Supplementary Material (ESI) for *Faraday Discussions*

Supplementary data

Table 1.

a) relative energy and the most important geometrical and topological parameters of ρ(**r**) in CP (3,-1) for **1POC** at different θ angle values.

Θ	Δ E_{rel}, kcal $mole^{-1}$	C1-C2, Å	C1-Ph, Å	C2...B3, Å	C2…B6, Å	ρ(**r**) (C1…C2), e/$Å^3$	∇^2(**r**) (C1...C2), e/$Å^5$.
0	0.238	1.641	1.510	1.714	1.715	1.23	-4.38
10	0.144	1.642	1.511	1.713	1.716	1.22	-4.36
20	0.138	1.642	1.511	1.713	1.716	1.22	-4.34
30	0.000	1.645	1.512	1.712	1.717	1.21	-4.23
40	0.001	1.648	1.513	1.711	1.717	1.21	-4.12
50	0.075	1.652	1.514	1.711	1.717	1.20	-3.97
60	0.207	1.657	1.514	1.710	1.713	1.18	-3.78
70	0.207	1.663	1.514	1.708	1.711	1.17	-3.60
80	0.276	1.669	1.513	1.706	1.708	1.16	-3.39
90	0.270	1.672	1.513	1.705	1.706	1.15	-3.30

b) relative energy and the most important geometrical and topological parameters of ρ(**r**) in CP (3,-1) for **3POC** at different θ angle values.

Θ	Δ E_{rel}, kcal $mole^{-1}$	C2-C6, Å	B1-C6, Å	B1-C2, Å	B1-C13, Å	ρ(**r**) (B1…C6), e/$Å^3$.	∇^2(**r**) (B1...C6), e/$Å^5$.
0	0.389	1.621	1.731	1.745	1.572	0.79	-1.02
10	0.338	1.621	1.731	1.742	1.572	0.79	-0.98
20	0.226	1.622	1.732	1.739	1.572	0.79	-0.95
30	0.136	1.623	1.733	1.735	1.572	0.79	-0.94
40	0.171	1.624	1.736	1.732	1.572	0.78	-1.03
50	0.277	1.624	1.739	1.730	1.572	0.79	-1.19
60	0.375	1.622	1.743	1.730	1.572	0.78	-1.40
70	0.375	1.620	1.747	1.731	1.572	0.77	-1.60
80	0.304	1.618	1.749	1.734	1.573	0.77	-1.74
90	0.156	1.616	1.751	1.737	1.573	0.77	-1.83
100	0.046	1.615	1.750	1.739	1.573	0.77	-1.87
110	0.002	1.616	1.747	1.741	1.574	0.78	-1.87
120	0.000	1.616	1.745	1.744	1.574	0.78	-1.86
130	0.010	1.616	1.743	1.746	1.574	0.78	-1.82
140	0.009	1.617	1.739	1.748	1.574	0.78	-1.72
150	0.084	1.617	1.737	1.748	1.573	0.79	-1.57
160	0.210	1.619	1.734	1.748	1.573	0.79	-1.37
170	0.338	1.620	1.732	1.747	1.572	0.79	-1.18

c) relative energy and the most important geometrical and topological parameters of ρ(**r**) in CP

Supplementary data

(3,-1) for **1PMC** at different θ angle values.

Θ	Δ E_{rel}, kcal $mole^{-1}$	C1-B2, Å	C1-B3, Å	C1-B4, Å	C1-B5, Å	C1-B6, Å
0	0.23	1.713	1.710	1.735	1.736	1.733
10	0.06	1.716	1.712	1.734	1.734	1.734
20	0.18	1.714	1.711	1.736	1.734	1.735
30	0.00	1.715	1.712	1.736	1.730	1.734
40	0.09	1.713	1.711	1.739	1.732	1.734
50	0.13	1.712	1.712	1.74	1.731	1.735
60	0.12	1.71	1.711	1.741	1.733	1.736
70	0.10	1.711	1.71	1.739	1.732	1.738
80	0.11	1.71	1.71	1.737	1.733	1.741
90	0.19	1.711	1.71	1.736	1.732	1.74
100	0.02	1.712	1.713	1.734	1.732	1.74
110	0.09	1.709	1.713	1.735	1.734	1.737
120	0.07	1.714	1.716	1.734	1.729	1.736
130	0.10	1.712	1.715	1.734	1.733	1.734
140	0.17	1.712	1.714	1.734	1.734	1.735
150	0.22	1.713	1.714	1.732	1.734	1.735
160	0.26	1.711	1.711	1.734	1.739	1.735
170	0.25	1.712	1.711	1.734	1.739	1.734

Table 2.

a) The geometrical parameters of C_{ph}-H…H-C and C_{ph}-H…H-B contacts, their energy and also topological parameters of ρ(**r**) in the corresponding CP (3,-1) for **1POC** according to the B3LYP/6-31G** calculations.

Θ	H(14)…H(X), Å	X[a)]	ρ(**r**), e/$Å^3$	∇^2(**r**), e/$Å^5$	H(18)…H(Y), Å	Y [a)]	ρ(**r**), e/$Å^3$	∇^2(**r**), e/$Å^5$
0	2.007	2	0.079	1.13	N/A			
10	2.030	2	0.076	1.11	2.264	4	0.063	0.87
20	2.086	2	0.072	1.09	2.166	4	0.070	0.94
30	N/A				2.106	4	0.076	0.99
40	2.232	6	0.067	0.94	2.092	4	0.078	1.01
50	2.110	6	0.079	1.06	2.122	4	0.075	0.99
60	2.041	6	0.086	1.12	2.206	4	0.068	0.93

Supplementary data

70	2.023	6	0.094	1.14	N/A			
80	2.043	6	0.086	1.13	2.266	3	0.067	0.98
90	2.105	6	0.080	1.09	2.134	3	0.078	1.07

[a)]X and Y denote hydrogen atom number according to Fig. 1 of the manuscript

b) The geometrical parameters of C_{ph}-H…H-C and C_{ph}-H…H-B contacts, their energy and also topological parameters of ρ(**r**) in the corresponding CP (3,-1) for **3POC** according to the B3LYP/6-31G** calculations.

Θ	H(14)…H(X), Å	X[a)]	ρ(**r**), e/Å^3	∇^2(**r**), e/Å^5	H(18)…H(Y), Å	Y [a)]	ρ(**r**), e/Å^3	∇^2(**r**), e/Å^5
0	2.188	6	0.055	0.79	N/A			
10	2.214	6	0.053	0.77	N/A			
20	2.281	6	0.049	0.74	N/A			
30	N/A				N/A			
40	N/A				N/A			
50	2.247	2	0.051	0.75	N/A			
60	2.199	2	0.054	0.78	N/A			
70	2.189	2	0.055	0.79	N/A			
80	2.216	2	0.053	0.79	N/A			
90	N/A				N/A			
100	N/A				2.357	5	0.049	0.63
110	N/A				2.331	5	0.050	0.65
120	2.371	3	0.048	0.64	2.353	5	0.049	0.64
130	2.334	3	0.050	0.65	N/A			
140	2.342	3	0.049	0.64	N/A			
150	2.380	3	0.047	0.63	N/A			
160	N/A				N/A			
170	N/A				2.206	6	0.054	0.78

[a)]X and Y denote hydrogen atom number according to Fig. 1 of the manuscript

c) The geometrical parameters of C_{ph}-H…H-C and C_{ph}-H…H-B contacts, their energy and also topological parameters of ρ(**r**) in the corresponding CP (3,-1) for **1PMC** according to the B3LYP/6-31G** calculations.

Θ	H(14)…H(X), Å	X[a)]	ρ(**r**), e/Å^3	∇^2(**r**), e/Å^5	H(18)…H(Y), Å	Y [a)]	ρ(**r**), e/Å^3	∇^2(**r**), e/Å^5
0	2.071	6	0.081	1.05	N/A			

Supplementary data

10	2.096	6	0.108	1.03	N/A			
20	2.169	6	0.072	0.98	2.195	3	0.070	0.95
30	2.283	6	0.063	0.90	2.139	3	0.074	0.99
40	N/A				2.123	3	0.076	1.00
50	2.189	5	0.070	0.95	2.150	3	0.074	0.98
60	2.106	5	0.077	1.02	2.230	3	0.067	0.92
70	2.071	5	0.081	1.05	N/A			
80	2.085	5	0.080	1.03	2.289	2	0.063	0.89
90	2.144	5	0.074	0.99	2.179	2	0.071	0.96
100	2.257	5	0.065	0.90	2.130	2	0.075	0.99
110	N/A				2.133	2	0.075	0.99
120	2.201	4	0.069	0.95	2.165	2	0.072	0.98
130	2.116	4	0.076	1.01	2.265	2	0.065	0.91
140	2.082	4	0.080	1.04	N/A		0.000	0.00
150	2.074	4	0.081	1.05	2.300	6	0.062	0.88
160	2.115	4	0.077	1.02	2.169	6	0.072	0.98
170	2.209	4	0.069	0.94	2.097	6	0.078	1.03

[a)]X and Y denote hydrogen atom number according to Fig. 1 of the manuscript

Table 3. Intermolecular H...H contacts according to the X-ray diffraction experiment and PBE calculation of **1POC**.

	Experimental data				**Calculated data**			
Contact	**Symm. trans.[a)]**	**H…H**	**X-H…H**	**X...H-X**	**Symm trans.[a)]**	**H…H**	**X-H…H**	**X...H-X**
C(2)-H(2)…H(7')-B(7')	**3655** **3645**	**2.280**	**156.4**	**104.8**	**3655** **3645**	**2.614**	**147.4**	**110.2**
C(2)-H(2)…H(12')-B(12')	**3655** **3645**	**2.578**	**111.5**	**101.7**				
B(3)-H(3)…H(8')-B(8')					**3555** **3545**	**2.241**	**166.6**	**155.7**
B(3)-H(3)…H(11')-B(11')	**1455** **1655**	**2.583**	**115.6**	**145.3**				
B(3)-H(3)…H(17')-C(17')	**3545** **3555**	**2.427**	**128.3**	**124.7**	**3545** **3555**	**2.423**	**116.2**	**120.0**
B(3)-H(3)…H(18')-C(18')					**3545** **3555**	**2.513**	**113.5**	**117.2**

Supplementary data

B(4)-H(4)…H(10')-B(10')	**1455 1655**	**2.491**	**158.9**	**109.1**				
B(5)-H(5)…H(10')-B(10')	**2655 2655**	**2.519**	**108.7**	**172.8**	**2655 2655**	**2.191**	**113.4**	**174.7**
B(6)-H(6)…H(15')-C(15')	**2565 2565**	**2.327**	**150.6**	**127.7**				
B(7)-H(7)…H(12')-B(12')	**3655 3645**	**2.450**	**112.4**	**117.1**	**3655 3645**	**2.365**	**122.4**	**129.0**
B(8)-H(8)…H(11')-B(11')	**3645 3655**	**2.430**	**139.2**	**120.8**				
B(9)-H(9)…H(14')-C(14')	**2555 2555**	**2.411**	**114.8**	**118.1**				
B(9)-H(9)…H(15')-C(15')	**2555 2555**	**2.360**	**160.1**	**120.5**	**2555 2555**	**2.387**	**157.9**	**132.6**
B(10)-H(10)…H(10')-B(10')	**2655**	**2.601**	**109.7**	**109.7**				
B(12)-H(12)…H(17')-C(17')	**1645 1465**	**2.323**	**146.5**	**130.0**	**1645 1465**	**2.254**	**152.0**	**128.5**

[a)] Symmetrical transformations, where 3655 = 1-x, 0.5+y, 0.5-z; 3645 = 1–x, -0.5+y, 0.5-z; 1455 = -1+x, y, z; 1655 = 1+x, y, z; 2655 = 1-x, -y, -z; 2565 = –x, 1-y, -z; 2555 = –x, -y, -z; 1645 = 1+x, -1+y, z; 1465 = -1+x, 1+y, z; 3545= –x, -0.5+y, 0.5-z; 3555 = –x, 0.5+y, 0.5-z.

Table 4. Topological parameters of intermolecular H…H contacts in the crystal of **1POC** according to the X-ray diffraction experiment.

Contact	Symm. trans. [a)]	ρ(r), e/Å^3	$\nabla^2\rho$(r), e/Å^5	ε	g(r)	V(r)	h_e(r)	$E_{cont.}$ kcal/mole
C(2)-H(2)…H(7')-B(7')	**3655**	**0.041**	**0.55**	**0.057**	**0.0044**	**-0.003**	**0.0013**	**0.94**
C(2)-H(2)…H(12')-B(12')	**3655**	**0.032**	**0.4**	**0.762**	**0.0032**	**-0.0022**	**0.001**	**0.69**
B(3)-H(3)…H(11')-B(11')	**1455**	**0.023**	**0.28**	**0.229**	**0.0022**	**-0.0014**	**0.0007**	**0.44**
B(3)-H(3)…H(17')-C(17')	**3545**	**0.03**	**0.38**	**0.068**	**0.003**	**-0.0020**	**0.001**	**0.63**
B(4)-H(4)…H(10')-B(10')	**1455**	**0.029**	**0.39**	**0.151**	**0.003**	**-0.0020**	**0.001**	**0.63**
B(5)-H(5)…H(10')-B(10')	**2655**	**0.021**	**0.42**	**0.723**	**0.0031**	**-0.0018**	**0.0013**	**0.56**
B(6)-H(6)…H(15')-C(15')	**2565**	**0.029**	**0.39**	**0.143**	**0.003**	**-0.0020**	**0.001**	**0.63**
B(7)-H(7)…H(12')-B(12')	**3655**	**0.041**	**0.44**	**0.079**	**0.0036**	**-0.0027**	**0.0009**	**0.85**
B(8)-H(8)…H(11')-B(11')	**3645**	**0.032**	**0.37**	**0.187**	**0.003**	**-0.0021**	**0.0009**	**0.66**
B(9)-H(9)…H(14')-C(14')	**2555**	**0.036**	**0.45**	**0.076**	**0.0036**	**-0.0025**	**0.0011**	**0.78**
B(9)-H(9)…H(15')-C(15')	**2555**	**0.027**	**0.41**	**0.16**	**0.0031**	**-0.0020**	**0.0011**	**0.63**
B(10)-H(10)…H(10')-B(10')	**2655**	**0.039**	**0.36**	**0.336**	**0.003**	**-0.0023**	**0.0007**	**0.72**
B(12)-H(12)…H(17')-C(17')	**1645**	**0.031**	**0.42**	**0.033**	**0.0033**	**-0.0022**	**0.0011**	**0.69**

a) For symmetry transformations see Table 3.