SUPPORTING INFORMATION

Effect of the donor component nature on the extraction ability of a tributyl phosphate-based deep eutectic solvent

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Data of extraction experiments

Table S1. Extraction of Zr(IV) as a function of phase contact time.
Conditions: $[HCl]_0$ = 6.5 mol/L, $[Zr(IV)]_0$ = 0.004 mol/L, $V_{aq} = V_{org}$, T = 25°C.

	TBP/Ph	TBP/Thy	TBP/PTBP	TBP/BHT	TBP/Men
Time (min)	E (%) / D	E (%) / D	E (%) / D	E (%) / D	E (%) / D
1	15.67 / 0.186	44.06 / 0.788	34.89 / 0.536	60.56 / 1.535	21.54 / 0.274
3	43.21 / 0.761	63.45 / 1.736	54.61 / 1.203	79.87 / 3.968	27.67 / 0.383
5	58.76 / 1.425	72.45 / 2.63	65.73 / 1.918	81.02 / 4.269	30.23 / 0.433
10	65.74 / 1.919	76.64 / 3.28	68.99 / 2.225	81.23 / 4.328	30.56 / 0.440
30	67.56 / 2.083	78.65 / 3.684	70.34 / 2.372	81.67 / 4.456	30.36 / 0.436
60	67.46 / 2.073	79.13 / 3.792	71.1 / 2.46	82.45 / 4.698	30.66 / 0.442

Table S2. Extraction of Zr(IV) as a function of initial HCl concentration.
Conditions: $[Zr(IV)]_0$ = 0.004 mol/L, $V_{aq} = V_{org}$, phase contact time = 10 min, 25°C.

	TBP/Ph	TBP/Thy	TBP/PTBP	TBP/BHT	TBP/Men
$C(HCl)_{init}$	E (%) / D	E (%) / D	E (%) / D	E (%) / D	E (%) / D
4.5	0 / 0	0 / 0	0 / 0	0 / 0	0 / 0
5	2.68 / 0.028	5.36 / 0.057	4.46 / 0.047	4.91 / 0.052	0 / 0
5.5	8.48 / 0.093	17.86 / 0.217	14.29 / 0.167	14.29 / 0.167	0 / 0
5.75	18.3 / 0.224	23.21 / 0.302	20.54 / 0.258	20.54 / 0.258	1.34 / 0.014
6	26.34 / 0.358	34.6 / 0.529	29.69 / 0.422	35.71 / 0.555	5.36 / 0.057
6.5	64.56 / 1.822	78.65 / 3.684	70.34 / 2.372	81.67 / 4.456	30.56 / 0.44
6.75	80.65 / 4.168	89 / 8.091	82.34 / 4.663	89.56 / 8.579	40.23 / 0.673
7	87.5 / 7.0	93.67 / 14.80	89.21 / 8.27	94.54 / 17.32	52.232 / 1.09
7.5	95.7 / 22.25	97.59 / 40.49	96.16 / 25.04	97.41 / 37.61	76.12 / 3.188

Table S3. Extraction of Zr(IV) as a function of H^+ concentration at constant $[Cl^-]$ = 6.5 mol/L
Conditions: $[Cl^-]$ = 6.5 mol/L (LiCl + HCl), $[Zr(IV)]_0$ = 0.004 mol/L, $V_{aq} = V_{org}$, phase contact time = 10 min, 25°C.

	TBP/Ph	TBP/Thy	TBP/PTBP	TBP/BHT	TBP/Men
$C(H^+)_{init}$	E (%) / D	E (%) / D	E (%) / D	E (%) / D	E (%) / D
0	0 / 0	0 / 0	0 / 0	0 / 0	0 / 0
0.1	16.98 / 0.205	6.98 / 0.075	12.79 / 0.147	6.28 / 0.067	24.88 / 0.331
0.25	30 / 0.429	22.09 / 0.284	23.72 / 0.311	11.63 / 0.132	51.63 / 1.067
0.5	49.77 / 0.991	41.86 / 0.720	45.12 / 0.822	30.23 / 0.433	66.98 / 2.03
0.75	72.09 / 2.583	64.19 / 1.792	64.42 / 1.81	53.72 / 1.161	90.7 / 9.75
1	75.58 / 3.095	75.81 / 3.134	72.09 / 2.583	66.74 / 2.01	90.05 / 9.05
1.5	75.72 / 3.119	80 / 4.0	73.02 / 2.706	73.67 / 2.798	86.51 / 6.413
2	74.88 / 2.981	80.09 / 4.023	73.3 / 2.745	76.65 / 3.283	83.16 / 4.94
4	72.65 / 2.656	79.91 / 3.978	72.33 / 2.614	80.28 / 4.071	61.4 / 1.591
6	70.88 / 2.434	79.07 / 3.778	70.42 / 2.381	80.37 / 4.094	37.67 / 0.604

Table S4. Extraction of Zr(IV) as a function of Cl^- concentration at constant $[H^+]$ = 1 mol/L
Conditions: $[H^+]$ = 1 mol/L (HCl + LiCl to adjust Cl^-), $[Zr(IV)]_0$ = 0.004 mol/L, $V_{aq} = V_{org}$, phase contact time = 10 min, 25°C.

	TBP/Ph	TBP/Thy	TBP/PTBP	TBP/BHT	TBP/Men
$C(Cl^-)_{init}$	E (%) / D	E (%) / D	E (%) / D	E (%) / D	E (%) / D

5	0.68 / 0.007	1.13 / 0.011	0.9 / 0.009	0.9 / 0.009	4.75 / 0.050
5.5	9.28 / 0.102	7.69 / 0.083	7.99 / 0.087	3.39 / 0.035	26.24 / 0.356
5.75	14.93 / 0.176	13.12 / 0.151	12.67 / 0.145	5.43 / 0.057	38.24 / 0.619
6	26.92 / 0.368	24.66 / 0.327	23.76 / 0.312	14.03 / 0.163	57.47 / 1.351
6.5	64.71 / 1.834	65.32 / 1.884	60.18 / 1.511	57.47 / 1.351	79.64 / 3.912
6.75	85.16 / 5.739	86.99 / 6.686	84.16 / 5.313	83.71 / 5.139	92.85 / 12.99
7	91.86 / 11.285	92.49 / 12.316	91.4 / 10.628	91.95 / 11.422	95.11 / 19.45
7.5	96.47 / 27.329	96.47 / 27.329	96.2 / 25.31	97.01 / 32.445	—
8	100 / —	100 / —	100 / —	100 / —	—

Table S5. Extraction of HCl as a function of equilibrium HCl concentration
Conditions: $V_{aq} = V_{org}$, phase contact time = 10 min, T = 25°C.

TBP/Ph		TBP/Thy		TBP/PTBP		TBP/BHT		TBP/Men	
[HCl]	E (%) / D	[HCl]	E (%) / D	[HCl]	E (%) / D	[HCl]	E (%) / D	[HCl]	E (%) / D
3.24	0 / 0	3.22	0 / 0	3.22	0 / 0	3.22	0 / 0	3.2	1.27 / 0.0129
5.3	0 / 0	5.24	0 / 0	5.24	0 / 0	5.2	0 / 0	5.02	8.29 / 0.0904
6.24	1.89 / 0.019	6.3	0.94 / 0.0095	6.28	1.26 / 0.0128	6.04	0.33 / 0.0033	5.88	16.79 / 0.202
7.44	3.02 / 0.031	7.34	1.87 / 0.019	7.3	2.41 / 0.0247	7.1	1.25 / 0.0127	6.74	22.28 / 0.287

Table S6. Extraction of Zr(IV) as a function of TBP mole fraction in HDES
Conditions: $[HCl]_0 = 6.5$ mol/L, $[Zr(IV)]_0 = 0.004$ mol/L, $V_{aq} = V_{org}$, phase contact time = 10 min, T = 25°C.

	TBP/Ph	TBP/Thy	TBP/PTBP	TBP/BHT	TBP/Men
χ(TBP)	E (%) / D	E (%) / D	E (%) / D	E (%) / D	E (%) / D
0.1	7.25 / 0.078	—	—	—	—
0.2	27.05 / 0.371	8.91 / 0.098	—	—	36.63 / 0.578
0.3	35.89 / 0.560	12.87 / 0.148	—	—	74.58 / 2.934
0,35	—	—	24.75 / 0.329	—	—
0.4	43.32 / 0.764	20.80 / 0.263	32.87 / 0.490	21.05 / 0.267	76.9 / 3.329
0.5	65.79 / 1.923	59.01 / 1.440	58.91 / 1.434	44.94 / 0.816	79.76 / 3.941
0.6	86.63 / 6.479	89.60 / 8.615	86.26 / 6.278	78.59 / 3.671	91.88 / 11.315
0.7	90.79 / 9.858	91.78 / 11.17	90.40 / 9.417	87.72 / 7.143	93.47 / 14.314
0.8	92.18 / 11.79	93.07 / 13.43	92.28 / 11.95	90.79 / 9.858	93.96 / 15.56
0.9	92.97 / 13.23	93.76 / 15.03	92.97 / 13.22	92.38 / 12.12	94.55 / 17.35

Table S7. Extraction of Zr(IV) as a function of aqueous/organic phase volume ratio
Conditions: $[HCl]_0 = 6.5$ mol/L, $[Zr(IV)]_0 = 0.004$ mol/L, phase contact time = 10 min, T = 25°C.

	TBP/Ph	TBP/Thy	TBP/PTBP	TBP/BHT	TBP/Men
V_{aq}/V_{HDES}	E (%) / D	E (%) / D	E (%) / D	E (%) / D	E (%) / D
1	64.06 / 1.78	78.77 / 3.71	70.31 / 2.368	81.03 / 4.272	30.80 / 0.445
3	36.22 / 1.704	50.10 / 3.012	43.88 / 2.346	54.76 / 3.631	24.23 / 0.959
5	26.02 / 1.759	41.07 / 3.485	32.38 / 2.395	45.40 / 4.158	17.09 / 1.031

FT-IR spectra

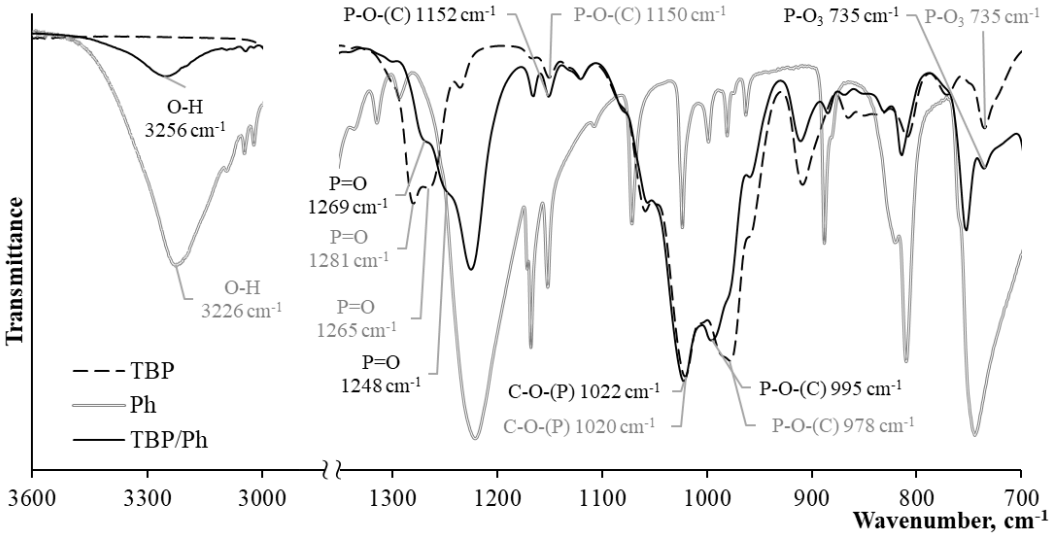

Fig. S1. FT-IR spectra of HDES TBP/Ph.

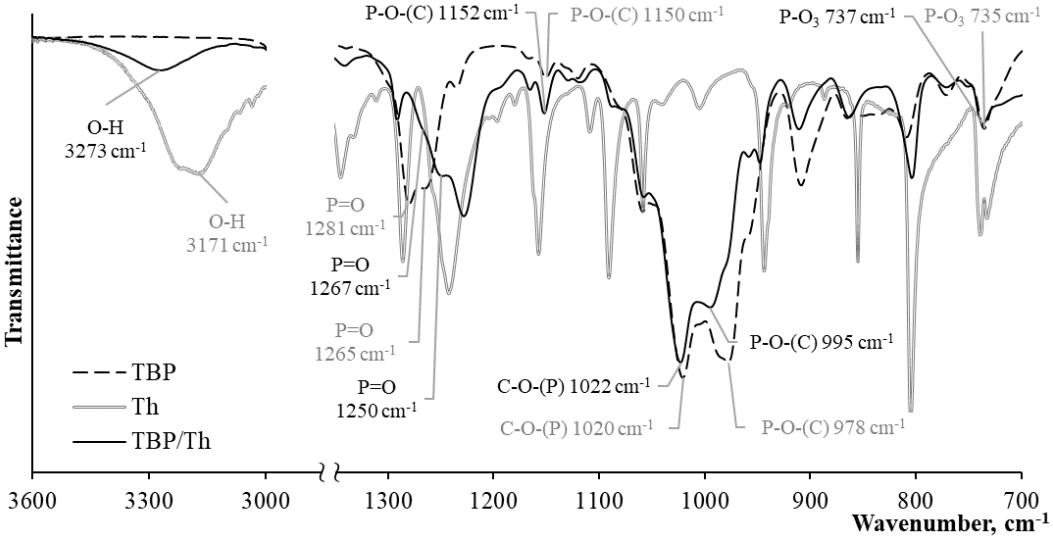

Fig. S2. FT-IR spectra of HDES TBP/Th.

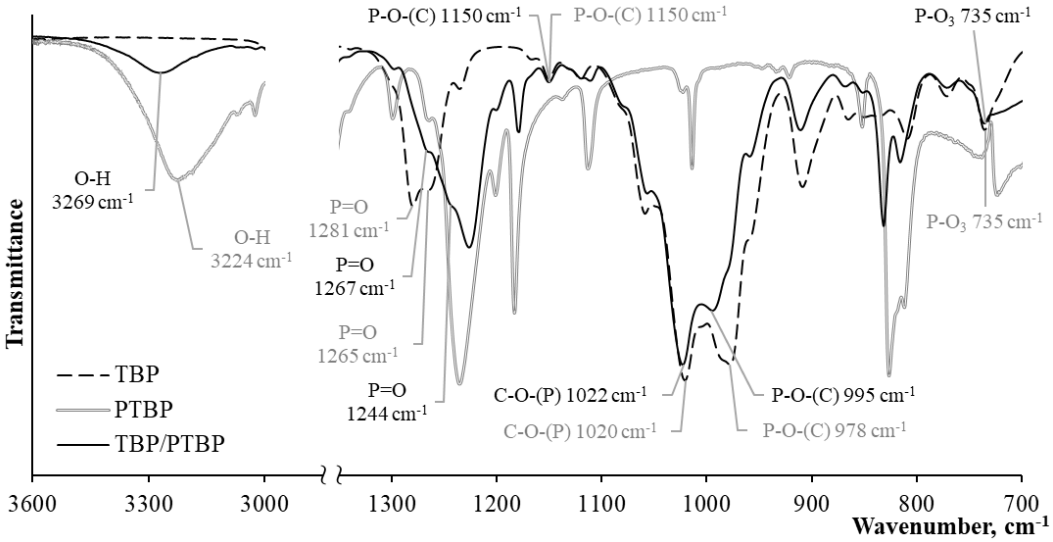

Fig. S3. FT-IR spectra of HDES TBP/PTBP.

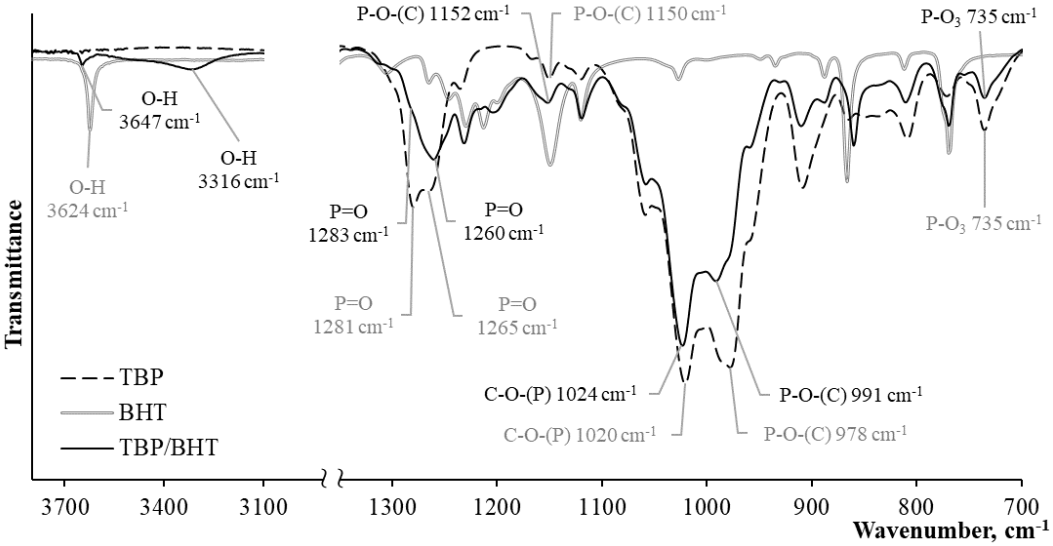

Fig. S4. FT-IR spectra of HDES TBP/BHT.

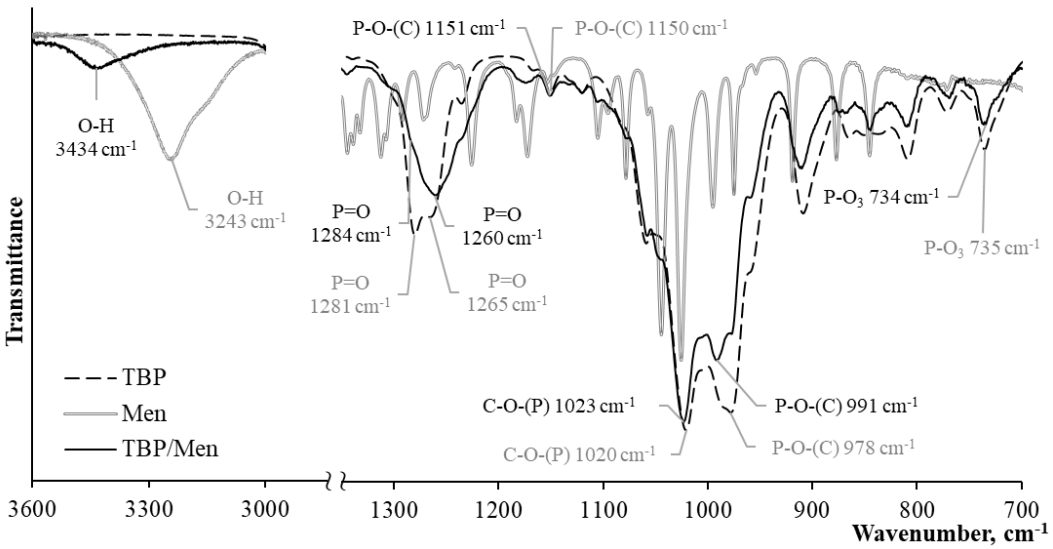

Fig. S5. FT-IR spectra of HDES TBP/Men.

^{1}H,^{1}H-NOESY NMR spectra

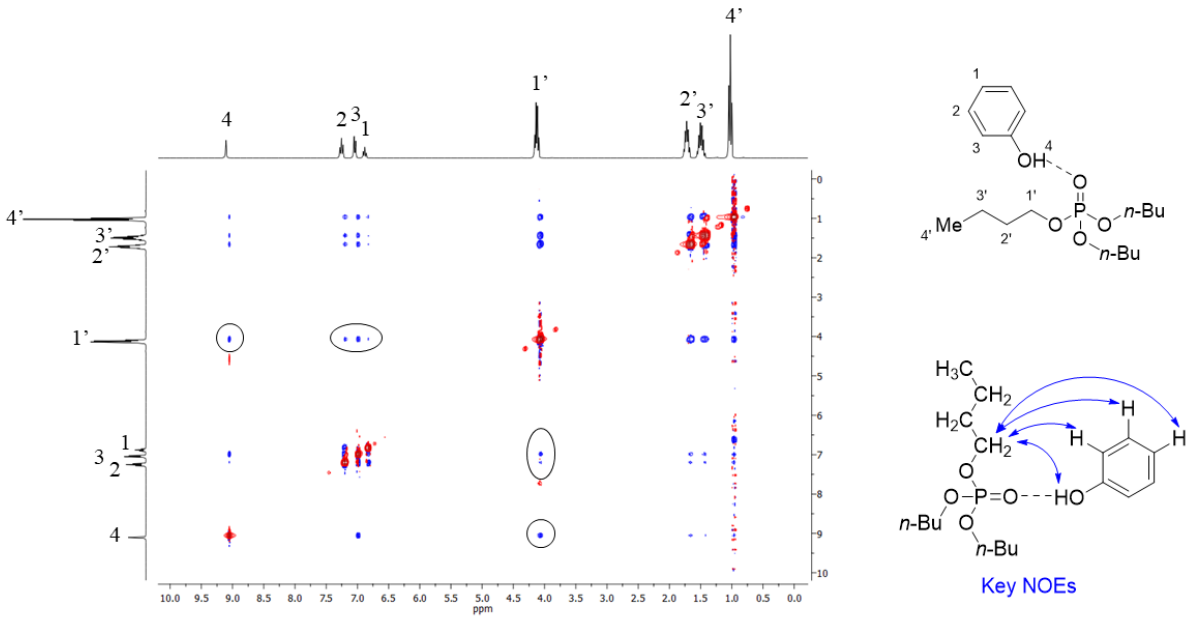

Fig. S6. ^{1}H,^{1}H-NOESY spectra of HDES TBP/Ph

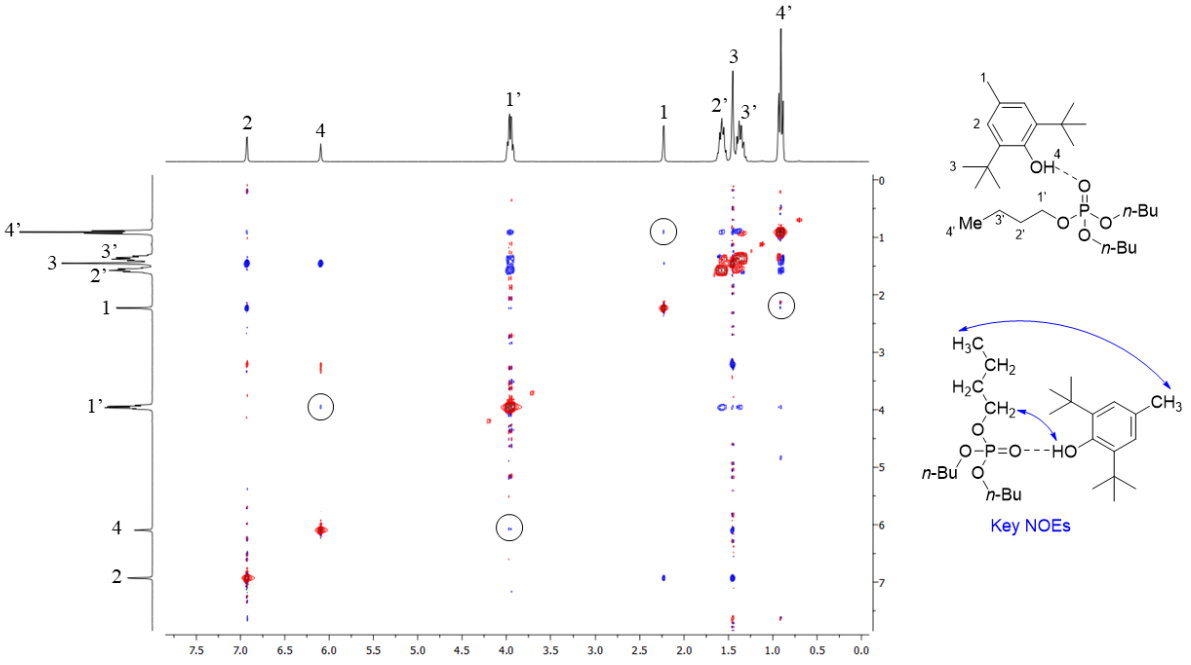

Fig. S7. ^{1}H,^{1}H-NOESY spectra of HDES TBP/BHT

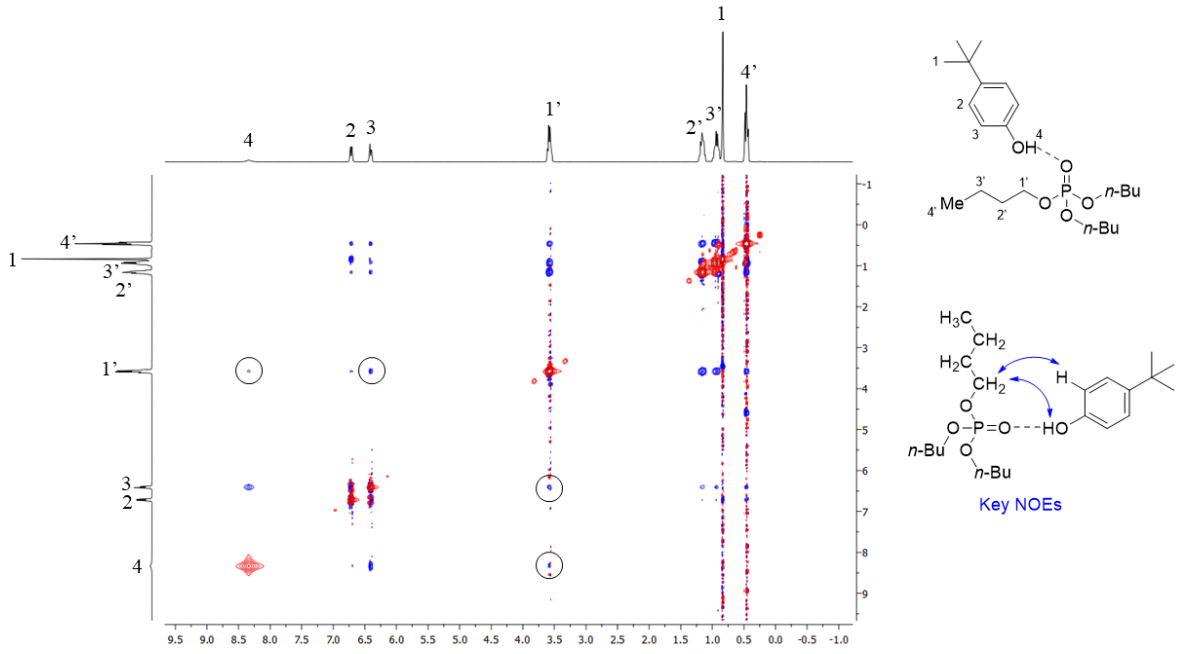

Fig. S8. ^{1}H,^{1}H-NOESY spectra of HDES TBP/PTBP

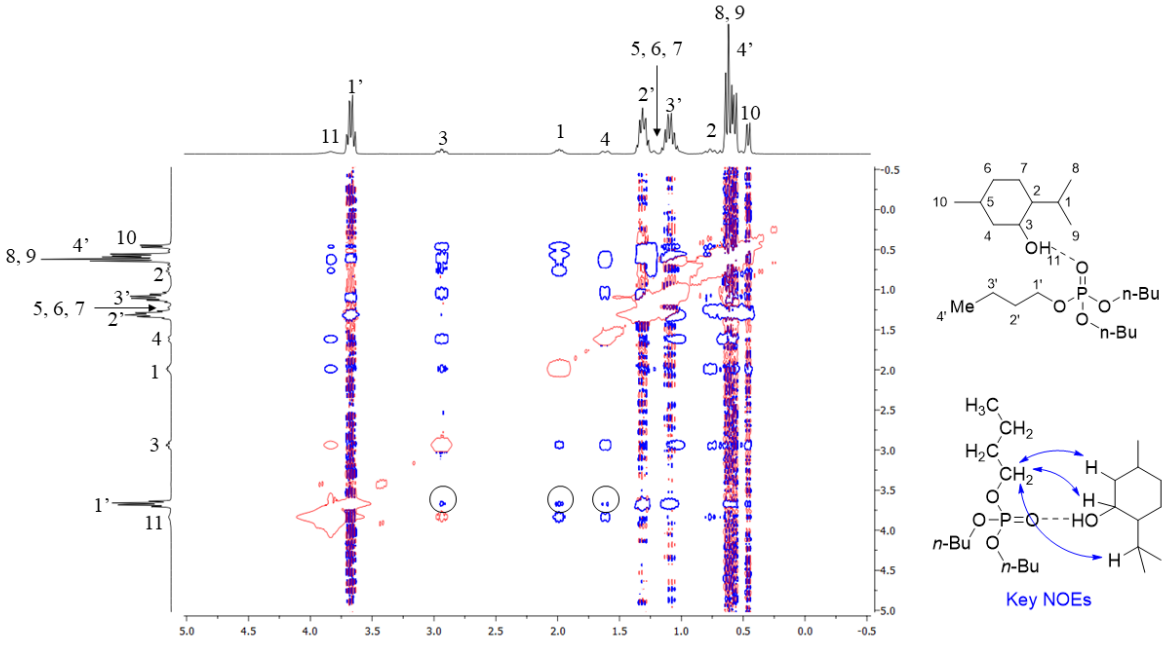

Fig. S9. ^{1}H,^{1}H-NOESY spectra of HDES TBP/Men

Born-Oppenheimer molecular dynamics

Table S8. The average number of selected types of hydrogen bonds.

Formal type of the associate (Ph)	N_{HB}	Formal type of the associate (Thy)	N_{HB}
–OH…O= (Ph/TBP)	3.87	–OH…O= (Thy/TBP)	4.08
–OH…O– (Ph/TBP)	0.18	–OH…O– (Thy/TBP)	0.03
Ph/Ph	0.42	Thy/Thy	0.49

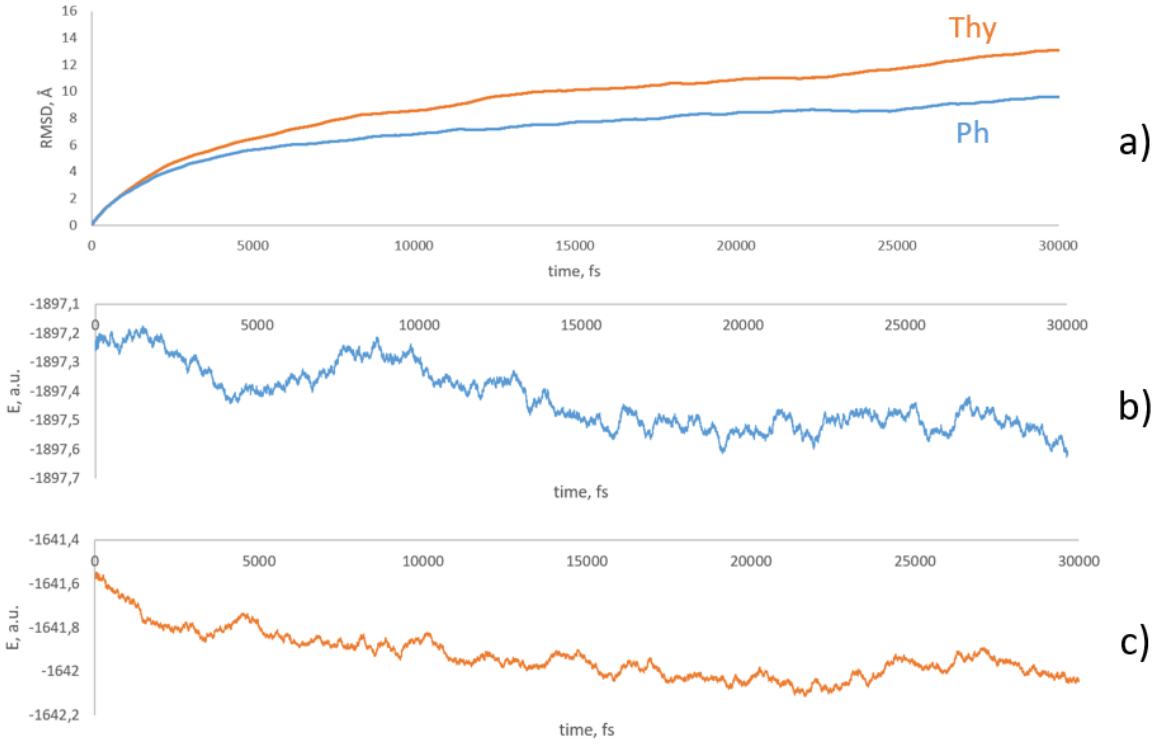

Fig. S10. Dependence of RMSD (a) and total energy of the system (b – Ph, c – Thy) on the simulation time.

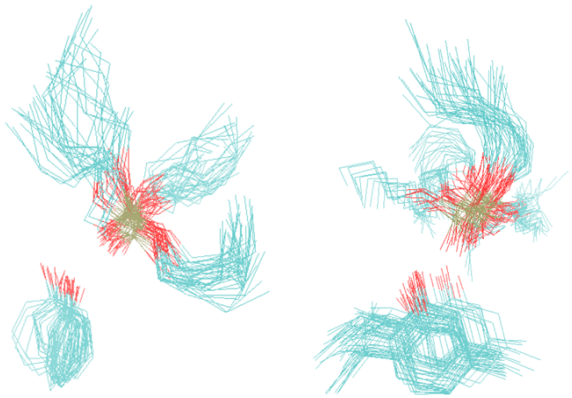

Fig. S11. The geometry of the "–OH...O=" type dimers for Ph and Thy.

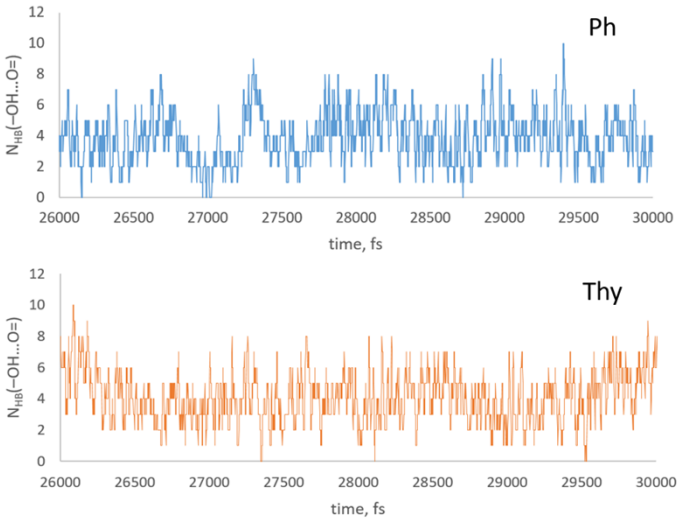

Fig. S12. Dependence of the number of hydrogen bonds of the "–OH...O=" type on the simulation time for Ph and Thy.

Combined DFT+D and DLPNO-CCSD calculations

Below are the coordinates of the atomic nuclei of dimers (Tables S2-S6) and the values of the total electron energy calculated at the theoretical level DLPNO-CCSD(T)/def2-TZVP.

Table S9. Men/TBP. E = -1581.640345295498 a.u.

O	-1.79258	-0.19132	0.93179
C	-5.64844	-1.05116	-0.63489
C	-5.15530	-1.88304	0.54535
C	-3.64506	-1.72247	0.68981
C	-3.20082	-0.26936	0.80658
C	-3.71709	0.56278	-0.37335
C	-5.23318	0.40772	-0.49903
H	-1.40526	-0.67427	0.18130
P	1.05053	-0.83665	-1.09950
O	-0.30805	-1.41600	-1.12202
O	2.09714	-1.72020	-1.89528
O	1.62236	-0.58482	0.36984
O	1.25530	0.59620	-1.75240
C	3.46429	-1.31265	-2.09761
H	3.77800	-1.83823	-3.00206
H	3.49000	-0.23750	-2.30033
C	0.50440	1.72798	-1.25790
H	0.00866	1.45908	-0.31925
H	-0.26355	1.94748	-2.00288
C	1.29802	-1.44700	1.47997
H	0.30433	-1.87245	1.32512
H	2.03840	-2.25545	1.50245
C	1.34466	-0.61659	2.73818
H	0.58672	0.17037	2.65318
H	1.03486	-1.25789	3.57299
C	2.71613	-0.01847	3.02136
H	3.44638	-0.82988	3.14009
H	3.03812	0.56057	2.14972
C	2.72499	0.86755	4.25774
H	2.42320	0.30889	5.14980
H	3.71821	1.28448	4.44661

H	2.02869	1.70490	4.14409
C	4.34927	-1.67648	-0.92478
H	4.26831	-2.75399	-0.73934
H	3.98588	-1.16651	-0.02677
C	5.80285	-1.29667	-1.17572
H	5.86593	-0.22152	-1.38619
H	6.16692	-1.80596	-2.07673
C	6.70250	-1.63724	0.00335
H	6.68165	-2.71055	0.21730
H	7.74119	-1.35645	-0.19036
H	6.37801	-1.11368	0.90839
C	1.44152	2.89482	-1.06260
H	0.82761	3.77753	-0.84186
H	1.95355	3.10091	-2.01062
C	2.45909	2.67951	0.04923
H	1.92530	2.49431	0.98921
H	3.02669	1.76604	-0.15672
C	3.40878	3.85556	0.21411
H	4.12596	3.67963	1.02079
H	3.97845	4.03545	-0.70365
H	2.86465	4.77622	0.44925
C	-3.24531	2.02613	-0.30870
C	-3.36300	2.71278	-1.66567
H	-2.84164	2.14599	-2.44419
H	-4.40795	2.81728	-1.97683
H	-2.93298	3.71944	-1.63507
C	-3.94233	2.84945	0.77096
H	-5.00024	3.00806	0.53793
H	-3.88114	2.37237	1.75334
H	-3.47713	3.83650	0.85698
H	-5.60074	0.98485	-1.35423
H	-3.60137	0.14967	1.73910
H	-3.26084	0.12079	-1.27405
H	-5.62734	-1.48089	1.45504
H	-3.28031	-2.27341	1.56421
H	-5.71775	0.83039	0.39092
H	-6.73879	-1.12955	-0.71895
H	-5.23076	-1.46890	-1.56197
H	-3.15098	-2.16216	-0.18941
C	-5.54826	-3.34706	0.41172
H	-5.21077	-3.93081	1.27383
H	-6.63380	-3.46245	0.33031
H	-5.09719	-3.78707	-0.48480
H	-2.18275	1.98080	-0.04728

Table S10. Ph/TBP. E = -1421.08970875498 a.u.

O	2.80515100	-1.27908100	-1.50334800
C	6.04527300	1.15884500	-0.64974600
C	6.19491000	-0.21759600	-0.79821100
H	7.17418500	-0.67142500	-0.68194100
C	5.10389100	-1.02308900	-1.08779600
H	5.20870000	-2.09690400	-1.19751400
C	3.83590300	-0.45730300	-1.23515700
C	3.68111500	0.92524000	-1.09880700
H	2.69490000	1.36041800	-1.22227200
C	4.78271600	1.71984700	-0.80524000
H	4.64886700	2.79204900	-0.69849200
H	1.96488900	-0.78280000	-1.46332900

H	6.90102500	1.78379000	-0.41987900
P	-0.61501600	-0.30754600	-0.21404800
O	0.49113700	0.11895500	-1.09762000
O	-1.33716900	-1.59811600	-0.77485800
O	-1.71535400	0.83253100	0.00734000
O	-0.28532800	-0.72114900	1.27680100
C	-2.43150200	-2.24302700	-0.09426200
H	-2.30567100	-3.30760900	-0.30270200
H	-2.32682200	-2.09174100	0.98442000
C	0.19016900	0.22081500	2.26555700
H	-0.06987400	-0.24333400	3.21957900
H	-0.38040600	1.14887200	2.16401900
C	-2.06836500	1.71174600	-1.07993200
H	-1.15122200	2.13178100	-1.50059900
H	-2.56901900	1.12203300	-1.85730900
C	-2.98441200	2.78220100	-0.53988000
H	-2.45555700	3.34001800	0.24228000
H	-3.17731800	3.49234900	-1.35375700
C	-4.30288300	2.24586900	0.00160600
H	-4.81682400	1.69059400	-0.79380000
H	-4.09359000	1.52334100	0.79771800
C	-5.21158000	3.34600200	0.52841000
H	-5.45663900	4.06830200	-0.25702400
H	-6.15173900	2.93957700	0.91088900
H	-4.73167400	3.89616500	1.34420100
C	-3.76320300	-1.73810000	-0.60206700
H	-3.80441800	-1.87758100	-1.68852800
H	-3.83230100	-0.66226900	-0.41159800
C	-4.93588900	-2.44792200	0.06184600
H	-4.86538200	-2.32733400	1.15017700
H	-4.87028800	-3.52582800	-0.13089600
C	-6.27941000	-1.92186200	-0.42189500
H	-6.38858800	-2.05527800	-1.50281600
H	-7.11093100	-2.43996200	0.06306600
H	-6.38220500	-0.85292000	-0.20853600
C	1.67957300	0.45979900	2.17229800
H	1.93055900	1.17038000	2.97171500
H	1.92210300	0.95824100	1.22743200
C	2.52012400	-0.80152300	2.32215000
H	2.17191500	-1.36419300	3.19877600
H	2.35637700	-1.44826600	1.45435500
C	4.00335100	-0.49337500	2.46261100
H	4.59319000	-1.41089400	2.53384600
H	4.37454800	0.06841200	1.60145300
H	4.19827600	0.10068700	3.36234800

Table S11. PTBP/TBP. E = -1578.03463545115 a.u.

O	1.48997	-1.75398	-1.60031
C	5.03109	0.19507	-0.54733
C	4.96221	-1.19079	-0.73363
H	5.85105	-1.79770	-0.58888
C	3.78618	-1.82866	-1.08765
H	3.75007	-2.90506	-1.21646
C	2.61549	-1.09137	-1.27326
C	2.66398	0.29197	-1.11290
H	1.76155	0.87509	-1.26524
C	3.85567	0.91425	-0.75233
H	3.84913	1.99136	-0.62989

H	0.72546	-1.14897	-1.55014
P	-1.74492	-0.36730	-0.23951
O	-0.61365	-0.06132	-1.14073
O	-2.59923	-1.58528	-0.77688
O	-2.72405	0.87877	-0.01760
O	-1.43956	-0.79656	1.25233
C	-3.74159	-2.11344	-0.07527
H	-3.72611	-3.18642	-0.27803
H	-3.60528	-1.96739	1.00060
C	-0.85179	0.10158	2.22113
H	-1.17432	-0.29908	3.18493
H	-1.29605	1.09312	2.09208
C	-3.00156	1.77745	-1.11057
H	-2.05265	2.09777	-1.54821
H	-3.57033	1.23330	-1.87425
C	-3.79678	2.94103	-0.57161
H	-3.20310	3.45049	0.19691
H	-3.92818	3.65848	-1.39134
C	-5.15502	2.54714	-0.00658
H	-5.73401	2.03888	-0.78860
H	-5.00876	1.81523	0.79503
C	-5.93975	3.73921	0.51941
H	-6.12134	4.47475	-0.27097
H	-6.91080	3.43436	0.91879
H	-5.39500	4.24597	1.32251
C	-5.02410	-1.48078	-0.56651
H	-5.09563	-1.62096	-1.65133
H	-4.98263	-0.40247	-0.38216
C	-6.25138	-2.06681	0.11911
H	-6.15251	-1.94873	1.20550
H	-6.29660	-3.14678	-0.06787
C	-7.54301	-1.41157	-0.34798
H	-7.68124	-1.53811	-1.42641
H	-8.41459	-1.84210	0.15207
H	-7.53561	-0.33679	-0.13939
C	0.65625	0.14156	2.13229
H	0.99560	0.83834	2.91101
H	0.96471	0.57271	1.17377
C	1.32362	-1.21346	2.32794
H	0.90480	-1.69565	3.22152
H	1.07524	-1.86145	1.48134
C	2.83460	-1.09864	2.46240
H	3.29896	-2.08218	2.57164
H	3.27449	-0.62484	1.58120
H	3.10726	-0.50083	3.33941
C	6.34647	0.84455	-0.12661
C	6.78389	0.27086	1.22858
H	6.92853	-0.81166	1.17866
H	7.72892	0.72253	1.54968
H	6.02852	0.47070	1.99454
C	6.22011	2.36096	0.01542
H	7.18377	2.78328	0.31602
H	5.93031	2.83262	-0.92849
H	5.48500	2.63565	0.77814
C	7.42580	0.54946	-1.17689
H	8.37901	1.00346	-0.88474
H	7.58903	-0.52490	-1.29595
H	7.13690	0.95314	-2.15175

Table S12. Thy/TBP. E = -1578.03793271864 a.u.

O	2.20784	-1.02308	-1.09570
C	5.10034	1.82521	-0.35866
C	5.39438	0.46553	-0.28334
H	6.40005	0.16354	-0.01017
C	4.43737	-0.51111	-0.52632
C	3.14346	-0.07754	-0.86516
C	2.84625	1.28066	-0.94623
H	1.83360	1.57505	-1.20807
C	3.81751	2.24768	-0.68980
H	1.32762	-0.60746	-1.17458
H	5.87485	2.55774	-0.15289
P	-1.34885	-0.25548	-0.12255
O	-0.25334	0.16255	-1.02296
O	-1.91312	-1.67843	-0.52148
O	-2.56637	0.78209	-0.09334
O	-1.04556	-0.42889	1.42026
C	-2.96365	-2.33987	0.21011
H	-2.72622	-3.40383	0.14483
H	-2.91445	-2.04315	1.26223
C	-0.70852	0.68112	2.28351
H	-0.98450	0.33353	3.28168
H	-1.34685	1.53089	2.02349
C	-2.95709	1.46619	-1.30112
H	-2.06796	1.91563	-1.75058
H	-3.36668	0.72936	-2.00261
C	-3.99306	2.50207	-0.93989
H	-3.55231	3.21152	-0.22921
H	-4.22071	3.07191	-1.84949
C	-5.27422	1.91366	-0.36401
H	-5.69991	1.20640	-1.08768
H	-5.02804	1.33079	0.53002
C	-6.30525	2.97740	-0.01913
H	-6.58752	3.55802	-0.90337
H	-7.21621	2.53353	0.39135
H	-5.91369	3.67882	0.72466
C	-4.31893	-2.04266	-0.39101
H	-4.30549	-2.32164	-1.45101
H	-4.50122	-0.96427	-0.34307
C	-5.43959	-2.78015	0.33010
H	-5.42245	-2.51649	1.39506
H	-5.26021	-3.86120	0.28017
C	-6.80946	-2.46084	-0.25068
H	-6.86397	-2.74013	-1.30763
H	-7.60320	-2.99665	0.27652
H	-7.02576	-1.38989	-0.18003
C	0.75899	1.03718	2.22565
H	0.90452	1.86673	2.93119
H	1.01470	1.42488	1.23338
C	1.69035	-0.11337	2.58504
H	1.32919	-0.59687	3.50271
H	1.64449	-0.87161	1.79691
C	3.12765	0.34720	2.77500
H	3.78939	-0.49725	2.98582
H	3.50641	0.84349	1.87778
H	3.20785	1.05117	3.61074
C	4.71934	-1.99326	-0.45119
H	3.83200	-2.45472	-0.00120
C	5.92402	-2.34265	0.41357

H	5.84352	-1.90568	1.41342
H	6.00554	-3.42822	0.52219
H	6.85990	-1.99241	-0.03474
C	4.87057	-2.58101	-1.85733
H	5.01279	-3.66602	-1.81206
H	3.98389	-2.37650	-2.46094
H	5.73946	-2.14411	-2.36113
C	3.46873	3.70597	-0.76995
H	3.11178	3.97381	-1.76963
H	2.67344	3.96269	-0.06200
H	4.33433	4.33242	-0.54307

Table S13. BHT/TBP. E = -1774.20815068261 a.u.

O	1.88764	0.65548	-1.96469
C	4.29870	0.42567	1.42508
C	4.25783	-0.61770	0.50915
H	4.86778	-1.49088	0.70687
C	3.46729	-0.57746	-0.63875
C	2.68487	0.57584	-0.85256
C	2.76052	1.68553	0.01280
C	3.56111	1.56950	1.14911
H	1.01441	0.26211	-1.77677
P	-1.64455	-0.68739	-0.46481
O	-0.58242	-0.31991	-1.42098
O	-2.56270	-1.83931	-1.04499
O	-2.58015	0.54182	-0.04924
O	-1.23455	-1.25809	0.95127
C	-3.65150	-2.41812	-0.29948
H	-3.71537	-3.44931	-0.65353
H	-3.39079	-2.43711	0.76317
C	-0.51243	-0.46662	1.92563
H	-1.09004	-0.55250	2.85022
H	-0.51188	0.58104	1.61519
C	-2.95590	1.53295	-1.02642
H	-2.07179	1.81106	-1.60480
H	-3.69337	1.08683	-1.70460
C	-3.53816	2.71553	-0.29283
H	-2.77255	3.12524	0.37663
H	-3.75215	3.49335	-1.03657
C	-4.80115	2.38649	0.49187
H	-5.55458	1.98024	-0.19572
H	-4.57655	1.59026	1.20962
C	-5.36947	3.59445	1.22088
H	-5.62523	4.39638	0.52069
H	-6.27518	3.33747	1.77687
H	-4.64511	3.99935	1.93494
C	-4.94815	-1.67779	-0.54213
H	-5.13936	-1.64285	-1.62105
H	-4.84018	-0.64394	-0.19851
C	-6.12163	-2.33201	0.17541
H	-5.90429	-2.39128	1.24927
H	-6.23415	-3.36678	-0.17108
C	-7.42472	-1.57574	-0.03847
H	-7.68113	-1.52580	-1.10145
H	-8.25721	-2.05597	0.48251
H	-7.34738	-0.54829	0.33165
C	0.88988	-0.99354	2.09526
H	1.39265	-0.35198	2.83018

H	1.44176	-0.86433	1.15890
C	0.93863	-2.44644	2.54603
H	0.36884	-2.55768	3.47831
H	0.42941	-3.06657	1.80053
C	2.36057	-2.94644	2.74832
H	2.37621	-3.99386	3.06203
H	2.93804	-2.86074	1.82376
H	2.88206	-2.36007	3.51207
C	3.47376	-1.75185	-1.62599
C	4.49022	-2.82510	-1.22339
H	4.24759	-3.28813	-0.26165
H	4.48276	-3.61762	-1.97730
H	5.50820	-2.42740	-1.17082
C	3.86788	-1.26215	-3.02774
H	3.88850	-2.10902	-3.72239
H	3.16671	-0.51811	-3.40259
H	4.86810	-0.81777	-3.00751
C	2.09746	-2.43195	-1.66726
H	1.80755	-2.77725	-0.66910
H	1.31165	-1.77557	-2.03718
H	2.13955	-3.30776	-2.32404
C	2.03832	3.00346	-0.29781
C	2.35200	4.08474	0.74033
H	2.00956	3.80791	1.74256
H	3.42176	4.30801	0.78881
H	1.83450	5.00675	0.45891
C	2.50344	3.53350	-1.66322
H	3.58490	3.70091	-1.65663
H	2.26644	2.83162	-2.46190
H	2.01444	4.49055	-1.87678
C	0.51557	2.81591	-0.30214
H	0.02568	3.77118	-0.52289
H	0.19750	2.08747	-1.04551
H	0.16729	2.48423	0.68172
C	5.11103	0.31282	2.68287
H	6.02130	-0.27030	2.51957
H	5.40161	1.29645	3.06064
H	4.54279	-0.18860	3.47539
H	3.62840	2.39883	1.84323

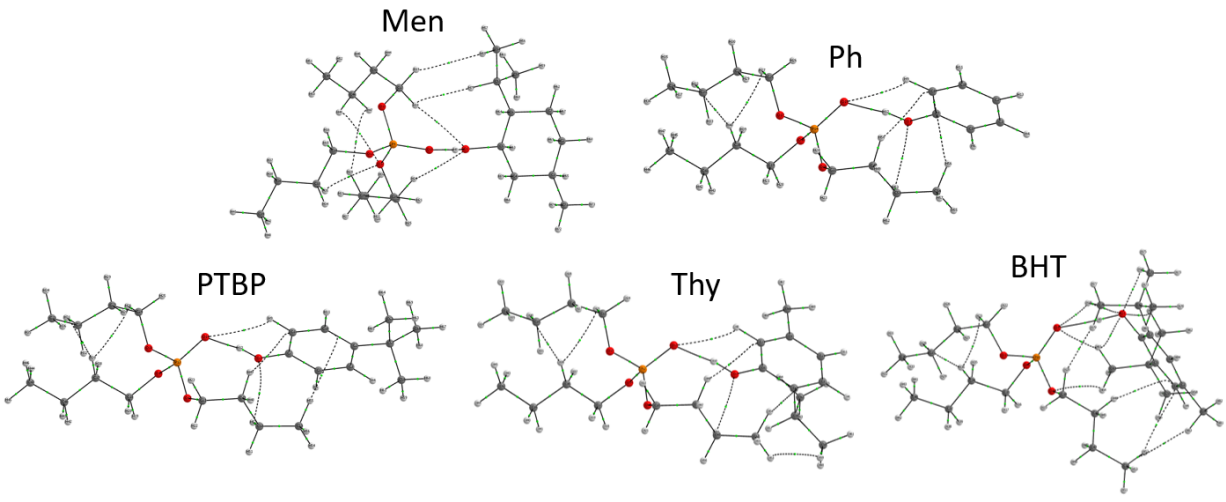

Fig. S13. Atomic bonding graphs for associates of TBP. Small green spheres denote (3,-1) critical points of electron density.