SUPPLEMENTARY MATERIAL

BONDS OR (3,-1), RINGS OR (3,1) AND CAGES OR (3,3) CRITICAL POINTS:

CP type	Bond (if b.c.p.)		Rho ($e/Å^3$)	Hessian Eigenvalues ($e/Å^5$)			Bond ellipt.	Bond length(Å)
(3,-1)	1 O33	10 C32	1.633	-8.711	-8.280	18.414	0.052	1.400
(3,-1)	1 O33	21 C34	1.775	-9.337	-8.972	16.496	0.041	1.349
(3,-1)	2 O5	14 C5	1.642	-8.614	-8.566	18.302	0.006	1.394
(3,-1)	3 C61	15 C6	1.054	-4.646	-4.632	11.396	0.003	1.591
(3,-1)	4 C3	6 C4	1.231	-5.519	-5.337	11.873	0.034	1.512
(3,-1)	4 C3	8 C31	1.466	-6.922	-6.711	11.516	0.031	1.403
(3,-1)	4 C3	17 C2	1.505	-7.100	-6.740	11.393	0.053	1.391
(3,-1)	5 C8	9 C7	1.304	-6.064	-5.996	11.731	0.011	1.467
(3,-1)	5 C8	18 C9	1.178	-5.381	-5.304	11.708	0.015	1.525
(3,-1)	6 C4	11 C41	1.122	-5.021	-5.009	11.616	0.002	1.555
(3,-1)	6 C4	14 C5	1.219	-5.390	-5.283	11.844	0.020	1.518
(3,-1)	6 C4	18 C9	1.146	-5.091	-5.036	11.689	0.011	1.548
(3,-1)	7 C22	10 C32	1.560	-7.430	-7.207	11.038	0.031	1.364
(3,-1)	7 C22	12 C23	1.172	-5.380	-5.286	11.738	0.018	1.528
(3,-1)	7 C22	13 C21	1.470	-6.954	-6.743	11.456	0.031	1.400
(3,-1)	8 C31	10 C32	1.475	-6.951	-6.564	11.509	0.059	1.403
(3,-1)	8 C31	20 C35	1.288	-5.944	-5.586	11.878	0.064	1.484
(3,-1)	9 C7	15 C6	1.196	-5.382	-5.319	11.777	0.012	1.522
(3,-1)	13 C21	17 C2	1.525	-7.255	-7.079	11.183	0.025	1.377
(3,-1)	14 C5	15 C6	1.123	-4.928	-4.881	11.680	0.010	1.561
(3,-1)	14 C5	16 C1	1.139	-5.030	-4.891	11.664	0.029	1.553
(3,-1)	15 C6	19 C62	1.170	-5.280	-5.276	11.704	0.001	1.531
(3,-1)	16 C1	17 C2	1.286	-5.947	-5.691	11.833	0.045	1.481
(3,-1)	20 C35	21 C34	1.650	-7.931	-7.668	10.246	0.034	1.327
(3,+1)			0.552	-1.911	3.428	3.995		
(3,+1)			0.450	-1.246	2.608	2.764		
(3,+1)			0.318	-0.904	1.754	2.285		
(3,+1)			0.227	-0.500	1.263	1.558		

The CHARACTERISTIC SET of the (sub)molecular graph is:
(nucleus, bonds, rings, cages) = (21, 24, 4, 0)

The topological consistency has been checked:
nucleus - bonds + rings - cages = 1

The Poincare-Hopf relationship is satisfied.

Table 7. Numerical critical point properties of the Fourier map for compound 5.

BONDS OR (3,-1), RINGS OR (3,1) AND CAGES OR (3,3) CRITICAL POINTS:

CP type	Bond (if b.c.p.)		Rho ($e/Å^3$)	Hessian Eigenvalues ($e/Å^5$)			Bond ellipt.	Bond length(Å)
(3,-1)	1 S33	4 C32	1.213	-4.670	-4.495	8.910	0.039	1.670
(3,-1)	1 S33	5 C34	1.156	-4.443	-4.258	9.098	0.044	1.700
(3,-1)	2 O2	15 C2	2.178	-12.162	-11.979	34.639	0.015	1.214
(3,-1)	3 O5	10 C5	1.607	-8.270	-6.655	18.345	0.243	1.432
(3,-1)	3 O5	19 C1	1.526	-7.863	-5.925	18.380	0.327	1.464
(3,-1)	4 C32	9 C31	1.534	-7.288	-7.018	11.129	0.039	1.375
(3,-1)	5 C34	12 C35	1.359	-6.366	-6.146	11.686	0.036	1.446
(3,-1)	6 C4	7 C41	1.176	-5.318	-5.292	11.719	0.005	1.528
(3,-1)	6 C4	8 C3	1.114	-4.892	-4.735	11.614	0.033	1.568
(3,-1)	6 C4	10 C5	1.187	-5.261	-5.112	11.813	0.029	1.533
(3,-1)	6 C4	14 C9	1.192	-5.337	-5.301	11.770	0.007	1.524
(3,-1)	8 C3	9 C31	1.212	-5.513	-5.455	11.841	0.011	1.513
(3,-1)	8 C3	15 C2	1.204	-5.478	-5.240	11.819	0.045	1.520
(3,-1)	9 C31	12 C35	1.448	-6.833	-6.565	11.521	0.041	1.410
(3,-1)	10 C5	16 C6	1.237	-5.564	-5.502	11.876	0.011	1.505
(3,-1)	10 C5	19 C1	1.348	-6.023	-3.162	11.202	0.905	1.492
(3,-1)	11 C61	16 C6	1.117	-4.980	-4.971	11.600	0.002	1.558
(3,-1)	13 C7	16 C6	1.162	-5.193	-5.126	11.723	0.013	1.539
(3,-1)	13 C7	17 C8	1.194	-5.483	-5.411	11.722	0.013	1.517
(3,-1)	14 C9	17 C8	1.191	-5.456	-5.383	11.720	0.014	1.519
(3,-1)	15 C2	19 C1	1.331	-6.181	-5.960	11.821	0.037	1.460
(3,-1)	16 C6	18 C62	1.169	-5.257	-5.252	11.708	0.001	1.532
(3,+1)			1.323	-6.042	4.327	8.090		
(3,+1)			0.455	-1.364	2.498	2.929		
(3,+1)			0.420	-1.105	2.432	2.615		
(3,+1)			0.228	-0.515	1.223	1.624		

The CHARACTERISTIC SET of the (sub)molecular graph is:
(nucleus, bonds, rings, cages) = (19, 22, 4, 0)

The topological consistency has been checked:
nucleus - bonds + rings - cages = 1

The Poincare-Hopf relationship is satisfied.

Table 8. Numerical critical point properties of the Fourier map for compound 6.

BONDS OR (3,-1), RINGS OR (3,1) AND CAGES OR (3,3) CRITICAL POINTS:

CP type	Bond (if b.c.p.)		Rho ($e/Å^3$)	Hessian Eigenvalues ($e/Å^5$)			Bond ellipt.	Bond length(Å)
(3,-1)	1 O10	6 C10	2.193	-12.323	-12.038	35.849	0.024	1.210
(3,-1)	2 O6	12 C5	1.634	-8.645	-8.410	18.050	0.028	1.396
(3,-1)	2 O6	13 C7	1.748	-9.252	-8.840	17.159	0.047	1.359
(3,-1)	3 O7	13 C7	2.281	-13.631	-13.418	46.525	0.016	1.184
(3,-1)	4 N4	6 C10	1.567	-8.022	-7.842	16.439	0.023	1.416
(3,-1)	4 N4	9 C3	1.498	-7.555	-7.348	16.739	0.028	1.445
(3,-1)	4 N4	12 C5	1.416	-7.089	-6.953	16.637	0.020	1.473
(3,-1)	5 C11	6 C10	1.307	-6.051	-5.872	11.932	0.030	1.471
(3,-1)	5 C11	8 C12	1.607	-7.682	-7.475	10.704	0.028	1.345
(3,-1)	5 C11	10 C16	1.468	-6.938	-6.715	11.481	0.033	1.402
(3,-1)	7 C17	12 C5	1.184	-5.297	-5.252	11.797	0.009	1.529
(3,-1)	7 C17	16 C18	1.189	-5.356	-5.334	11.739	0.004	1.523
(3,-1)	7 C17	21 C19	1.180	-5.318	-5.302	11.729	0.003	1.527
(3,-1)	7 C17	22 C20	1.201	-5.437	-5.412	11.754	0.005	1.517
(3,-1)	8 C12	11 C13	1.457	-6.902	-6.733	11.468	0.025	1.404
(3,-1)	9 C3	13 C7	1.276	-5.858	-5.590	11.932	0.048	1.487
(3,-1)	9 C3	14 C1	1.402	-6.258	-4.035	11.257	0.551	1.476
(3,-1)	9 C3	19 C2	1.374	-6.164	-3.618	11.097	0.704	1.491
(3,-1)	10 C16	15 C15	1.474	-7.007	-6.859	11.334	0.022	1.395
(3,-1)	11 C13	17 C14	1.615	-7.749	-7.595	10.531	0.020	1.339
(3,-1)	14 C1	18 C9	1.137	-5.143	-5.058	11.674	0.017	1.548
(3,-1)	14 C1	19 C2	1.455	-6.632	-4.723	11.195	0.404	1.442
(3,-1)	14 C1	20 C8	1.216	-5.579	-5.504	11.790	0.014	1.509
(3,-1)	15 C15	17 C14	1.365	-6.409	-6.241	11.719	0.027	1.442
(3,+1)			1.310	-5.633	4.203	5.832		
(3,+1)			0.487	-1.572	2.976	4.145		
(3,+1)			0.315	-0.895	1.950	2.061		

The CHARACTERISTIC SET of the (sub)molecular graph is:
(nucleus, bonds, rings, cages) = (22, 24, 3, 0)

The topological consistency has been checked:
nucleus - bonds + rings - cages = 1

The Poincare-Hopf relationship is satisfied.

Table 9. Numerical critical point properties of the Fourier map for compound 7.

BONDS OR (3,-1), RINGS OR (3,1) AND CAGES OR (3,3) CRITICAL POINTS:

CP type	Bond (if b.c.p.)		Rho ($e/Å^3$)	Hessian Eigenvalues ($e/Å^5$)			Bond ellipt.	Bond length(Å)
(3,-1)	1 MN1	6 P1	0.468	-1.374	-1.369	6.617	0.003	2.220
(3,-1)	1 MN1	7 P2	0.369	-1.009	-1.003	5.172	0.006	2.359
(3,-1)	1 MN1	28 C1	0.756	-3.459	-3.436	16.207	0.007	1.828
(3,-1)	1 MN1	29 C2	0.731	-3.301	-3.278	15.641	0.007	1.844
(3,-1)	1 MN1	23 N1	0.485	-2.067	-2.007	12.005	0.030	2.045
(3,-1)	1 MN1	24 N2	0.472	-1.983	-1.927	11.581	0.029	2.058
(3,+1)			0.231	-0.599	0.961	2.105		
(3,-1)	2 CL1	9 P4	0.857	-2.386	-2.378	4.856	0.004	1.981
(3,-1)	3 CL2	9 P4	0.829	-2.336	-2.332	5.005	0.001	2.005
(3,-1)	4 CL3	10 P5	0.827	-2.334	-2.331	5.004	0.001	2.006
(3,-1)	5 CL4	10 P5	0.830	-2.339	-2.336	4.986	0.002	2.004
(3,-1)	6 P1	20 O3	1.096	-4.061	-4.047	19.844	0.004	1.599
(3,-1)	6 P1	21 O4	1.117	-4.288	-4.238	21.657	0.012	1.585
(3,-1)	6 P1	22 O5	1.148	-4.582	-4.554	24.233	0.006	1.567
(3,-1)	7 P2	8 P3	0.541	-1.391	-1.381	3.703	0.007	2.256
(3,-1)	7 P2	58 C61	0.782	-2.390	-2.339	4.943	0.022	1.865
(3,-1)	7 P2	64 C71	0.802	-2.442	-2.397	4.829	0.019	1.847
(3,+1)			0.245	-0.561	1.278	1.426		
(3,-1)	8 P3	25 N3	1.097	-3.776	-3.711	15.879	0.017	1.613
(3,-1)	8 P3	27 N5	1.148	-4.222	-4.159	19.585	0.015	1.580
(3,-1)	8 P3	70 C81	0.849	-2.549	-2.486	4.562	0.025	1.806
(3,-1)	9 P4	25 N3	1.216	-4.847	-4.783	24.544	0.013	1.540
(3,-1)	9 P4	26 N4	1.207	-4.754	-4.684	23.832	0.015	1.546
(3,-1)	10 P5	26 N4	1.169	-4.400	-4.326	21.034	0.017	1.568
(3,-1)	10 P5	27 N5	1.213	-4.826	-4.761	24.370	0.014	1.542
(3,-1)	18 O1	28 C1	2.565	-18.504	-18.503	82.801	0.000	1.113
(3,-1)	19 O2	29 C2	2.600	-19.129	-19.128	87.102	0.000	1.106
(3,-1)	20 O3	40 C31	1.594	-8.538	-8.262	18.815	0.033	1.411
(3,-1)	21 O4	46 C41	1.623	-8.663	-8.432	18.479	0.027	1.401
(3,-1)	22 O5	52 C51	1.648	-8.806	-8.545	18.319	0.031	1.392
(3,-1)	23 N1	30 C12	1.661	-8.543	-8.222	15.868	0.039	1.386
(3,+1)			0.333	-0.982	1.998	2.419		
(3,-1)	23 N1	34 C16	1.820	-9.301	-9.112	13.783	0.021	1.327
(3,-1)	24 N2	35 C22	1.766	-9.052	-8.707	14.912	0.040	1.351
(3,+1)			0.341	-1.012	2.161	2.367		
(3,-1)	24 N2	39 C26	1.779	-9.124	-8.918	14.301	0.023	1.342
(3,-1)	30 C12	31 C13	1.515	-7.208	-7.013	11.231	0.028	1.381
(3,-1)	30 C12	35 C22	1.328	-6.173	-5.925	11.899	0.042	1.463
(3,-1)	31 C13	32 C14	1.553	-7.418	-7.249	10.978	0.023	1.364
(3,-1)	32 C14	33 C15	1.556	-7.427	-7.238	10.975	0.026	1.364
(3,-1)	33 C15	34 C16	1.522	-7.260	-7.092	11.136	0.024	1.376
(3,-1)	35 C22	36 C23	1.585	-7.572	-7.360	10.857	0.029	1.354
(3,-1)	36 C23	37 C24	1.573	-7.519	-7.334	10.876	0.025	1.357
(3,-1)	37 C24	38 C25	1.548	-7.387	-7.202	11.019	0.026	1.367
(3,-1)	38 C25	39 C26	1.506	-7.175	-7.010	11.212	0.024	1.382
(3,-1)	40 C31	41 C32	1.571	-7.497	-7.255	10.955	0.033	1.360
(3,+1)			0.345	-0.997	2.080	2.285		
(3,-1)	40 C31	45 C36	1.597	-7.633	-7.410	10.791	0.030	1.349
(3,-1)	41 C32	42 C33	1.554	-7.416	-7.235	10.990	0.025	1.365
(3,-1)	42 C33	43 C34	1.549	-7.398	-7.221	10.988	0.024	1.366
(3,-1)	43 C34	44 C35	1.425	-6.724	-6.535	11.579	0.029	1.418
(3,-1)	44 C35	45 C36	1.615	-7.744	-7.567	10.572	0.023	1.340
(3,-1)	46 C41	47 C42	1.527	-7.266	-7.056	11.176	0.030	1.376
(3,+1)			0.330	-0.945	2.044	2.143		
(3,-1)	46 C41	51 C46	1.492	-7.081	-6.871	11.351	0.030	1.391
(3,-1)	47 C42	48 C43	1.533	-7.309	-7.132	11.100	0.025	1.373
(3,-1)	48 C43	49 C44	1.574	-7.528	-7.361	10.844	0.023	1.356
(3,-1)	49 C44	50 C45	1.479	-7.020	-6.845	11.365	0.026	1.395
(3,-1)	50 C45	51 C46	1.537	-7.332	-7.163	11.056	0.024	1.371
(3,-1)	52 C51	53 C52	1.531	-7.287	-7.066	11.172	0.031	1.375
(3,+1)			0.331	-0.946	1.997	2.199		
(3,-1)	52 C51	57 C56	1.560	-7.445	-7.243	10.995	0.028	1.363
(3,-1)	53 C52	54 C53	1.545	-7.379	-7.208	11.000	0.024	1.367

(3,-1)	54 C53	55 C54	1.382	-6.497	-6.325	11.688	0.027	1.435
(3,-1)	55 C54	56 C55	1.587	-7.601	-7.438	10.742	0.022	1.351
(3,-1)	56 C55	57 C56	1.546	-7.376	-7.190	11.040	0.026	1.368
(3,-1)	58 C61	59 C62	1.662	-7.971	-7.773	10.255	0.026	1.324
(3,+1)			0.343	-0.989	2.073	2.266		
(3,-1)	58 C61	63 C66	1.435	-6.754	-6.531	11.600	0.034	1.416
(3,-1)	59 C62	60 C63	1.451	-6.856	-6.654	11.530	0.030	1.408
(3,-1)	60 C63	61 C64	1.716	-8.266	-8.092	9.730	0.022	1.302
(3,-1)	61 C64	62 C65	1.488	-7.065	-6.879	11.355	0.027	1.392
(3,-1)	62 C65	63 C66	1.564	-7.475	-7.300	10.894	0.024	1.360
(3,-1)	64 C71	65 C72	1.557	-7.420	-7.218	11.005	0.028	1.365
(3,+1)			0.329	-0.942	1.976	2.199		
(3,-1)	64 C71	69 C76	1.478	-6.997	-6.788	11.409	0.031	1.397
(3,-1)	65 C72	66 C73	1.526	-7.276	-7.109	11.120	0.024	1.375
(3,-1)	66 C73	67 C74	1.468	-6.960	-6.778	11.419	0.027	1.399
(3,-1)	67 C74	68 C75	1.625	-7.797	-7.634	10.483	0.021	1.336
(3,-1)	68 C75	69 C76	1.481	-7.033	-6.862	11.353	0.025	1.394
(3,-1)	70 C81	71 C82	1.552	-7.384	-7.169	11.051	0.030	1.368
(3,+1)			0.329	-0.942	1.987	2.189		
(3,-1)	70 C81	75 C86	1.519	-7.210	-7.002	11.230	0.030	1.381
(3,-1)	71 C82	72 C83	1.481	-7.031	-6.854	11.357	0.026	1.394
(3,-1)	72 C83	73 C84	1.573	-7.525	-7.362	10.843	0.022	1.356
(3,-1)	73 C84	74 C85	1.513	-7.203	-7.028	11.200	0.025	1.381
(3,-1)	74 C85	75 C86	1.500	-7.133	-6.961	11.257	0.025	1.386
(3,-1)	11 P6	12 F1	1.072	-3.667	-3.539	18.689	0.036	1.606
(3,-1)	11 P6	13 F2	1.310	-5.849	-5.616	35.448	0.042	1.498
(3,-1)	11 P6	14 F3	1.221	-4.929	-4.777	28.266	0.032	1.538
(3,-1)	11 P6	15 F4	1.185	-4.680	-4.511	25.739	0.037	1.555
(3,-1)	11 P6	16 F5	1.357	-6.507	-6.091	39.732	0.068	1.477
(3,-1)	11 P6	17 F6	1.562	-8.902	-8.751	57.659	0.017	1.404

The CHARACTERISTIC SET of the (sub)molecular graphs is:

(nucleus, bonds, rings, cages) = (68, 77, 10, 0) (sub)molecular graph no. 1

(nucleus, bonds, rings, cages) = (7, 6, 0, 0) (sub)molecular graph no. 2

The topological consistency has been checked. The Poincare-Hopf relationship is satisfied.

Table 10. Numerical critical point properties of the Fourier map for compound 8.