Electronic supporting Information

Chemometrics-assisted mechanism study of the room-temperature phosphorescence on nanoscopic boronate assemblies

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Contents

1. General

The absorption and emission were measured using Shimadzu UV-3600 UV/vis/NIR spectrometer and JASCO FP-8500 spectrofluorometers, respectively. Quantum yields were measured with an integrating sphere unit (JASCO ILF-835 60 mm φ) on FP-8500. Fluorescence lifetimes were measured using Hamamatsu Photonics Quantaurus-Tau C11367 and TDC unit M12977-01. Powder X-ray diffraction (PXRD) data were collected by a Rigaku RINT-TTR III X-ray diffractometer with Cu Kα radiation. Field-emission scanning electron microscopy (FE-SEM) was performed using a JEOL JSM-7500F (acceleration voltage of 5 kV). The sample was coated with Os on a Meiwafosis Neoc-Pro osmium coater. Transmission electron microscopy (TEM) was performed using a JEOL JEM-3200FS (acceleration voltage 300 kV). Fourier-transform infrared (FT-IR) spectroscopy was performed using a JASCO FT/IR-4600 type A with ATR PRO 450-S. Photographic images were taken with a digital camera (Canon EOS Kiss X8i). X-ray photoelectron spectra was measured with a JEOL JPS9010MX.

2. Materials

Unless otherwise indicated, reagents used for the synthesis were commercially available and were used as supplied.

3. Synthesis and preparations

Preparation of BFs

To a MeOH solution (50 mL) of **PE** (20 mM) was added MeOH/H_2O=4/1 v/v solution (50 mL) of **BDBA** dropwise over 4 h while stirring. The resultant white solid was collected by filtration, washed with MeOH and dried in vacuo.

Preparation of BSs

To a THF dispersion (50 mL) of ball milled **PE** (20 mM) was added THF solution (50 mL) of **BDBA** in one portion. The resultant dispersed solution was allowed to stand for 24 h at room-temperature under dark condition. The white precipitate was collected by filtration, washed with MeOH and dried in ambient condition over 2 days.

Synthesis of 3,9-diphenyl-2,4,8,10-tetraoxa-3,9-diboraspiro[5.5] undecane (1)

It was synthesized according to the methods previously reported[1]. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.79 (dd, *J*=8.03 and 1.33 Hz, 4H), 7.45 (tt, *J*=7.41 and 1.68 Hz, 2H), 7.35-7.38 (m, 4H), 4.07 (s, 8H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) 133.94, 131.12, 127.67, 64.93, 36.67. ^{11}B NMR (128 MHz, $CDCl_3$): δ (ppm) 25.28. FAB-MS (positive mode): *m/z*=308 $[M]^+$.

4. Measurement of BDBA/PE ratio and estimation of the degree of polymerizations (X_n)

Boronate assembly was decomposed and dissolved into 1 M NaOH solution (MeOH/H_2O = 1:1 v/v). The concentration of **BDBA** was then measured by UV/Vis. Herein, a calibration curve of **BDBA** was obtained in identical solvent condition. Note that, all of the experiments were conducted in glovebox to avoid the oxidation of boronate salts. The ratio of **BDBA/PE** was calculated from the concentration of **BDBA** and the dissolved weight of boronate assemblies. Degree of polymerization (X_n) was calculated by the equation below, assuming that both sides of polymer chain are capped with **PE** (Fig. S1); the structure was estimated from the ATR-FTIR (Fig. 2b) and XPS (Fig. S2).

$$\frac{m_{\mathrm{BDBA}}}{m_{\mathrm{PE}}} = \frac{161.714 \cdot X_n}{68.013 \cdot (X_n - 1) + 204.136} \quad \text{(Eq. S1)}$$

Where m_{BDBA} and m_{PE} are the weights of BDBA and PE in an assembly, respectively.

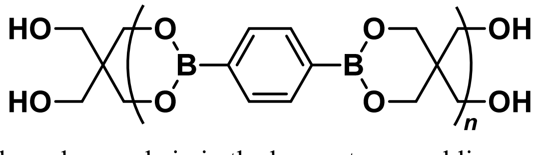


Fig. S1. Plausible structure of the polymer chain in the boronate assemblies, estimated from the FTIR spectra.

5. X-ray photoelectron spectroscopy (XPS) measurements

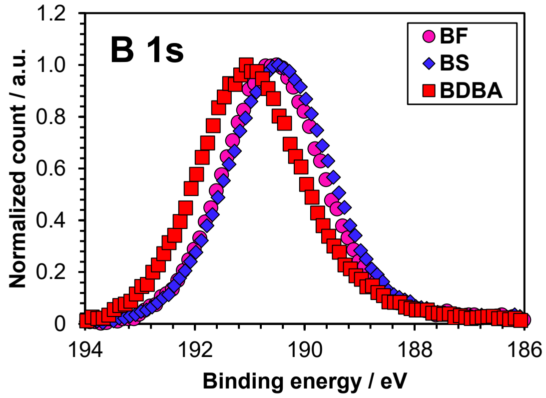


Fig. S2. XPS spectra of B 1s bands of **BF**, **BS** and **BDBA**.

6. Temperature dependent delayed emission spectra

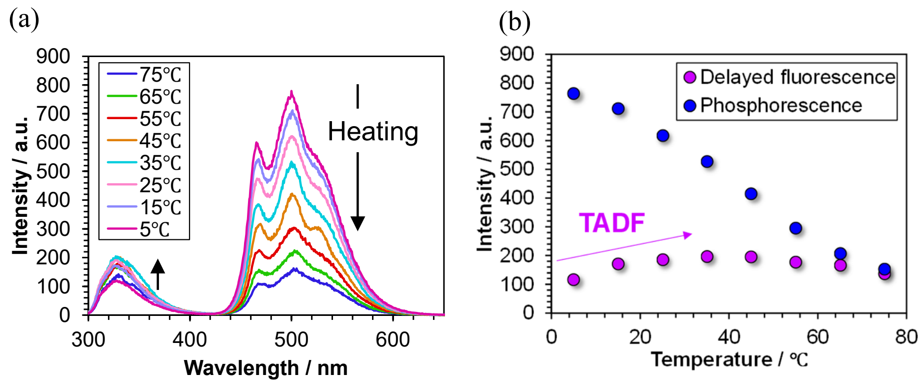


Fig. S3. Temperature dependent delayed emission spectra and (b) the temperature dependence of RTP and TADF intensity of **BF**. (λ_{ex} = 254 nm, delay time: 50 ms, MeOH dispersion)

7. Diffusion reflection absorption spectra of boronate assemblies

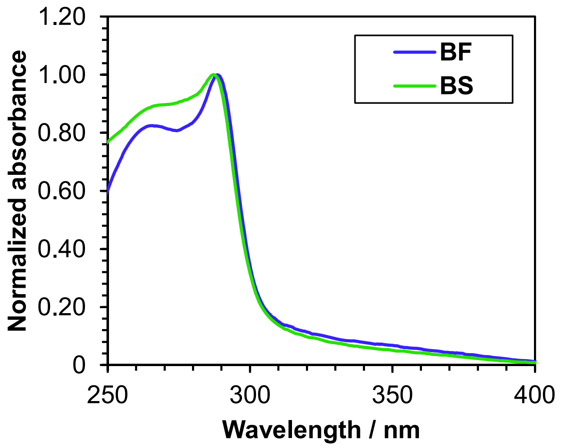


Fig. S4. Diffusion reflection absorption spectra of boronate assemblies.

8. Steady-state emission spectra of boronate assemblies

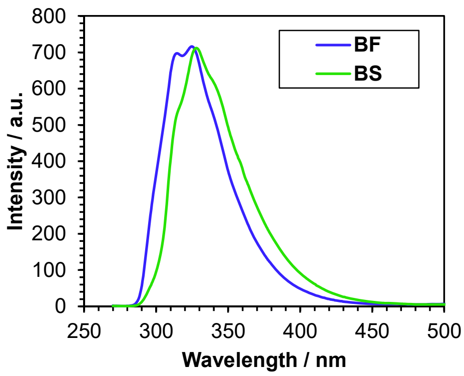
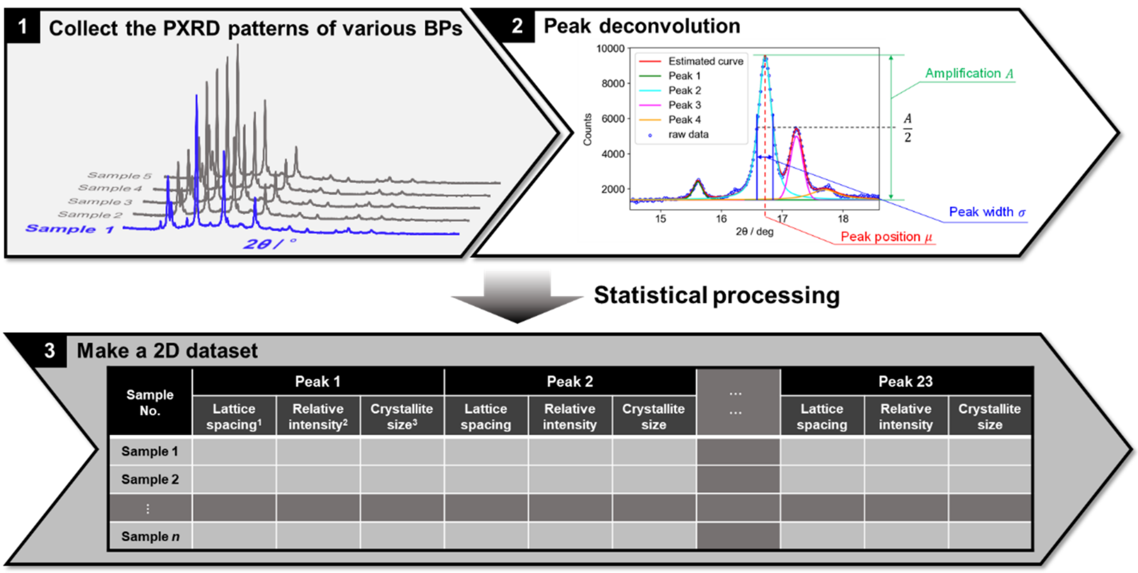


Fig. S5. Steady-state emission spectra of boronate assemblies. (λ_{ex} = 254 nm, MeOH dispersion)

9. Chemometrics analysis

All the chemometrics analyses in this work were performed using Python 3.7.9[2], Pandas[3], Numpy[4], Scikit-learn[5, 6], Matplotlib[7], and Scipy[8]. The dataset for the chemometrics QSPR analyses was prepared from the PXRD patterns of boronate assemblies. The PXRD patterns consisted of a maximum of 23 diffractions to be deconvoluted by 23 pseudo-Voigt functions. Peak amplification, peak width, and peak positions were extracted from the fitting result. Then the two-dimensional dataset was constructed from those parameters. The procedure so far is schematically illustrated in Fig. S4. Some missing data in the 2D-dataset was interpolated by MissForest in which the non-parametric missing value imputation method based on random forest[9]. The interpolated 2D-dataset was then auto-scaled and used for further chemometrics analyses. The RTP intensities at 500 nm at 50 ms of delay were used for the visualizations of chemometrics analyses. The additional two samples were prepared as out-of-sample prediction dataset, to evaluate the performance of PCR; whose PXRD patterns were analyzed by same procedure.

PCA of the 2D-dataset was performed by 7 principal components, and all of the components were used for PCR by using the RTP intensities at 500 nm at 50 ms of delay as response variables. To analyze the contributions of each peak parameter, inner product of the PCA loading vectors and the standardize regression coefficients were calculated. *t*-SNE analysis were performed with 5 of perplexity and 2 of components (meaning of 2 dimension).



[1]Calculated from the peak position by Bragg's law. [2]Relative intensity to the largest peak. [3]Calculated from the peak width by Scherrer equation.

Fig. S6. Schematic drawing of the chemometrics analysis procedure.

10. Contribution coefficients

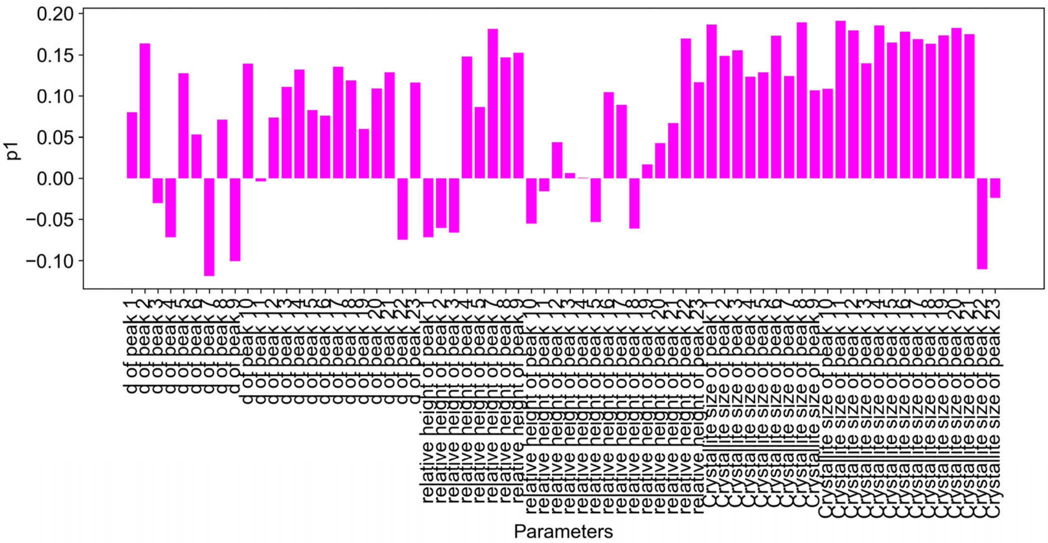


Fig. S7. Loading vectors (contributions) of each parameter in 1st principal component of PCA.

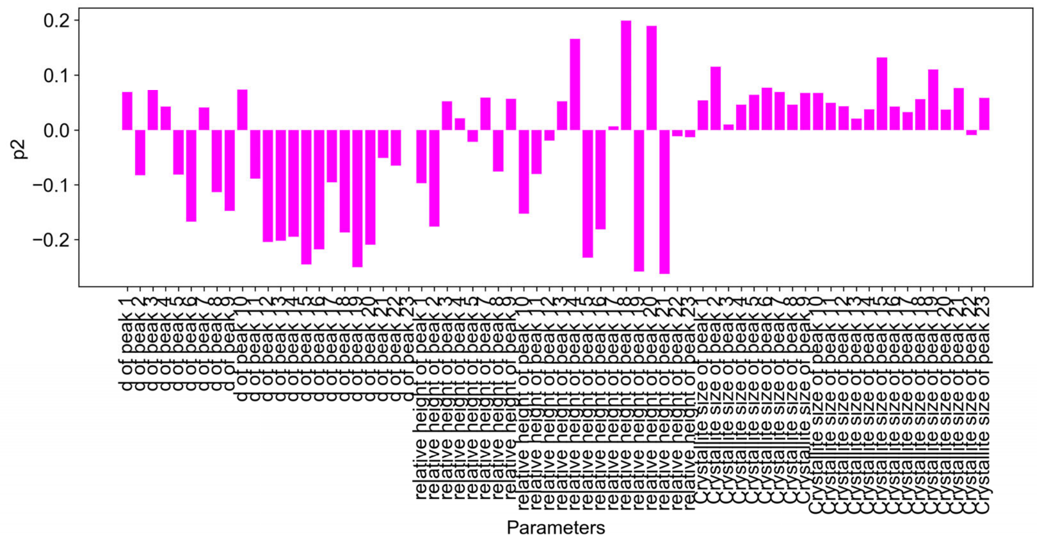


Fig. S8. Loading vectors (contributions) of each parameter in 2nd principal component of PCA.

11. Relationship between the RTP intensity and peak 2 parameters

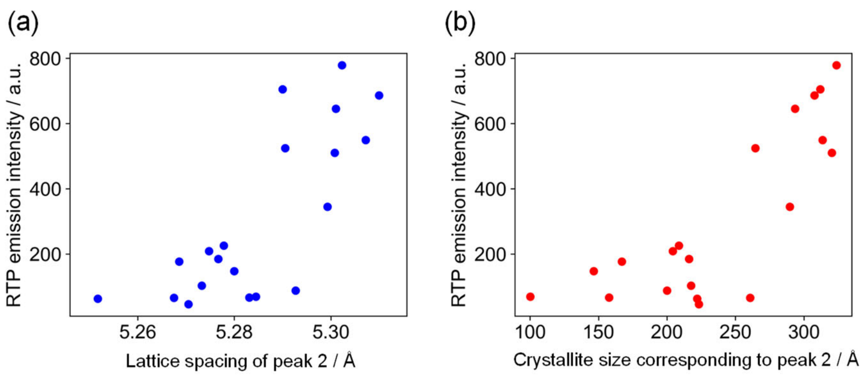


Fig. S9. Relationship between RTP intensity and the lattice spacing of peak 2 or crystallize size corresponding to peak 2.

12. Crystal structure simulation of boronate assemblies by compound 1

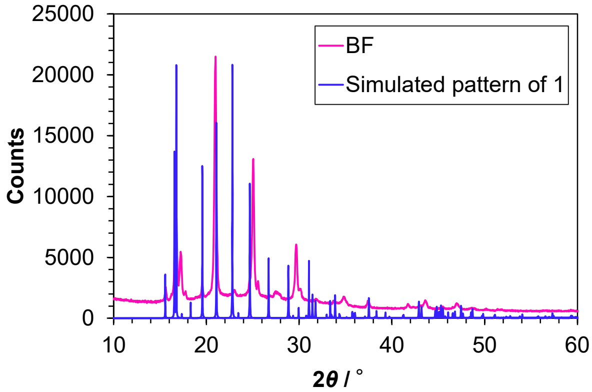


Fig. S10. PXRD pattern of **BF** compared to the simulated PXRD pattern of model compound **1**.

13. DFT calculations

Density functional theory (DFT) calculations were performed in Orca 4.2.1 software[10, 11]. The structure of dimer model was extracted from the single crystal of compound **1** (CCDC No. 1968918). Only the positions of hydrogens were optimized at B3LYP-D3BJ/def2-TZVP level. Distance between the molecules in a dimer was modified along the normal vector of (011) lattice plane. TD-DFT calculation was performed for the dimer models at ωB97X-D3/def2-TZVP level with RI and COSX approximation. The contribution of CT transition was extracted from the configuration interaction (CI) coefficients in S_1 state. The molecular orbitals were visualized using Avogadro 1.2.0 program[12, 13].

14. Fluorescence decay profiles of boronate assemblies

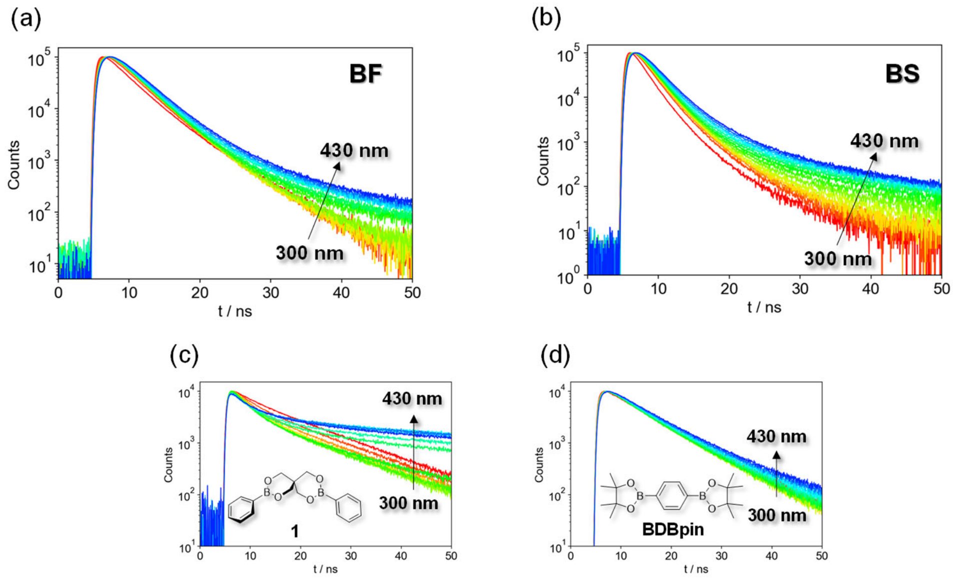


Fig. S11. Emission wavelength dependent fluorescence decay profiles of boronate assemblies, model compound **1**, and benzene-1,4-diboronic acid bis(pinacol) ester (BDBpin). (λ_{ex} = 280 nm, room-temperature, solid-state)

Table S1. Deconvoluted fluorescence decay parameters at λ_{em} = 400 nm.

Emission wavelength / nm	BF				BS			
	τ_1	τ_2	A_1	A_2	τ_1	τ_2	A_1	A_2
300	3.418917	7.58518	107525.6	5834.057	1.988512	6.730099	118358	1488.089
310	3.660027	13.12051	115907.8	672.0315	2.197124	7.207001	115203.6	1529.175
320	3.670594	17.60218	116681.9	299.1434	2.287124	8.557602	122184.3	1163.441
330	3.646579	16.62814	116793.5	281.6032	2.341464	9.460951	125264.1	1058.839
340	3.642737	21.21848	117591	269.7206	2.304106	8.909403	119588.3	1474.123
350	3.594707	17.13545	113411.9	516.3218	2.359804	10.78619	122419.9	1252.566
360	3.627367	20.69567	116386.5	499.4754	2.376785	11.47014	119182.5	1358.593
370	3.607194	18.98669	114839.1	768.5688	2.399879	12.35389	117861.5	1465.718
380	3.661949	21.03801	117328	781.8108	2.46237	13.54887	118803.9	1477.218
390	3.689806	19.81537	115848.2	978.8943	2.512634	13.96027	118954.6	1611.719
400	3.717663	19.75016	112904.6	1113.634	2.584634	14.54171	118632.7	1673.525
410	3.831974	21.93461	116002.7	993.1673	2.664785	14.68027	119323	1738.969
420	3.882886	21.61673	114932.8	1123.328	2.697389	13.92767	115573.5	2063.899
430	4.021212	24.72225	117967.2	946.6471	2.814898	14.51686	118184.4	2028.438

15. Absorption spectrum of BDBA crystal

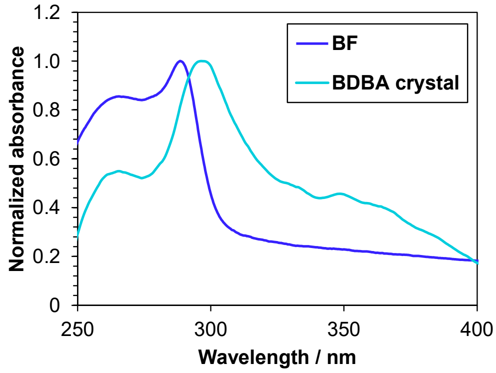


Fig. S12. Diffusion reflection absorption spectra of **BF** and **BDBA** crystal.

16. Errors of the predicted RTP intensities of unknown samples

Table S2. Errors of the predicted RTP intensities of out-of-sample unknown samples.

	Actual intensity / a.u.	Estimated intensity / a.u.	Error / a.u.
Sample 1 (Class: BF)	705.165	691.325	−13.840
Sample 2 (Class: BS)	148.321	136.634	−.11.687

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17. Preparation conditions of boronate assemblies

Table S3. Preparation conditions of boronate assemblies.

Sample	Solvent	**PE**	Addition of **BDBA** solution	Note
Sample 1	$MeOH/H_2O$ = 9/1 (V/V)	Commercial	20 mM in 50 mL Dropwise	Stirred 4 h
Sample 2	$MeOH/H_2O$ = 9/1 (V/V)	Commercial	20 mM in 50 mL Rapidly	Stand for overnight
Sample 3	$MeOH/H_2O/THF$=85/10/5 (V/V/V)	Commercial	20 mM in 50 mL Rapidly	Stand for overnight
Sample 4	THF	Ground	20 mM in 50 mL Rapidly	Stand for overnight
Sample 5	THF	Ground	20 mM in 50 mL Rapidly	Stand for overnight
Sample 6	DMSO	Ground	20 mM in 50 mL Rapidly	Stand for overnight
Sample 7	1,4-dioxane	Ground	20 mM in 50 mL Rapidly	Stand for overnight
Sample 8	Acetonitrile	Ground	20 mM in 50 mL Rapidly	Stand for overnight
Sample 9	Ethyl acetate	Ground	20 mM in 50 mL Rapidly	Stand for overnight
Sample 10	Acetone	Ground	20 mM in 50 mL Rapidly	Stand for overnight
Sample 11	MeOH	Comercial	20 mM in 50 mL Dropwise	Stirred 2 days
Sample 12	MeOH	Comercial	20 mM in 50 mL Rapidly	Stirred overnight
Sample 13	$MeOH/H_2O$ = 99/1 (V/V)	Comercial	100 mM in 10 mL Rapidly	Stand for overnight
Sample 14	$MeOH/H_2O$ = 99/1 (V/V)	Comercial	20 mM in 50 mL Rapidly	Stand for overnight
Sample 15	$MeOH/H_2O$ = 99/1 (V/V)	Comercial	20 mM in 50 mL Rapidly	Stand for overnight and calcined at 300°C under nitrogen
Sample 16	$MeOH/H_2O$ = 9/1 (V/V)	Comercial	20 mM in 50 mL Dropwise	Stirred 4 h
Sample 17	$MeOH/H_2O$ = 9/1 (V/V)	Comercial	20 mM in 50 mL Dropwise	Stirred 4 h
Sample 18	$MeOH/H_2O$ = 9/1 (V/V)	Comercial	20 mM in 50 mL Dropwise	Stirred 4 h
Out-of-sample data				
Sample 19	$MeOH/H_2O$ = 9/1 (V/V)	Comercial	20 mM in 50 mL Dropwise	Stirred 4 h
Sample 20	MeOH	Comercial	20 mM in 50 mL Rapidly	Stand for overnight

18. Entire dataset for chemometrics analyses before auto-scaling

Table S4. Input dataset for chemometrics analyses before auto-scaling (lattice spacing *d*).

	Lattice spacings *d*																						
Peak no.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**
Sample 1	5.672	5.302	5.145	5.005	4.537	4.236	3.865	3.555	3.483	3.235	3.008	2.963	2.807	2.656	2.580	2.401	2.165	2.137	2.075	1.995	1.933	1.873	1.816
Sample 2	5.664	5.301	5.144	5.017	4.520	4.234	3.865	3.558	3.486	3.217	3.011	2.966	2.804	2.648	2.573	2.400	2.163	2.132	2.074	1.998	1.935	1.874	1.818
Sample 3	5.667	5.299	5.142	5.013	4.475	4.234	3.873	3.557	3.486	3.214	3.012	2.965	2.804	2.645	2.569	2.401	2.156	2.116	2.069	1.994	1.932	1.875	1.818
Sample 4	5.654	5.268	5.166	5.008	4.442	4.230	3.870	3.556	3.486	3.208	3.008	2.926	2.728	2.580	2.392	2.315	2.156	2.072	2.058	1.929	1.928	1.875	1.814
Sample 5	5.630	5.252	5.151	5.008	4.435	4.221	3.870	3.546	3.486	3.195	3.006	2.795	2.628	2.556	2.397	2.156	2.156	2.079	1.987	1.925	1.927	1.875	1.814
Sample 6	5.589	5.284	5.140	5.007	4.492	4.263	3.868	3.561	3.487	3.189	3.012	2.962	2.784	2.644	2.598	2.398	2.160	2.127	2.088	1.987	1.927	1.875	1.815
Sample 7	5.660	5.271	5.187	5.007	4.449	4.231	3.869	3.554	3.486	3.194	3.014	2.956	2.757	2.616	2.580	2.390	2.157	2.103	2.079	1.972	1.927	1.874	1.814
Sample 8	5.674	5.269	5.146	5.003	4.548	4.241	3.866	3.566	3.488	3.211	3.011	2.971	2.818	2.655	2.599	2.407	2.164	2.149	2.083	1.993	1.932	1.872	1.817
Sample 9	5.646	5.277	5.164	5.008	4.374	4.219	3.869	3.544	3.486	3.206	3.000	2.914	2.796	2.618	2.579	2.397	2.156	2.102	2.076	1.993	1.927	1.874	1.814
Sample 10	5.673	5.273	5.198	5.004	4.551	4.240	3.867	3.550	3.486	3.204	3.007	2.959	2.786	2.639	2.587	2.399	2.160	2.148	2.079	1.978	1.932	1.873	1.816
Sample 11	5.665	5.293	5.131	5.011	4.446	4.215	3.870	3.539	3.486	3.219	2.993	2.935	2.804	2.644	2.558	2.398	2.154	2.109	2.069	1.991	1.924	1.875	1.811
Sample 12	5.658	5.291	5.130	5.005	4.514	4.253	3.867	3.570	3.487	3.200	3.027	2.963	2.791	2.652	2.581	2.400	2.165	2.132	2.085	1.994	1.941	1.881	1.814
Sample 13	5.475	5.275	5.129	5.008	4.456	4.230	3.870	3.555	3.487	3.207	3.010	2.967	2.795	2.641	2.563	2.394	2.157	2.107	2.083	1.985	1.929	1.875	1.814
Sample 14	5.482	5.278	5.128	5.006	4.449	4.231	3.870	3.556	3.487	3.207	3.074	3.009	2.788	2.635	2.570	2.387	2.157	2.107	2.072	1.986	1.928	1.875	1.814
Sample 15	5.675	5.283	5.132	5.008	4.455	4.222	3.869	3.546	3.487	3.197	2.996	2.938	2.798	2.641	2.565	2.406	2.157	2.112	2.083	1.987	1.929	1.874	1.814
Sample 16	5.665	5.301	5.143	4.998	4.518	4.234	3.866	3.558	3.486	3.210	3.013	2.972	2.806	2.645	2.571	2.399	2.161	2.137	2.073	1.996	1.936	1.875	1.816
Sample 17	5.670	5.307	5.146	5.003	4.524	4.243	3.866	3.564	3.487	3.217	3.017	2.969	2.809	2.646	2.571	2.403	2.163	2.141	2.081	1.996	1.936	1.879	1.820
Sample 18	5.688	5.310	5.145	4.994	4.549	4.241	3.863	3.560	3.486	3.208	3.013	2.969	2.859	2.706	2.610	2.405	2.165	2.138	2.081	1.995	1.934	1.867	1.817

Table S5. Input dataset for chemometrics analyses before auto-scaling (Relative height).

	Relative height																						
Peak no.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**
Sample 1	5.051	40.425	19.541	2.748	6.848	100.000	2.242	61.253	5.825	2.281	2.281	3.982	1.200	1.434	3.506	2.831	2.014	0.542	3.371	0.841	2.336	0.517	0.589
Sample 2	4.744	70.507	30.751	2.063	0.000	100.000	1.130	44.806	0.000	2.967	15.867	0.000	1.702	2.238	2.838	2.482	1.755	0.000	3.691	1.282	2.465	0.549	0.707
Sample 3	4.398	68.067	29.945	2.052	0.000	100.000	1.160	43.986	0.000	3.080	14.817	0.000	1.494	2.082	2.604	2.297	1.103	0.000	2.611	1.077	2.002	0.485	0.589
Sample 4	8.419	70.035	46.267	0.000	0.000	100.000	0.000	38.264	0.000	2.453	12.468	0.000	0.000	2.807	1.572	0.000	0.000	2.623	0.000	1.724	0.000	0.000	0.000
Sample 5	7.814	53.349	39.921	0.000	0.000	100.000	0.000	40.293	0.000	3.238	13.126	1.373	3.140	3.470	2.031	1.398	0.000	3.934	0.785	2.442	0.000	0.000	0.000
Sample 6	24.424	141.822	0.000	0.000	0.000	100.000	0.000	45.177	0.000	4.979	15.420	0.000	0.000	0.000	5.995	2.634	0.000	0.000	5.433	0.000	3.056	0.000	0.000
Sample 7	11.299	74.695	61.921	0.000	0.000	100.000	0.000	40.990	0.000	3.292	13.353	0.000	0.000	0.000	4.272	1.996	0.000	0.000	3.970	0.000	1.993	0.000	0.000
Sample 8	0.000	58.488	46.098	0.000	26.604	100.000	0.000	48.480	0.000	2.303	15.843	0.000	0.000	0.000	4.031	1.817	0.000	2.410	4.070	1.275	2.843	0.000	0.000
Sample 9	6.759	44.556	39.719	0.000	10.797	100.000	0.000	39.582	0.000	2.959	13.878	0.000	1.035	0.000	3.150	2.010	1.366	0.000	3.577	0.938	2.199	0.000	0.000
Sample 10	7.759	58.283	55.600	0.000	7.690	100.000	0.000	46.501	0.000	3.365	14.404	0.000	0.000	0.000	4.125	2.286	0.000	1.374	3.534	0.000	2.265	0.000	0.000
Sample 11	5.705	58.985	20.928	0.000	0.000	100.000	0.000	45.850	0.000	4.832	18.168	0.000	3.193	2.080	4.126	2.383	1.350	0.000	3.486	1.014	2.193	0.000	0.376
Sample 12	7.183	84.991	40.900	0.000	0.000	100.000	0.000	54.129	0.000	5.054	21.862	0.000	1.760	0.000	4.052	3.117	1.591	0.000	4.960	1.643	3.272	0.658	0.891
Sample 13	10.254	75.081	36.728	0.000	0.000	100.000	0.000	46.801	0.000	5.088	17.092	0.000	3.151	2.895	4.208	2.149	1.274	0.000	3.337	0.000	2.005	0.000	0.000
Sample 14	9.935	82.136	37.808	0.000	0.000	100.000	0.000	45.852	0.000	4.781	2.581	14.063	2.211	0.000	4.099	2.219	0.000	0.000	3.165	0.000	2.669	0.000	0.000
Sample 15	5.257	78.069	38.904	0.000	0.000	100.000	0.000	47.082	0.000	6.287	17.183	0.000	2.968	4.082	4.303	2.931	0.000	0.000	3.727	0.000	2.359	0.000	0.000
Sample 16	4.855	66.453	29.270	1.955	0.000	100.000	1.137	43.161	0.000	3.056	14.553	0.000	1.739	2.151	2.704	2.386	1.013	0.000	3.500	1.126	2.222	0.555	0.740
Sample 17	5.081	74.917	32.679	0.000	0.000	100.000	1.015	44.890	0.000	3.129	14.974	0.000	1.498	2.225	2.603	2.348	0.000	0.914	2.501	0.890	1.767	0.437	0.527
Sample 18	7.365	62.290	30.237	8.174	56.540	100.000	1.258	57.893	3.883	4.351	20.425	8.816	2.132	1.498	2.458	3.187	0.000	0.000	2.560	1.544	2.701	0.717	0.000

Table S6. Input dataset for chemometrics analyses before auto-scaling (Crystallite size).

	Crystallite size																						
Peak no.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**
Sample 1	468.0	323.7	318.7	304.4	588.0	348.1	316.5	411.3	579.1	141.4	354.3	343.8	228.2	373.0	194.4	319.5	458.5	523.9	220.4	321.3	217.5	168.4	552.5
Sample 2	254.7	293.5	288.8	93.0	511.5	261.1	179.5	250.5	446.4	115.3	209.7	282.1	159.7	159.4	126.9	214.7	515.7	130.7	113.0	153.3	104.0	127.6	144.2
Sample 3	252.6	289.8	284.1	95.6	502.7	267.8	180.2	253.6	444.5	115.5	199.7	259.5	150.3	169.7	117.2	210.8	206.4	92.8	77.8	143.7	111.3	229.4	156.0
Sample 4	124.6	260.7	73.9	136.6	441.5	144.5	195.6	103.8	442.2	124.8	88.0	194.4	134.4	58.0	96.9	98.0	144.2	42.7	88.8	91.8	83.2	302.7	368.6
Sample 5	118.9	221.9	74.5	136.7	402.8	142.2	194.4	99.4	440.7	93.6	83.4	145.6	93.3	95.4	88.9	98.9	133.3	59.7	104.1	78.3	83.0	299.9	379.5
Sample 6	57.3	100.2	113.5	136.8	355.0	62.8	194.4	58.2	440.8	111.2	56.8	145.3	91.0	76.1	50.3	77.0	117.2	89.9	40.5	98.5	41.7	312.2	410.9
Sample 7	129.8	223.3	71.2	136.9	379.6	100.3	194.4	78.3	440.7	116.1	75.2	158.5	127.6	73.9	53.5	81.9	118.7	60.9	43.8	95.4	51.9	312.0	393.0
Sample 8	129.5	167.0	62.3	129.7	501.6	107.4	195.3	95.6	441.8	113.1	83.1	175.8	131.1	111.5	61.0	100.7	204.3	46.5	67.8	70.4	75.6	271.4	336.7
Sample 9	122.4	216.1	76.8	144.9	204.0	156.6	197.2	119.4	440.8	136.6	101.9	163.4	165.3	106.3	57.4	127.1	88.7	89.9	66.5	122.8	87.0	315.7	416.0
Sample 10	111.4	217.6	68.9	131.8	529.5	122.7	194.9	96.7	444.9	112.9	86.5	178.7	133.8	113.7	54.1	75.6	214.6	76.9	76.1	100.4	95.4	233.7	306.2
Sample 11	227.8	200.0	250.0	137.7	421.5	214.4	193.4	177.3	448.3	108.6	127.0	170.4	68.6	143.6	71.5	180.6	128.1	94.0	61.7	138.6	83.6	271.0	555.0
Sample 12	253.6	264.5	159.1	121.5	491.8	180.6	192.0	196.9	444.9	98.2	151.9	197.9	104.6	144.0	54.0	214.3	234.9	68.7	104.8	143.0	124.8	213.8	126.4
Sample 13	68.2	204.2	120.0	136.8	376.1	152.7	194.4	123.4	440.7	83.3	91.6	154.9	92.3	107.8	75.3	106.4	89.8	71.2	62.8	105.7	101.4	302.0	388.3
Sample 14	67.6	208.7	125.6	136.8	355.3	154.0	194.4	125.8	440.8	69.1	104.9	109.8	119.8	82.7	45.2	94.6	118.8	89.0	46.8	105.6	75.6	312.2	410.6
Sample 15	130.7	157.7	122.0	136.8	385.2	132.6	194.4	114.4	440.7	104.4	91.8	152.3	57.4	57.0	73.7	71.4	117.7	68.0	58.3	102.0	64.6	312.2	396.7
Sample 16	283.7	320.3	306.1	138.1	513.1	289.3	206.1	260.4	447.1	120.6	197.8	290.6	177.7	181.3	121.4	228.0	250.2	140.4	136.0	164.2	108.7	164.5	188.5
Sample 17	271.9	313.7	318.8	133.2	504.7	266.3	171.2	262.7	450.0	132.0	206.2	300.1	167.7	183.8	122.2	223.9	305.6	62.4	106.4	162.0	110.5	201.3	208.3
Sample 18	417.7	307.6	228.9	335.0	484.7	279.8	221.1	343.8	419.0	129.3	284.5	464.3	517.8	356.9	136.0	220.5	346.2	248.1	178.8	224.2	189.7	312.8	401.6

19. Emission intensities of each boronate assembly (Response variables for PCR)

Table S7. Emission intensities of each boronate assembly (Response variables for PCR).

Sample	RTP intensity
1	778.549
2	645.454
3	345.5
4	66.1899
5	63.5087
6	69.2849
7	46.599
8	177.137
9	185.008
10	103.851
11	88.1631
12	524.421
13	209.637
14	226.36
15	67.1545
16	510.855
17	549.608
18	686.65

20. Score of PCA

Table S8. Scores of PCA.

	Principal components						
	1	2	3	4	5	6	7
Sample 1	12.18452	3.368828	3.59851	-2.77796	-3.83315	1.920927	-0.90575
Sample 2	4.257979	0.015525	-3.92248	-1.02096	-0.12823	-0.44193	0.359647
Sample 3	1.98378	0.799355	-2.77373	-1.71222	0.562065	-0.9176	1.333937
Sample 4	-4.72272	6.095075	-0.60158	2.049507	-0.87697	0.574159	0.639347
Sample 5	-6.33831	8.564614	-0.09264	0.878756	1.958432	1.949653	-2.13866
Sample 6	-4.0866	-5.82786	1.694921	0.261462	-0.96085	1.899626	-3.60517
Sample 7	-4.41213	-0.87214	1.014107	1.316993	-2.33629	-0.91346	0.730651
Sample 8	-1.09084	-2.24622	-0.51289	4.029987	-1.612	-0.55603	0.458691
Sample 9	-3.17446	0.678557	1.595929	-0.8451	-1.19592	-3.08519	1.012321
Sample 10	-1.65654	-1.34245	0.031287	2.930034	-2.88854	-0.88545	0.326216
Sample 11	-1.60369	0.471105	1.132638	-4.40172	0.775464	-2.77766	-0.75223
Sample 12	1.725863	-3.70298	-3.75516	-0.1046	1.17251	1.865837	-1.86207
Sample 13	-3.28561	-1.52004	1.056849	-2.27084	1.521342	0.300322	0.391752
Sample 14	-3.69195	-2.61862	2.564476	-1.51336	1.271322	4.132063	4.107137
Sample 15	-3.55244	-1.56039	1.074276	-1.80785	1.505371	-2.03311	-1.06743
Sample 16	4.221012	0.190021	-2.722	-0.24114	0.513262	-0.12233	0.327008
Sample 17	3.751314	-0.17404	-3.75857	0.813913	0.222588	0.395956	0.655898
Sample 18	9.490813	-0.31833	4.376058	4.4151	4.329607	-1.30578	-0.0113

21. Loadings of PCA

Table S9. Loadings of PCA.

	Principal components						
	1	**2**	**3**	**4**	**5**	**6**	**7**
d of peak 1	0.079215	0.070519	-0.10165	0.131398	-0.10419	-0.2841	-0.17784
d of peak 2	0.162613	-0.08012	-0.06159	-0.09086	0.094534	-0.0742	0.017014
d of peak 3	-0.03581	0.064839	0.015419	0.217189	-0.29511	-0.14445	0.067399
d of peak 4	-0.06984	0.04242	-0.11078	-0.24393	-0.10768	-0.04462	0.007197
d of peak 5	0.131035	-0.08369	-0.07235	0.17973	-0.05419	0.088416	-0.08769
d of peak 6	0.053496	-0.17198	-0.06582	0.172985	-0.06447	0.237833	-0.20495
d of peak 7	-0.13647	0.046583	-0.00298	-0.1888	0.013111	-0.03975	0.084173
d of peak 8	0.07049	-0.11736	-0.15348	0.191809	0.018922	0.250161	0.000661
d of peak 9	-0.12863	-0.15034	-0.10896	0.100398	0.157284	0.032487	0.023468
d of peak 10	0.138561	0.077776	-0.01493	-0.13609	-0.11852	-0.04078	0.186398
d of peak 11	-0.00501	-0.09077	0.009588	0.016386	0.082023	0.391561	0.336488
d of peak 12	0.077051	-0.2153	-0.00607	-0.01468	-0.06268	0.047192	0.268825
d of peak 13	0.11652	-0.19074	0.035555	-0.01641	0.018116	-0.17912	0.148554
d of peak 14	0.134894	-0.18943	0.057749	0.022904	0.09196	-0.09785	0.031883
d of peak 15	0.08391	-0.24402	0.046782	-0.01885	-0.05474	-0.12056	0.062469
d of peak 16	0.079179	-0.22646	0.004926	-0.0574	-0.09648	-0.16597	0.151463
d of peak 17	0.144381	-0.07975	-0.05187	0.182653	-0.0358	0.113021	-0.11634
d of peak 18	0.125058	-0.1696	-0.06426	0.100661	-0.08768	-0.02905	-0.03582
d of peak 19	0.057134	-0.24217	0.014721	-0.00839	-0.10537	-0.12216	0.100581
d of peak 20	0.108165	-0.20984	-0.01928	-0.10855	-0.00489	-0.13049	0.087909
d of peak 21	0.129306	-0.05356	-0.22082	0.10388	0.045541	0.090648	-0.01548
d of peak 22	-0.04942	-0.03587	-0.2527	-0.15681	-0.03761	0.170162	-0.07649
d of peak 23	0.115193	-0.0201	-0.14903	0.157472	-0.02598	0.030396	0.125391
relative height of peak 1	-0.0718	-0.10111	0.124981	-0.00471	-0.01673	0.189925	-0.2335
relative height of peak 2	-0.05939	-0.18343	-0.03269	0.004598	0.06537	0.195379	-0.20899
relative height of peak 3	-0.06652	0.053832	-0.05547	0.179867	-0.07866	-0.09511	0.269121
relative height of peak 4	0.144831	0.022434	0.120601	0.116347	0.200034	-0.07096	0.016642
relative height of peak 5	0.085002	-0.02121	0.178669	0.260508	0.149838	-0.13874	0.029024
relative height of peak 7	0.178429	0.062156	-0.01325	-0.05024	-0.04052	0.033973	0.030348
relative height of peak 8	0.146781	-0.07359	0.133741	7.51E-05	0.03218	0.098001	-0.12361
relative height of peak 9	0.15008	0.060237	0.218946	0.00636	-0.05239	0.065426	-0.07316
relative height of peak 10	-0.05307	-0.15564	0.091442	-0.14012	0.279688	0.010673	-0.14691
relative height of peak 11	-0.01399	-0.08155	-0.13886	0.102212	0.235043	-0.2833	-0.2556
relative height of peak 12	0.041768	-0.01986	0.214915	0.021564	0.173131	0.255228	0.294766
relative height of peak 13	0.007097	0.054288	0.023966	-0.23339	0.366414	-0.01218	-0.02182
relative height of peak 14	0.000281	0.164866	-0.06239	-0.12521	0.221355	-0.07878	-0.09607
relative height of peak 15	-0.05066	-0.2351	0.11559	-0.08953	-0.12834	0.045977	-0.1717
relative height of peak 16	0.105784	-0.17938	0.045227	-0.09449	0.111884	-0.03744	-0.13823
relative height of peak 17	0.089293	0.011171	-0.07721	-0.27311	-0.07163	-0.05968	-0.04296
relative height of peak 18	-0.06123	0.197333	-0.03643	0.196885	-0.05608	0.117181	-0.09533

relative height of peak 19	0.019525	-0.25872	0.004004	-0.07477	-0.11056	-0.03307	-0.15104
relative height of peak 20	0.041801	0.191375	-0.1265	0.10294	0.154563	0.01526	-0.12968
relative height of peak 21	0.06896	-0.26379	0.035588	-0.03422	-0.0129	-0.02126	-0.01305
relative height of peak 22	0.167691	-0.00912	-0.13309	0.018197	0.131709	0.042098	-0.03004
relative height of peak 23	0.117098	-0.00967	-0.25693	-0.15551	-0.00839	0.052477	-0.05649
Crystallite size of peak 1	0.184549	0.058561	-0.0012	-0.02053	0.036106	-0.04339	-0.05139
Crystallite size of peak 2	0.145535	0.1204	-0.12631	0.007723	0.0391	0.018433	0.17302
Crystallite size of peak 3	0.154666	0.01302	-0.11455	-0.1642	0.067532	-0.01228	0.024071
Crystallite size of peak 4	0.127864	0.045965	0.270249	0.078831	0.047595	0.019283	-0.0684
Crystallite size of peak 5	0.133664	0.032644	-0.13647	0.078201	-0.078	0.091015	-0.04741
Crystallite size of peak 6	0.170938	0.082353	-0.05916	-0.11503	0.067019	-0.02093	0.093848
Crystallite size of peak 7	0.115732	0.070529	0.217112	-0.06675	-0.18274	0.110437	-0.0984
Crystallite size of peak 8	0.186889	0.050442	-0.01014	-0.0696	0.05966	0.009394	0.033092
Crystallite size of peak 9	0.105322	0.074044	0.086893	-0.161	-0.28775	0.142969	-0.0806
Crystallite size of peak 10	0.10685	0.070717	-0.00234	0.093629	-0.2044	-0.24507	-0.0932
Crystallite size of peak 11	0.188473	0.053306	0.011666	-0.0521	0.026944	0.0232	0.028484
Crystallite size of peak 12	0.176987	0.042951	0.003626	0.098847	0.100948	-0.07093	-0.00376
Crystallite size of peak 13	0.135805	0.023357	0.135708	0.194575	0.15112	-0.06426	0.078257
Crystallite size of peak 14	0.184017	0.039845	0.093752	0.010047	0.036435	0.001608	-0.03077
Crystallite size of peak 15	0.161572	0.135717	-0.00697	-0.04663	-0.00874	0.01887	-0.02225
Crystallite size of peak 16	0.176449	0.045173	-0.08058	-0.10929	0.016172	0.018448	-0.01799
Crystallite size of peak 17	0.167053	0.029832	-0.08956	0.030154	-0.05898	0.047048	-0.01554
Crystallite size of peak 18	0.154691	0.054594	0.173956	-0.08444	-0.12046	0.083814	-0.06674
Crystallite size of peak 19	0.170631	0.114629	0.03808	0.036209	0.013324	0.069271	-0.08656
Crystallite size of peak 20	0.17965	0.038076	0.086172	-0.09556	-0.03832	0.031528	-0.03536
Crystallite size of peak 21	0.174668	0.070243	0.07468	-0.00224	0.036116	0.04391	-0.00129
Crystallite size of peak 22	-0.12767	-0.01413	0.240681	0.079987	0.133723	-0.04619	0.007856
Crystallite size of peak 23	-0.02751	0.050836	0.348036	-0.09176	-0.08253	-0.03713	-0.06509

22. Contribution ratios of each principal component

Table S10. Contribution ratios of each principal component.

	Principal components						
	1	**2**	**3**	**4**	**5**	**6**	**7**
contribution ratio	0.387323	0.164557	0.093451	0.081593	0.056761	0.050419	0.039201
cumulative contribution ratio	0.387323	0.55188	0.645331	0.726924	0.783685	0.834103	0.873304

23. Standardized correlation coefficients of PCR

Table S11. Standardized correlation coefficients of PCR.

	Principal components						
	1	**2**	**3**	**4**	**5**	**6**	**7**
Standardized correlation coefficient	45.78293	-0.70222	-16.7413	-3.26284	14.6271	21.21973	8.785027

24. Contributions of each parameter (Inner product of the PCA loading vector and the standardized correlation coefficients of PCR)

Table S12. Contributions of each parameter (Inner product of the PCA loading vector and the standardized correlation coefficients of PCR).

Parameter	Coefficient
d of peak 1	-4.26461
d of peak 2	8.78648
d of peak 3	-9.44143
d of peak 4	-3.03533
d of peak 5	6.995886
d of peak 6	5.410771
d of peak 7	-5.52699
d of peak 8	10.84421
d of peak 9	-1.09097
d of peak 10	6.021619
d of peak 11	12.08511
d of peak 12	6.274529
d of peak 13	2.696136
d of peak 14	4.816274
d of peak 15	0.481053
d of peak 16	0.286449
d of peak 17	7.791154
d of peak 18	4.378386
d of peak 19	-0.68325
d of peak 20	3.708173
d of peak 21	11.76923
d of peak 22	4.893609
d of peak 23	8.635727
relative height of peak 1	-3.55917
relative height of peak 2	1.207961
relative height of peak 3	-3.54614
relative height of peak 4	5.782739
relative height of peak 5	-0.43199
relative height of peak 7	8.906027
relative height of peak 8	5.996817
relative height of peak 9	3.121944
relative height of peak 10	-0.36707
relative height of peak 11	-3.41091
relative height of peak 12	8.795701
relative height of peak 13	5.556609
relative height of peak 14	2.072307
relative height of peak 15	-6.20723
relative height of peak 16	4.14794
relative height of peak 17	3.57248

relative height of peak 18	-2.14566
relative height of peak 19	-2.39331
relative height of peak 20	5.006638
relative height of peak 21	2.103865
relative height of peak 22	12.40841
relative height of peak 23	10.6712
Crystallite size of peak 1	7.651115
Crystallite size of peak 2	11.15097
Crystallite size of peak 3	10.46412
Crystallite size of peak 4	1.544663
Crystallite size of peak 5	8.500027
Crystallite size of peak 6	10.49451
Crystallite size of peak 7	0.63808
Crystallite size of peak 8	10.2805
Crystallite size of peak 9	1.95732
Crystallite size of peak 10	-4.43308
Crystallite size of peak 11	9.702755
Crystallite size of peak 12	7.627998
Crystallite size of peak 13	4.828744
Crystallite size of peak 14	7.091348
Crystallite size of peak 15	7.647912
Crystallite size of peak 16	10.22218
Crystallite size of peak 17	9.027336
Crystallite size of peak 18	3.837264
Crystallite size of peak 19	7.880221
Crystallite size of peak 20	6.865245
Crystallite size of peak 21	8.153282
Crystallite size of peak 22	-9.08058
Crystallite size of peak 23	-9.38925

25. Cartesian coordinates of the dimer models

Table S13 *d* of peak 2 = 5.25 Å.

	x	y	z
O	2.1687	0.2578	9.6421
B	2.7459	1.4574	9.3528
C	1.9625	2.4337	8.4111
C	0.6761	2.0861	7.9842
H	0.261	1.1252	8.2988
C	-0.083	2.935	7.1903
H	-1.0924	2.6454	6.8869
C	0.4409	4.1557	6.789
H	-0.1541	4.837	6.1754
C	1.7254	4.5216	7.187
H	2.1359	5.4864	6.8769
C	2.4761	3.6745	8.0031
H	3.4781	3.972	8.325

O	3.9381	1.8655	9.8803
C	4.6641	1.0016	10.7716
H	5.4342	0.4646	10.1898
H	5.1835	1.6444	11.5002
C	3.7562	-0.0002	11.4858
C	2.8878	0.6998	12.5334
H	2.137	1.3602	12.0789
O	2.1686	-0.2582	13.3317
B	2.7458	-1.4578	13.6211
O	3.9381	-1.8659	13.0936
C	1.9624	-2.4341	14.5627
C	0.676	-2.0866	14.9895
H	0.2563	-1.1337	14.6625
C	-0.0831	-2.9355	15.7833
C	0.4408	-4.1562	16.1846
H	-0.149	-4.8296	16.8129
C	1.7253	-4.522	15.7867
H	2.1408	-5.4831	16.1027
H	-1.0924	-2.643	16.087
C	2.476	-3.6749	14.9706
H	3.4766	-3.9743	14.647
H	3.5179	1.3182	13.1963
C	4.6641	-1.0019	12.2023
H	5.1858	-1.6447	11.4749
H	5.4332	-0.4614	12.7828
C	2.8879	-0.7002	10.4404
H	3.5167	-1.3197	9.7773
H	2.1411	-1.3555	10.9096
O	-0.9514	5.5741	9.6272
B	-0.3742	6.7738	9.3379
C	-1.1576	7.7501	8.3962
C	-2.444	7.4025	7.9693
H	-2.8567	6.4395	8.2814
C	-3.2031	8.2513	7.1754
H	-4.2099	7.9573	6.8655
C	-2.6793	9.472	6.7741
H	-3.2687	10.145	6.1449
C	-1.3947	9.838	7.1721
H	-0.9791	10.7989	6.8555
C	-0.6441	8.9907	7.9883
H	0.3564	9.2893	8.3131
O	0.818	7.1819	9.8655
C	1.544	6.318	10.7567
H	2.307	5.7744	10.1722
H	2.066	6.9605	11.4841
C	0.6361	5.3161	11.4709
C	-0.2323	6.0162	12.5185

H	-0.9784	6.6723	12.0491
O	-0.9515	5.0581	13.3168
B	-0.3743	3.8584	13.6062
O	0.818	3.4504	13.0787
C	-1.1577	2.8821	14.5478
C	-2.4441	3.2297	14.9747
H	-2.8584	4.1924	14.6638
C	-3.2032	2.3808	15.7684
C	-2.6794	1.1602	16.1698
H	-3.2675	0.4887	16.8019
C	-1.3948	0.7942	15.7719
H	-0.9739	-0.1576	16.1021
H	-4.2098	2.6754	16.0784
C	-0.6442	1.6415	14.9557
H	0.3528	1.3329	14.6292
H	0.3973	6.6356	13.1814
C	1.544	4.3143	12.1874
H	2.0671	3.6747	11.4583
H	2.3122	4.8541	12.7699
C	-0.2322	4.6161	10.4255
H	0.394	4.0017	9.7638
H	-0.9794	3.9612	10.8952

Table S14 *d* of peak 2 = 5.27 Å.

	x	y	z
O	2.1687	0.2578	9.6421
B	2.7459	1.4574	9.3528
C	1.9625	2.4337	8.4111
C	0.6761	2.0861	7.9842
H	0.261	1.1252	8.2988
C	-0.083	2.935	7.1903
H	-1.0924	2.6454	6.8869
C	0.4409	4.1557	6.789
H	-0.1541	4.837	6.1754
C	1.7254	4.5216	7.187
H	2.1359	5.4864	6.8769
C	2.4761	3.6745	8.0031
H	3.4781	3.972	8.325
O	3.9381	1.8655	9.8803
C	4.6641	1.0016	10.7716
H	5.4342	0.4646	10.1898
H	5.1835	1.6444	11.5002
C	3.7562	-0.0002	11.4858
C	2.8878	0.6998	12.5334
H	2.137	1.3602	12.0789
O	2.1686	-0.2582	13.3317
B	2.7458	-1.4578	13.6211

O	3.9381	-1.8659	13.0936
C	1.9624	-2.4341	14.5627
C	0.676	-2.0866	14.9895
H	0.2563	-1.1337	14.6625
C	-0.0831	-2.9355	15.7833
C	0.4408	-4.1562	16.1846
H	-0.149	-4.8296	16.8129
C	1.7253	-4.522	15.7867
H	2.1408	-5.4831	16.1027
H	-1.0924	-2.643	16.087
C	2.476	-3.6749	14.9706
H	3.4766	-3.9743	14.647
H	3.5179	1.3182	13.1963
C	4.6641	-1.0019	12.2023
H	5.1858	-1.6447	11.4749
H	5.4332	-0.4614	12.7828
C	2.8879	-0.7002	10.4404
H	3.5167	-1.3197	9.7773
H	2.1411	-1.3555	10.9096
O	-0.9514	5.5938	9.6303
B	-0.3742	6.7935	9.341
C	-1.1576	7.7698	8.3993
C	-2.444	7.4222	7.9724
H	-2.8567	6.4592	8.2845
C	-3.2031	8.271	7.1785
H	-4.2099	7.977	6.8686
C	-2.6793	9.4917	6.7772
H	-3.2687	10.1647	6.148
C	-1.3947	9.8577	7.1752
H	-0.9791	10.8186	6.8586
C	-0.6441	9.0104	7.9914
H	0.3564	9.309	8.3162
O	0.818	7.2016	9.8686
C	1.544	6.3377	10.7598
H	2.307	5.7941	10.1753
H	2.066	6.9802	11.4872
C	0.6361	5.3358	11.474
C	-0.2323	6.0359	12.5216
H	-0.9784	6.692	12.0522
O	-0.9515	5.0778	13.3199
B	-0.3743	3.8781	13.6093
O	0.818	3.4701	13.0818
C	-1.1577	2.9018	14.5509
C	-2.4441	3.2494	14.9778
H	-2.8584	4.2121	14.6669
C	-3.2032	2.4005	15.7715
C	-2.6794	1.1799	16.1729

H	-3.2675	0.5084	16.805
C	-1.3948	0.8139	15.775
H	-0.9739	-0.1379	16.1052
H	-4.2098	2.6951	16.0815
C	-0.6442	1.6612	14.9588
H	0.3528	1.3526	14.6323
H	0.3973	6.6553	13.1845
C	1.544	4.334	12.1905
H	2.0671	3.6944	11.4614
H	2.3122	4.8738	12.773
C	-0.2322	4.6358	10.4286
H	0.394	4.0214	9.7669
H	-0.9794	3.9809	10.8983

Table S15 *d* of peak 2 = 5.29 Å.

	x	y	z
O	2.1687	0.2578	9.6421
B	2.7459	1.4574	9.3528
C	1.9625	2.4337	8.4111
C	0.6761	2.0861	7.9842
H	0.261	1.1252	8.2988
C	-0.083	2.935	7.1903
H	-1.0924	2.6454	6.8869
C	0.4409	4.1557	6.789
H	-0.1541	4.837	6.1754
C	1.7254	4.5216	7.187
H	2.1359	5.4864	6.8769
C	2.4761	3.6745	8.0031
H	3.4781	3.972	8.325
O	3.9381	1.8655	9.8803
C	4.6641	1.0016	10.7716
H	5.4342	0.4646	10.1898
H	5.1835	1.6444	11.5002
C	3.7562	-0.0002	11.4858
C	2.8878	0.6998	12.5334
H	2.137	1.3602	12.0789
O	2.1686	-0.2582	13.3317
B	2.7458	-1.4578	13.6211
O	3.9381	-1.8659	13.0936
C	1.9624	-2.4341	14.5627
C	0.676	-2.0866	14.9895
H	0.2563	-1.1337	14.6625
C	-0.0831	-2.9355	15.7833
C	0.4408	-4.1562	16.1846
H	-0.149	-4.8296	16.8129
C	1.7253	-4.522	15.7867
H	2.1408	-5.4831	16.1027

H	-1.0924	-2.643	16.087
C	2.476	-3.6749	14.9706
H	3.4766	-3.9743	14.647
H	3.5179	1.3182	13.1963
C	4.6641	-1.0019	12.2023
H	5.1858	-1.6447	11.4749
H	5.4332	-0.4614	12.7828
C	2.8879	-0.7002	10.4404
H	3.5167	-1.3197	9.7773
H	2.1411	-1.3555	10.9096
O	-0.9514	5.6136	9.6334
B	-0.3742	6.8133	9.3441
C	-1.1576	7.7896	8.4024
C	-2.444	7.442	7.9755
H	-2.8567	6.479	8.2876
C	-3.2031	8.2908	7.1816
H	-4.2099	7.9968	6.8717
C	-2.6793	9.5115	6.7803
H	-3.2687	10.1845	6.1511
C	-1.3947	9.8775	7.1783
H	-0.9791	10.8384	6.8617
C	-0.6441	9.0302	7.9945
H	0.3564	9.3288	8.3193
O	0.818	7.2214	9.8717
C	1.544	6.3575	10.7629
H	2.307	5.8139	10.1784
H	2.066	7	11.4903
C	0.6361	5.3556	11.4771
C	-0.2323	6.0557	12.5247
H	-0.9784	6.7118	12.0553
O	-0.9515	5.0976	13.323
B	-0.3743	3.8979	13.6124
O	0.818	3.4899	13.0849
C	-1.1577	2.9216	14.554
C	-2.4441	3.2692	14.9809
H	-2.8584	4.2319	14.67
C	-3.2032	2.4203	15.7746
C	-2.6794	1.1997	16.176
H	-3.2675	0.5282	16.8081
C	-1.3948	0.8337	15.7781
H	-0.9739	-0.1181	16.1083
H	-4.2098	2.7149	16.0846
C	-0.6442	1.681	14.9619
H	0.3528	1.3724	14.6354
H	0.3973	6.6751	13.1876
C	1.544	4.3538	12.1936
H	2.0671	3.7142	11.4645

H	2.3122	4.8936	12.7761
C	-0.2322	4.6556	10.4317
H	0.394	4.0412	9.77
H	-0.9794	4.0007	10.9014

Table S16 *d* of peak 2 = 5.30 Å.

	x	y	z
O	2.1687	0.2578	9.6421
B	2.7459	1.4574	9.3528
C	1.9625	2.4337	8.4111
C	0.6761	2.0861	7.9842
H	0.261	1.1252	8.2988
C	-0.083	2.935	7.1903
H	-1.0924	2.6454	6.8869
C	0.4409	4.1557	6.789
H	-0.1541	4.837	6.1754
C	1.7254	4.5216	7.187
H	2.1359	5.4864	6.8769
C	2.4761	3.6745	8.0031
H	3.4781	3.972	8.325
O	3.9381	1.8655	9.8803
C	4.6641	1.0016	10.7716
H	5.4342	0.4646	10.1898
H	5.1835	1.6444	11.5002
C	3.7562	-0.0002	11.4858
C	2.8878	0.6998	12.5334
H	2.137	1.3602	12.0789
O	2.1686	-0.2582	13.3317
B	2.7458	-1.4578	13.6211
O	3.9381	-1.8659	13.0936
C	1.9624	-2.4341	14.5627
C	0.676	-2.0866	14.9895
H	0.2563	-1.1337	14.6625
C	-0.0831	-2.9355	15.7833
C	0.4408	-4.1562	16.1846
H	-0.149	-4.8296	16.8129
C	1.7253	-4.522	15.7867
H	2.1408	-5.4831	16.1027
H	-1.0924	-2.643	16.087
C	2.476	-3.6749	14.9706
H	3.4766	-3.9743	14.647
H	3.5179	1.3182	13.1963
C	4.6641	-1.0019	12.2023
H	5.1858	-1.6447	11.4749
H	5.4332	-0.4614	12.7828
C	2.8879	-0.7002	10.4404
H	3.5167	-1.3197	9.7773

H	2.1411	-1.3555	10.9096
O	-0.9514	5.6257	9.6353
B	-0.3742	6.8254	9.346
C	-1.1576	7.8017	8.4043
C	-2.444	7.4541	7.9774
H	-2.8567	6.4911	8.2895
C	-3.2031	8.3029	7.1835
H	-4.2099	8.0089	6.8736
C	-2.6793	9.5236	6.7822
H	-3.2687	10.1966	6.153
C	-1.3947	9.8896	7.1802
H	-0.9791	10.8505	6.8636
C	-0.6441	9.0423	7.9964
H	0.3564	9.3409	8.3212
O	0.818	7.2335	9.8736
C	1.544	6.3696	10.7648
H	2.307	5.826	10.1803
H	2.066	7.0121	11.4922
C	0.6361	5.3677	11.479
C	-0.2323	6.0678	12.5266
H	-0.9784	6.7239	12.0572
O	-0.9515	5.1097	13.3249
B	-0.3743	3.91	13.6143
O	0.818	3.502	13.0868
C	-1.1577	2.9337	14.5559
C	-2.4441	3.2813	14.9828
H	-2.8584	4.244	14.6719
C	-3.2032	2.4324	15.7765
C	-2.6794	1.2118	16.1779
H	-3.2675	0.5403	16.81
C	-1.3948	0.8458	15.78
H	-0.9739	-0.106	16.1102
H	-4.2098	2.727	16.0865
C	-0.6442	1.6931	14.9638
H	0.3528	1.3845	14.6373
H	0.3973	6.6872	13.1895
C	1.544	4.3659	12.1955
H	2.0671	3.7263	11.4664
H	2.3122	4.9057	12.778
C	-0.2322	4.6677	10.4336
H	0.394	4.0533	9.7719
H	-0.9794	4.0128	10.9033

Table S17 *d* of peak 2 = 5.32 Å.

	x	y	z
O	2.1687	0.2578	9.6421
B	2.7459	1.4574	9.3528

C	1.9625	2.4337	8.4111
C	0.6761	2.0861	7.9842
H	0.261	1.1252	8.2988
C	-0.083	2.935	7.1903
H	-1.0924	2.6454	6.8869
C	0.4409	4.1557	6.789
H	-0.1541	4.837	6.1754
C	1.7254	4.5216	7.187
H	2.1359	5.4864	6.8769
C	2.4761	3.6745	8.0031
H	3.4781	3.972	8.325
O	3.9381	1.8655	9.8803
C	4.6641	1.0016	10.7716
H	5.4342	0.4646	10.1898
H	5.1835	1.6444	11.5002
C	3.7562	-0.0002	11.4858
C	2.8878	0.6998	12.5334
H	2.137	1.3602	12.0789
O	2.1686	-0.2582	13.3317
B	2.7458	-1.4578	13.6211
O	3.9381	-1.8659	13.0936
C	1.9624	-2.4341	14.5627
C	0.676	-2.0866	14.9895
H	0.2563	-1.1337	14.6625
C	-0.0831	-2.9355	15.7833
C	0.4408	-4.1562	16.1846
H	-0.149	-4.8296	16.8129
C	1.7253	-4.522	15.7867
H	2.1408	-5.4831	16.1027
H	-1.0924	-2.643	16.087
C	2.476	-3.6749	14.9706
H	3.4766	-3.9743	14.647
H	3.5179	1.3182	13.1963
C	4.6641	-1.0019	12.2023
H	5.1858	-1.6447	11.4749
H	5.4332	-0.4614	12.7828
C	2.8879	-0.7002	10.4404
H	3.5167	-1.3197	9.7773
H	2.1411	-1.3555	10.9096
O	-0.9514	5.6432	9.6381
B	-0.3742	6.8429	9.3488
C	-1.1576	7.8192	8.4071
C	-2.444	7.4716	7.9802
H	-2.8567	6.5086	8.2923
C	-3.2031	8.3204	7.1863
H	-4.2099	8.0264	6.8764
C	-2.6793	9.5411	6.785

H	-3.2687	10.2141	6.1558
C	-1.3947	9.9071	7.183
H	-0.9791	10.868	6.8664
C	-0.6441	9.0598	7.9992
H	0.3564	9.3584	8.324
O	0.818	7.251	9.8764
C	1.544	6.3871	10.7676
H	2.307	5.8435	10.1831
H	2.066	7.0296	11.495
C	0.6361	5.3852	11.4818
C	-0.2323	6.0853	12.5294
H	-0.9784	6.7414	12.06
O	-0.9515	5.1272	13.3277
B	-0.3743	3.9275	13.6171
O	0.818	3.5195	13.0896
C	-1.1577	2.9512	14.5587
C	-2.4441	3.2988	14.9856
H	-2.8584	4.2615	14.6747
C	-3.2032	2.4499	15.7793
C	-2.6794	1.2293	16.1807
H	-3.2675	0.5578	16.8128
C	-1.3948	0.8633	15.7828
H	-0.9739	-0.0885	16.113
H	-4.2098	2.7445	16.0893
C	-0.6442	1.7106	14.9666
H	0.3528	1.402	14.6401
H	0.3973	6.7047	13.1923
C	1.544	4.3834	12.1983
H	2.0671	3.7438	11.4692
H	2.3122	4.9232	12.7808
C	-0.2322	4.6852	10.4364
H	0.394	4.0708	9.7747
H	-0.9794	4.0303	10.9061

Table S18 *d* of peak 2 = 5.34 Å.

	x	y	z
O	2.1687	0.2578	9.6421
B	2.7459	1.4574	9.3528
C	1.9625	2.4337	8.4111
C	2.4761	3.6745	8.0031
H	3.4781	3.972	8.325
C	1.7254	4.5216	7.187
H	2.1359	5.4864	6.8769
C	0.4409	4.1557	6.789
H	-0.1541	4.837	6.1754
C	-0.083	2.935	7.1903
H	-1.0924	2.6454	6.8869

C	0.6761	2.0861	7.9842
H	0.261	1.1252	8.2988
O	3.9381	1.8655	9.8803
C	4.6641	1.0016	10.7716
C	3.7562	-0.0002	11.4858
C	2.8878	0.6998	12.5334
H	2.137	1.3602	12.0789
H	3.5179	1.3182	13.1963
O	2.1686	-0.2582	13.3317
B	2.7458	-1.4578	13.6211
C	1.9624	-2.4341	14.5627
C	2.476	-3.6749	14.9706
H	3.4766	-3.9743	14.647
C	1.7253	-4.522	15.7867
H	2.1408	-5.4831	16.1027
C	0.4408	-4.1562	16.1846
H	-0.149	-4.8296	16.8129
C	-0.0831	-2.9355	15.7833
H	-1.0924	-2.643	16.087
C	0.676	-2.0866	14.9895
H	0.2563	-1.1337	14.6625
O	3.9381	-1.8659	13.0936
C	4.6641	-1.0019	12.2023
H	5.4332	-0.4614	12.7828
H	5.1858	-1.6447	11.4749
H	5.4342	0.4646	10.1898
H	5.1835	1.6444	11.5002
C	2.8879	-0.7002	10.4404
H	2.1411	-1.3555	10.9096
H	3.5167	-1.3197	9.7773
O	-0.9514	5.6618	9.641
B	-0.3742	6.8615	9.3517
C	-1.1576	7.8378	8.41
C	-0.6441	9.0784	8.0021
H	0.3564	9.377	8.3269
C	-1.3947	9.9257	7.1859
H	-0.9791	10.8866	6.8693
C	-2.6793	9.5597	6.7879
H	-3.2687	10.2327	6.1587
C	-3.2031	8.339	7.1892
H	-4.2099	8.045	6.8793
C	-2.444	7.4902	7.9831
H	-2.8567	6.5272	8.2952
O	0.818	7.2696	9.8793
C	1.544	6.4057	10.7705
C	0.6361	5.4038	11.4847
C	-0.2323	6.1039	12.5323

H	-0.9784	6.76	12.0629
H	0.3973	6.7233	13.1952
O	-0.9515	5.1458	13.3306
B	-0.3743	3.9461	13.62
C	-1.1577	2.9698	14.5616
C	-0.6442	1.7292	14.9695
H	0.3528	1.4206	14.643
C	-1.3948	0.8819	15.7857
H	-0.9739	-0.0699	16.1159
C	-2.6794	1.2479	16.1836
H	-3.2675	0.5764	16.8157
C	-3.2032	2.4685	15.7822
H	-4.2098	2.7631	16.0922
C	-2.4441	3.3174	14.9885
H	-2.8584	4.2801	14.6776
O	0.818	3.5381	13.0925
C	1.544	4.402	12.2012
H	2.3122	4.9418	12.7837
H	2.0671	3.7624	11.4721
H	2.307	5.8621	10.186
H	2.066	7.0482	11.4979
C	-0.2322	4.7038	10.4393
H	-0.9794	4.0489	10.909
H	0.394	4.0894	9.7776