821870	-0.025646
O	2.171640	3.051281	1.838363		H	-2.406492	-6.914739	-0.030261
C	0.861965	3.703107	-3.060471		N	-2.419297	-5.306679	-1.375753
O	0.202928	3.441361	-4.052166		C	-0.248295	-5.548499	1.097172
N	1.290398	4.459502	0.206844		H	0.050438	-5.278108	2.112415
C	1.632659	4.854424	-1.148137		H	-0.114934	-6.630542	0.946565
H	2.020726	5.883635	-1.154279		C	-1.369200	-5.683011	-2.302870
N	0.591899	4.711768	-2.142912		H	-1.742603	-5.476813	-3.308216
C	0.526000	5.291207	1.112041		H	-1.167418	-6.757907	-2.194639

H	0.770794	4.972251	2.127634	N	0.623710	-4.829863	0.190940
H	0.819917	6.342631	0.971806	C	0.892187	-5.260539	-1.170807
C	-0.528614	5.613648	-2.298182	H	1.126672	-6.335041	-1.187326
H	-0.919133	5.469773	-3.307880	N	-0.125087	-4.960163	-2.153538
H	-0.170704	6.646180	-2.181581	C	1.617212	-3.981556	0.676440
N	-0.911094	5.182640	0.965887	O	1.739650	-3.610103	1.831230
C	-1.677668	5.909217	-0.028195	C	0.270557	-3.976424	-3.051478
H	-1.392095	6.971338	-0.020280	O	-0.357866	-3.602661	-4.026956
N	-1.631581	5.395718	-1.381818	N	2.464253	-3.681004	-0.378194
C	-1.708111	4.665142	1.979297	C	2.095494	-4.355512	-1.602931
O	-1.317702	4.143529	3.009231	H	2.952424	-4.925026	-1.990551
C	-2.863254	4.920071	-1.814673	N	1.529592	-3.532444	-2.662983
O	-3.139952	4.558081	-2.944574	C	3.631982	-2.834433	-0.215583
N	-3.033061	4.893308	1.627094	H	4.491633	-3.316715	-0.699894
C	-3.162249	5.662840	0.407864	H	3.815669	-2.744729	0.856708
H	-3.717723	6.591175	0.606370	C	2.337882	-2.727062	-3.564263
N	-3.737440	4.975131	-0.733469	H	1.756085	-2.587742	-4.477979
C	-4.125744	4.607367	2.531235	H	3.265545	-3.273556	-3.792733
H	-4.755779	5.504492	2.620050	N	3.481178	-1.494820	-0.741788
H	-3.688013	4.366527	3.502431	C	3.757082	-1.167165	-2.129372
C	-5.158456	4.746181	-0.901655	H	4.679497	-1.665360	-2.450018
H	-5.332444	4.587603	-1.968163	N	2.676011	-1.416730	-3.064151
H	-5.709183	5.636223	-0.563936	C	3.591331	-0.382746	0.082679
N	-4.956049	3.481797	2.149466	O	3.641841	-0.391639	1.303666
C	-6.045392	3.574874	1.194585	C	2.199110	-0.254483	-3.653207
H	-6.674067	4.447157	1.425712	O	1.386764	-0.185857	-4.562458
N	-5.677147	3.587708	-0.205246	N	3.665777	0.739061	-0.730452
C	-5.047288	2.346631	2.948063	C	3.882299	0.388163	-2.122636
O	-4.371946	2.101788	3.932073	H	4.870065	0.743564	-2.440901
C	-6.096853	2.448930	-0.880908	N	2.852581	0.813954	-3.053691
O	-6.014067	2.251969	-2.080680	C	3.975781	2.046615	-0.190659
N	-6.080494	1.564063	2.446321	H	4.126059	1.924616	0.883683
C	-6.793275	2.208841	1.363521	H	4.899537	2.413694	-0.654738
H	-7.854824	2.323223	1.627527	C	2.731946	2.162573	-3.554879
N	-6.671076	1.594624	0.054346	H	3.737740	2.557487	-3.762634
C	-6.542582	0.374511	3.131743	H	2.153465	2.117218	-4.480153
H	-6.032518	0.342169	4.096882				

Inclusion complex of DSS and CB[7] Group F'

$E_{\text{DSS\_complex\_F'}} = -5525.8617108$ (a.u.)

C	1.829674	-0.114658	-0.970595	H	1.271586	-6.623091	-2.111709
Si	0.467015	-0.023893	0.339328	C	0.893489	-5.459285	1.312281
C	1.313244	-0.081174	2.041496	H	0.789566	-5.189124	2.365347
C	0.541097	0.279131	3.330923	H	1.077088	-6.540259	1.222963
C	-0.427408	-0.816261	3.778382	N	-0.192078	-5.171014	-1.795152
C	-0.489388	1.587324	0.098759	C	-0.798842	-5.715321	-0.593960
C	-0.715249	-1.462379	0.009942	H	-0.675923	-6.808157	-0.574382
S	-1.426647	-0.357682	5.239788	N	-0.364870	-5.145911	0.664803
O	-0.563413	-0.449614	6.444334	C	-1.127928	-4.594793	-2.646074
O	-1.943961	1.030900	4.939244	O	-0.929275	-4.215665	-3.786325
O	-2.599493	-1.310621	5.220311	C	-1.382893	-4.469732	1.325513
H	1.417090	-0.117256	-1.986631	O	-1.330009	-4.008891	2.450361
H	2.428458	-1.026880	-0.861924	N	-2.347432	-4.575433	-1.976836
H	2.514319	0.738670	-0.899112	C	-2.296833	-5.263635	-0.704074
H	1.787544	-1.064112	2.168567	H	-3.005104	-6.105376	-0.703262
H	2.148073	0.628633	1.967438	N	-2.492002	-4.449404	0.482099
H	1.268096	0.453989	4.132959	C	-3.573041	-4.198590	-2.646505
H	-0.005838	1.219356	3.203958	H	-3.330532	-4.056205	-3.701719
H	-1.159353	-1.059384	3.001914	H	-4.306263	-5.010222	-2.540226
H	0.086156	-1.748208	4.032271	C	-3.779440	-3.992038	0.952371
H	-1.231934	1.743537	0.889167	H	-3.665888	-3.743966	2.010164
H	-1.011711	1.591303	-0.866776	H	-4.516078	-4.801755	0.839449
H	0.190316	2.446454	0.109048	N	-4.179576	-2.968361	-2.177297
H	-1.158673	-1.367761	-0.990223	C	-5.003938	-2.859759	-0.999409
H	-0.178091	-2.416381	0.041137	H	-5.749141	-3.666783	-0.977073
H	-1.532031	-1.516921	0.736846	N	-4.302659	-2.803682	0.283860
Na	-3.698754	0.206222	3.710796	C	-4.137413	-1.790420	-2.914411
N	2.869322	4.619166	-1.478000	O	-3.575981	-1.626983	-3.981308
C	3.463760	4.812029	-0.174421	C	-4.606350	-1.650603	0.979309
H	3.796114	5.854760	-0.062702	O	-4.270126	-1.384789	2.130754
N	2.655862	4.424499	0.970735	N	-4.899136	-0.843420	-2.231669
C	3.504993	3.628704	-2.217898	C	-5.633000	-1.433983	-1.127328
O	3.280098	3.343790	-3.380473	H	-6.710423	-1.446598	-1.342321
C	3.296922	3.468898	1.758449	N	-5.397193	-0.851011	0.176308
O	2.953563	3.104274	2.868261	C	-5.256226	0.419025	-2.849934
N	4.476347	3.055933	-1.401942	H	-4.842368	0.409276	-3.860914
C	4.643118	3.782200	-0.155344	H	-6.352558	0.499551	-2.900449
H	5.634690	4.257738	-0.128316	C	-5.957963	0.408008	0.620645
N	4.420652	3.035335	1.063622	H	-5.997411	0.390001	1.709817
C	5.480506	2.158970	-1.942499	H	-6.980176	0.483280	0.231683

H	5.302240	2.088068	-3.017729		N	-4.723681	1.591535	-2.181889
H	6.478166	2.585163	-1.758822		C	-5.376307	2.243100	-1.061399
C	5.377036	2.106525	1.634956		H	-6.440921	2.407474	-1.278631
H	5.130948	1.997718	2.693466		N	-5.231291	1.595648	0.225100
H	6.385044	2.532820	1.530597		C	-3.828213	2.443104	-2.827204
N	5.439530	0.812883	-1.412561		O	-3.285103	2.237451	-3.896357
C	6.054992	0.410691	-0.164244		C	-4.371313	2.274147	1.069003
H	7.093299	0.772503	-0.125587		O	-4.110753	1.948503	2.225103
N	5.361672	0.776032	1.057400		N	-3.709014	3.589430	-2.049844
C	5.077431	-0.271690	-2.203332		C	-4.562790	3.566799	-0.888088
O	4.685086	-0.223520	-3.355183		H	-5.192589	4.466746	-0.858697
C	4.984718	-0.337014	1.802410		N	-3.901849	3.389939	0.405350
O	4.577198	-0.330272	2.949812		C	-2.951381	4.744979	-2.488288
N	5.295162	-1.424239	-1.456931		H	-3.578510	5.639285	-2.365328
C	5.947410	-1.153896	-0.192221		H	-2.721033	4.598238	-3.545635
H	6.926092	-1.655640	-0.161169		C	-3.226038	4.480720	1.102481
N	5.198267	-1.462547	1.012487		H	-3.155835	4.196005	2.154593
C	5.156918	-2.742917	-2.037103		H	-3.843227	5.386532	1.004627
H	6.087147	-3.305999	-1.869792		N	-1.693553	4.947689	-1.804746
H	4.994988	-2.608255	-3.108792		C	-1.568198	5.582792	-0.509372
C	5.027712	-2.801441	1.542474		H	-2.158585	6.510880	-0.487297
H	4.787652	-2.696600	2.602766		N	-1.884059	4.766555	0.648575
H	5.969527	-3.357585	1.428798		C	-0.477676	4.845614	-2.472562
N	4.039133	-3.517557	-1.531506		O	-0.320768	4.491915	-3.627516
C	4.096236	-4.300295	-0.310549		C	-0.788878	4.607493	1.496743
H	5.017478	-4.901100	-0.292805		O	-0.811839	4.116837	2.609405
N	3.959603	-3.570624	0.932572		N	0.516556	5.268536	-1.598581
C	2.995512	-3.912623	-2.363131		C	-0.024926	5.828636	-0.374238
O	2.813534	-3.553539	-3.512575		H	0.239057	6.894076	-0.302042
C	2.792673	-3.893573	1.615277		N	0.320087	5.148630	0.857314
O	2.491607	-3.529298	2.738310		C	1.874144	5.495017	-2.056712
N	2.223774	-4.829457	-1.657899		H	1.881095	5.323560	-3.135267
C	2.793311	-5.166848	-0.372019		H	2.153344	6.537280	-1.844393
H	2.987833	-6.248264	-0.318160		C	1.604427	5.263848	1.519490
N	2.045768	-4.740002	0.798634		H	1.928810	6.314781	1.483791
C	1.126170	-5.544681	-2.271916		H	1.458852	4.958011	2.557896
H	1.154486	-5.323597	-3.341074					

Optimized structure of inclusion complex of TSP and CB[7] using DFT calculation

The initial conformers of the inclusion complex of TSP and CB[7] were constructed, in which the trimethylsilyl group of Group A and B TSP was located in the CB[7] cavity based on the inclusion complex structure was estimated by NMR measurements. All conformations in water were optimized using a SAS model at B3LYP/6-31+g(d) level, the structures with the smallest energy were regarded as the optimized conformation of the inclusion complex (Fig. S14 Groups A' and B'). The stabilization energies E (kJ mol^{-1}) for the inclusion complexation were calculated using the following equation: $E = E_{\underline{TSP}\_complex} - (E_{TSP} + E_{CB[7]})$, where $E_{\underline{TSP}\_complex}$, E_{TSP}, and $E_{CB[7]}$ represent the total energy of the inclusion complex, TSP, and CB[7], respectively.

Group A'

2.27 Å
2.33 Å
2.24 Å
2.34 Å

$E = -32.2$ kJ mol^{-1}

Group B'

2.21 Å
2.21 Å

$E = +46.5$ kJ mol^{-1}
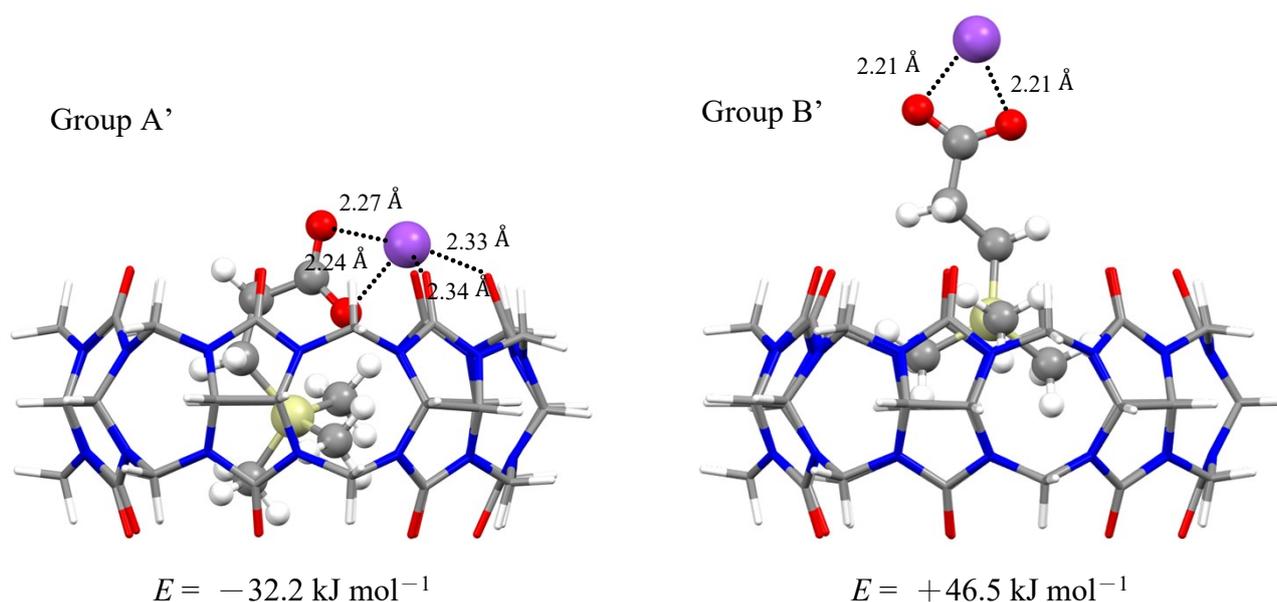
Fig. S14 Optimized structures of inclusion complex of TSP and CB[7].

Table S5 Atomic coordinates and energies of inclusion complex of TSP and CB[7] (Groups A and

B).

Inclusion complex of TSP and CB[7] Group A'

$E_{\text{TSP\_complex\_A'}} = -5051.2910134$ (a.u.)

C	0.025947	-1.801254	0.049229	H	-4.829658	2.646753	2.946546
Si	-0.248233	0.017071	0.483756	H	-5.961901	3.336721	1.740093
C	-1.434328	0.020850	1.967889	N	-3.976773	3.612150	-1.150226
C	1.362175	0.795720	1.093530	C	-4.037174	4.324555	0.107690
C	-1.088677	0.996999	-0.923444	H	-4.948885	4.939509	0.146265
C	-0.971598	0.462175	-2.363185	N	-3.930092	3.531357	1.318879
C	0.461534	0.286893	-2.860934	C	-2.861010	3.952698	-1.905841
O	1.387683	0.253856	-1.990966	O	-2.646990	3.626130	-3.059305
O	0.663349	0.147278	-4.109308	C	-2.828575	3.890906	2.088160
H	0.770155	-1.907562	-0.744518	O	-2.592242	3.521311	3.225096
H	-0.900285	-2.284397	-0.283842	N	-2.062578	4.781644	-1.123756
H	0.376906	-2.341356	0.936717	C	-2.719548	5.173481	0.108749
H	-1.659729	1.030335	2.333481	H	-2.903816	6.258540	0.106831
H	-2.387653	-0.460929	1.721192	N	-2.069709	4.788273	1.344710
H	-1.007550	-0.541948	2.808244	C	-0.911161	5.464244	-1.679192
H	1.211556	1.845775	1.373176	H	-0.864430	5.200385	-2.738000
H	2.120088	0.755215	0.307521	H	-1.050727	6.550887	-1.572817
H	1.735400	0.276016	1.985149	C	-0.948727	5.500269	1.922008
H	-2.155983	1.084555	-0.670978	H	-0.925280	5.262363	2.987636
H	-0.691211	2.021672	-0.892058	H	-1.109541	6.580858	1.786650
H	-1.458812	-0.518829	-2.454321	N	0.361563	5.100158	-1.087712
H	-1.499535	1.119028	-3.062505	C	0.868018	5.681417	0.136590
Na	2.857912	-0.155773	-3.625881	H	0.729029	6.773217	0.117004
N	1.894944	-4.781870	-1.052229	N	0.347131	5.142097	1.379356
C	1.644218	-5.572499	0.138563	C	1.352389	4.446929	-1.814686
H	2.242436	-6.495700	0.107150	O	1.253668	4.028655	-2.952565
N	1.828308	-4.908001	1.411488	C	1.352752	4.623647	2.188834
C	0.758087	-4.651123	-1.847650	O	1.239028	4.289110	3.354893
O	0.725521	-4.195473	-2.976334	N	2.500321	4.411960	-1.021732
C	0.645644	-4.797758	2.134619	C	2.373642	5.252895	0.155099
O	0.542552	-4.413442	3.286377	H	3.067765	6.104134	0.081320
N	-0.310427	-5.191749	-1.145049	N	2.524394	4.606705	1.440274
C	0.098982	-5.836246	0.085920	C	3.775560	4.019654	-1.581326
H	-0.156937	-6.905786	0.049560	H	3.608277	3.783404	-2.634166
N	-0.385430	-5.258144	1.325446	H	4.481420	4.860677	-1.498285
C	-1.623451	-5.333106	-1.739804	C	3.799092	4.229898	2.012601
H	-1.528683	-5.063482	-2.793961	H	3.640238	4.093838	3.084439

H	-1.941665	-6.382791	-1.651234		H	4.521443	5.041563	1.843935
C	-1.725257	-5.451846	1.844950		N	4.378031	2.846448	-0.969727
H	-1.683536	-5.254444	2.918297		C	5.126349	2.885126	0.283629
H	-2.026490	-6.495534	1.670525		H	5.877908	3.686367	0.234957
N	-2.650550	-4.479361	-1.173860		N	4.363182	2.995205	1.504173
C	-3.399009	-4.809308	0.024765		C	4.640627	1.700949	-1.691459
H	-3.748149	-5.851698	-0.028122		O	4.318752	1.480948	-2.856282
N	-2.735878	-4.575701	1.289767		C	4.422265	1.841290	2.278478
C	-3.288285	-3.508644	-1.941107		O	3.985334	1.708220	3.406368
O	-2.986757	-3.171261	-3.071616		N	5.397034	0.854843	-0.900232
C	-3.366669	-3.597972	2.052021		C	5.751877	1.452295	0.371450
O	-3.115418	-3.315569	3.209752		H	6.846027	1.460069	0.482533
N	-4.361122	-3.026712	-1.199852		N	5.131962	0.887685	1.553573
C	-4.567630	-3.766055	0.026760		C	5.914876	-0.408711	-1.380477
H	-5.564760	-4.231609	0.020130		H	6.968714	-0.490601	-1.084966
N	-4.372996	-3.039042	1.268011		H	5.848445	-0.400703	-2.469255
C	-5.314971	-2.088342	-1.753226		C	5.523289	-0.373418	2.148604
H	-6.327983	-2.502036	-1.637978		H	5.197641	-0.348827	3.190998
H	-5.079624	-1.977676	-2.814021		H	6.618832	-0.470231	2.105234
C	-5.366613	-2.144517	1.833105		N	5.216410	-1.585933	-0.906334
H	-5.163061	-2.070702	2.903650		C	5.467945	-2.214045	0.375459
H	-6.366479	-2.576155	1.674207		H	6.547720	-2.378842	0.500527
N	-5.276217	-0.762913	-1.168033		N	4.923422	-1.546532	1.540738
C	-5.966763	-0.403051	0.054955		C	4.332961	-2.306669	-1.687962
H	-7.001584	-0.776729	0.021985		O	4.011771	-2.025556	-2.841050
N	-5.342583	-0.796662	1.302504		C	4.048568	-2.364124	2.251758
C	-4.926586	0.352210	-1.924156		O	3.593922	-2.139666	3.358159
O	-4.522566	0.343916	-3.072581		N	3.927395	-3.415047	-0.972559
C	-5.009554	0.297535	2.095107		C	4.639852	-3.538816	0.294096
O	-4.661729	0.261962	3.261590		H	5.264209	-4.443703	0.278029
N	-5.170776	1.479620	-1.146429		N	3.833682	-3.509703	1.491599
C	-5.877697	1.161752	0.077799		C	3.211435	-4.522585	-1.589190
H	-6.863579	1.651112	0.075130		H	3.086262	-4.277207	-2.645739
N	-5.194231	1.441203	1.325486		H	3.826796	-5.429887	-1.490596
C	-5.058916	2.818245	-1.692748		C	3.117588	-4.656764	2.016437
H	-4.873306	2.714176	-2.764009		H	3.750546	-5.548434	1.897051
H	-6.007955	3.349505	-1.529465		H	2.941070	-4.468962	3.077710
C	-5.029773	2.768788	1.879755					

Inclusion complex of TSP and CB[7] Group B'

$E_{\text{TSP\_complex\_B'}} = -5051.2625154$ (a.u.)

C	0.520598	-1.493232	1.573726
Si	-0.099316	0.284313	1.454836
C	1.117671	1.275308	0.392671
C	-1.737467	0.253037	0.507924
C	-0.246327	1.019492	3.198779
C	-1.241203	0.304470	4.132091
C	-1.109017	0.634723	5.623133
O	-2.134388	0.451160	6.365279
O	0.007182	1.033617	6.090287
H	-0.198512	-2.127653	2.102188
H	1.465374	-1.557221	2.124121
H	0.676940	-1.923385	0.574728
H	0.718263	2.261351	0.127801
H	2.067781	1.426286	0.912227
H	1.328086	0.746227	-0.546673
H	-2.125139	1.262060	0.327020
H	-2.494853	-0.307620	1.062194
H	-1.605660	-0.231075	-0.469514
H	0.755684	0.991045	3.646743
H	-0.508412	2.082986	3.131626
H	-2.276898	0.502176	3.838926
H	-1.125154	-0.788093	4.067050
Na	-0.920289	1.096167	8.094470
N	3.408058	-4.160860	0.975420
C	4.160678	-4.276769	-0.256632
H	4.682096	-5.245292	-0.286212
N	3.428293	-4.073729	-1.492661
C	3.824626	-3.080950	1.747220
O	3.494922	-2.848253	2.896593
C	3.945168	-3.028342	-2.249393
O	3.641705	-2.751521	-3.396894
N	4.722339	-2.337913	0.984038
C	5.135313	-3.051437	-0.212007
H	6.193478	-3.341443	-0.128628
N	4.906175	-2.388971	-1.477157
C	5.481376	-1.244288	1.562868
H	5.173722	-1.161032	2.607520
H	6.554838	-1.482821	1.510708
C	5.748297	-1.340441	-2.013856
H	5.584770	-1.315373	-3.093394
H	0.243547	5.149086	-3.611213
H	0.158745	6.548474	-2.493223
N	-1.216476	5.021654	0.409049
C	-1.741924	5.447168	-0.874541
H	-1.779341	6.546125	-0.918059
N	-1.074389	4.930382	-2.050711
C	-2.167967	4.337755	1.163289
O	-2.072853	4.039653	2.339718
C	-1.894998	4.106956	-2.812239
O	-1.635150	3.647920	-3.910976
N	-3.264059	4.092159	0.339725
C	-3.156850	4.778219	-0.932397
H	-3.976855	5.504794	-1.035438
N	-3.085452	3.944082	-2.114570
C	-4.510296	3.554360	0.859562
H	-4.400438	3.478686	1.943611
H	-5.324196	4.252877	0.616126
C	-4.232013	3.288417	-2.705206
H	-3.972204	3.058277	-3.740793
H	-5.089727	3.977491	-2.681493
N	-4.864140	2.234010	0.378101
C	-5.474642	1.961594	-0.906239
H	-6.354692	2.606537	-1.048229
N	-4.612670	2.042941	-2.071413
C	-4.855283	1.119307	1.210249
O	-4.544499	1.104947	2.387136
C	-4.530674	0.835703	-2.755292
O	-4.017194	0.660461	-3.846703
N	-5.312133	0.035878	0.466953
C	-5.833419	0.436382	-0.826454
H	-6.915550	0.242817	-0.871676
N	-5.186750	-0.123442	-1.994942
C	-5.528721	-1.264172	1.071326
H	-5.327003	-1.152644	2.139033
H	-6.577422	-1.561484	0.921492
C	-5.433427	-1.456786	-2.502150
H	-5.175756	-1.453988	-3.563495
H	-6.501378	-1.688464	-2.379577
N	-4.673126	-2.330543	0.578520
C	-4.970421	-3.110574	-0.606279

H	6.798225	-1.589184	-1.802398
N	5.259901	0.048589	0.943301
C	5.954078	0.499241	-0.247791
H	7.031757	0.299578	-0.151834
N	5.468245	-0.012056	-1.512689
C	4.672644	1.100986	1.640740
O	4.173631	1.036519	2.749601
C	4.951393	0.985148	-2.330793
O	4.602133	0.855191	-3.491155
N	4.795292	2.246623	0.860237
C	5.612214	2.027595	-0.316469
H	6.501972	2.673659	-0.279652
N	4.955460	2.166886	-1.601142
C	4.424147	3.559990	1.356779
H	5.287007	4.233276	1.247279
H	4.177637	3.445673	2.414713
C	4.633253	3.438238	-2.213278
H	4.515723	3.257109	-3.283938
H	5.464589	4.138252	-2.043617
N	3.270839	4.165042	0.718898
C	3.310820	4.862864	-0.550788
H	4.120767	5.607610	-0.543768
N	3.406257	4.046769	-1.744620
C	2.083881	4.387910	1.409511
O	1.849896	4.069772	2.560371
C	2.295467	4.172875	-2.569009
O	2.178869	3.719769	-3.694506
N	1.227000	5.083731	0.560442
C	1.883386	5.502839	-0.661656
H	1.904503	6.601521	-0.719218
N	1.362235	4.955015	-1.898775
C	-0.040409	5.612889	1.023814
H	-0.100847	5.408565	2.095050
H	-0.057906	6.699895	0.851497
C	0.175164	5.450602	-2.563734
H	-6.026111	-3.420147	-0.595340
N	-4.648198	-2.501520	-1.880906
C	-3.715575	-2.940185	1.385382
O	-3.385445	-2.585530	2.502292
C	-3.681327	-3.208283	-2.583883
O	-3.328417	-3.002167	-3.732187
N	-3.232171	-4.054541	0.703139
C	-3.971714	-4.314717	-0.516382
H	-4.473723	-5.291432	-0.449550
N	-3.226126	-4.226532	-1.755447
C	-2.389893	-5.040838	1.354966
H	-2.873923	-6.026143	1.270567
H	-2.311008	-4.760084	2.407465
C	-2.321774	-5.250199	-2.231775
H	-2.189076	-5.084709	-3.303115
H	-2.773855	-6.238061	-2.061318
N	-1.035924	-5.126368	0.839589
C	-0.683685	-5.859654	-0.364006
H	-1.117457	-6.870406	-0.328024
N	-1.006214	-5.232755	-1.626754
C	0.068892	-4.925694	1.664580
O	0.041678	-4.577771	2.831273
C	0.124235	-4.856866	-2.340506
O	0.144308	-4.416417	-3.476797
N	1.205772	-5.241244	0.926725
C	0.882379	-5.859316	-0.342142
H	1.316706	-6.869427	-0.387558
N	1.231713	-5.120140	-1.541602
C	2.538081	-5.198808	1.499862
H	2.420029	-5.009524	2.568917
H	3.021779	-6.174359	1.347179
C	2.572057	-5.076959	-2.087048
H	3.040227	-6.066322	-1.967848
H	2.482389	-4.837428	-3.148900