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Isomer specific intercalation chemistry: potassium insertion into the D_2 and D_{2d} isomers of C_{84}

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Supplementary Material: Fractional coordinates for the D_2 and D_{2d} isomers of C_{84} with mirror plane normals (D_{2d}) and C_2 axes (D_2) oriented along the <1 0 0> and <1 1 0> directions, as described in the text. The coordinates are for carbon atoms in the asymmetric unit of an $Fm\bar{3}m$ unit cell with a = 16.54Å.

C_{84} -D_{2d} <1 1 0> Orientation

	x	y	z
C1	0.20129	0.85785	0.09029
C2	0.13356	0.93018	0.20658
C3	0.19846	0.92430	0.15001
C4	0.02945	0.02945	0.25808
C5	0.19811	0.13498	0.06143
C6	0.25754	0.02812	0.96955
C7	0.23226	0.11154	0.98524
C8	0.11207	0.01036	0.23212
C9	0.14392	0.08080	0.19235
C10	0.20052	0.07451	0.12788
C11	0.23223	0.99507	0.11218

C_{84} - D_2 <1 1 0> Orientation

	x	y	z
C1	-0.27204	0.60824	0.99245
C2	-0.30180	0.62565	0.07243
C3	-0.26369	0.38407	0.00774
C4	-0.24116	0.46775	0.02897
C5	-0.29922	0.34792	0.07834
C6	-0.30252	0.56054	0.13424
C7	-0.26755	0.48441	0.11189
C8	-0.29799	0.40898	0.14359
C9	-0.36531	0.56106	0.19786
C10	0.02812	0.96952	0.25788
C11	-0.35757	0.40943	0.20225
C12	-0.38843	0.48516	0.23265
C13	-0.02759	0.74341	0.02871
C14	-0.14174	0.81013	0.07843
C15	0.13559	0.79116	0.07215
C16	-0.00961	0.76817	0.11195
C17	-0.08015	0.80840	0.14295
C18	0.07057	0.79281	0.13471
C19	-0.07427	0.87243	0.20021
C20	0.07599	0.84968	0.19935
C21	0.00496	0.88783	0.23255

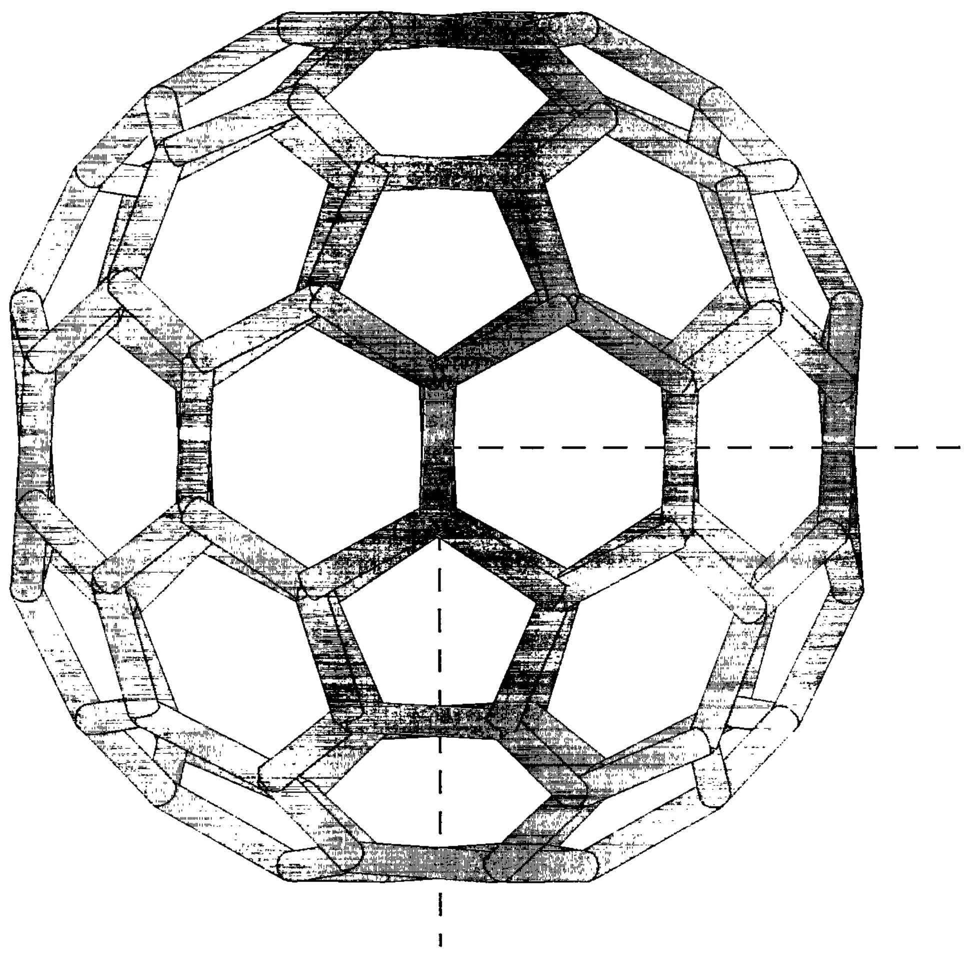
C_{84} - D_{2d} <1 0 0> Orientation

	x	y	z
C1	0.04182	0.75717	0.09029
C2	0.04507	0.85620	0.20658
C3	0.08679	0.80615	0.15000
C4	0.04165	0.00000	0.25807
C5	0.23552	0.95536	0.06142
C6	0.20198	0.83778	0.96955
C7	0.24309	0.91465	0.98525
C8	0.08657	0.92809	0.23211
C9	0.15890	0.95537	0.19234
C10	0.19447	0.91090	0.12787
C11	0.16072	0.83231	0.11218

C_{84} - D_2 <1 0 0> Orientation

	x	y	z
C1	0.26228	0.91535	0.50755
C2	0.41488	0.25093	0.99226
C3	0.53667	0.33525	0.20225
C4	0.49834	0.95856	0.75788
C5	0.56840	0.41061	0.23265
C6	0.57848	0.29280	0.14359
C7	0.53444	0.25049	0.07833
C8	0.65334	0.32462	0.11189
C9	0.63841	0.44793	0.19786
C10	0.68244	0.40317	0.13424
C11	0.66022	0.29417	0.02897
C12	0.72899	0.44870	0.07243
C13	0.42419	0.91717	0.73254
C14	0.44744	0.83998	0.69934
C15	0.35728	0.96230	0.70020
C16	0.30785	0.92119	0.64295
C17	0.40339	0.30359	0.13471
C18	0.32928	0.84286	0.61195
C19	0.44820	0.25645	0.07215
C20	0.26552	0.96597	0.57843
C21	0.29906	0.33807	0.02871

Figure 1·iii



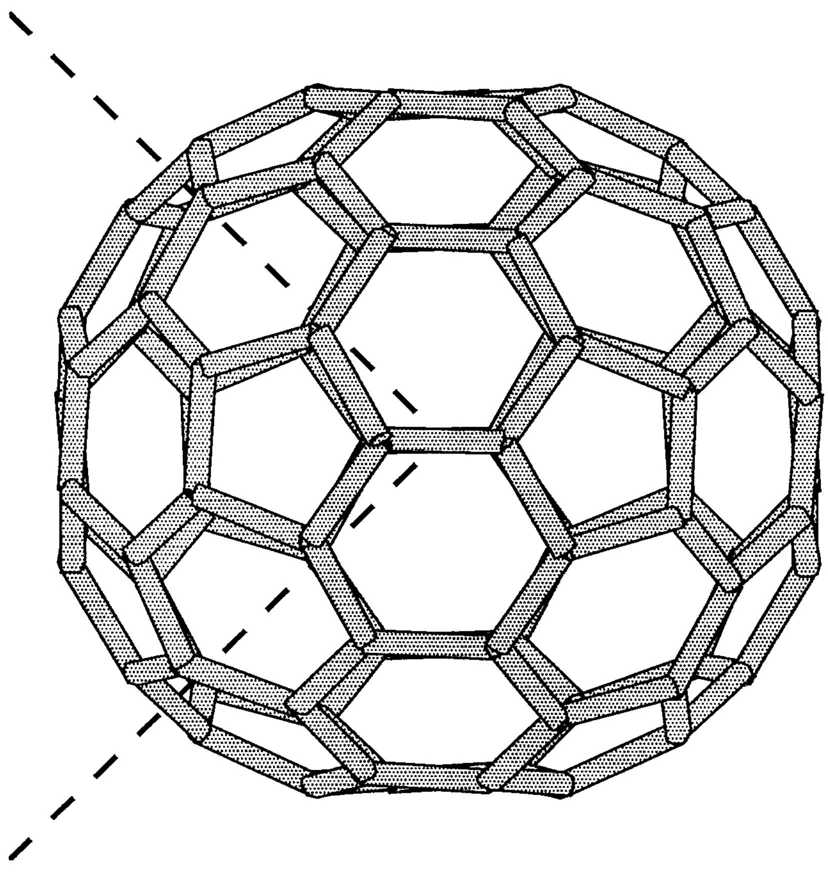
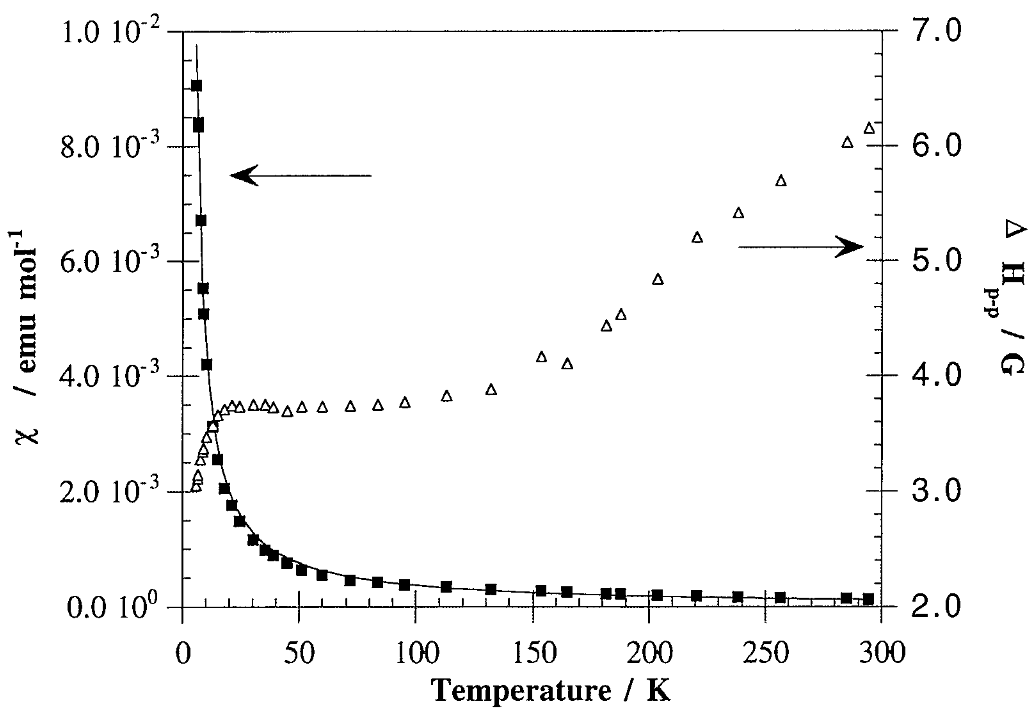


Figure 5



1.0 10^-2
8.0 10^-3
6.0 10^-3
4.0 10^-3
2.0 10^-3
0.0 10^0
χ / emu mol^-1
0
50
100
150
200
250
300
Temperature / K
7.0
6.0
5.0
4.0
3.0
2.0
Δ H_p-p / G

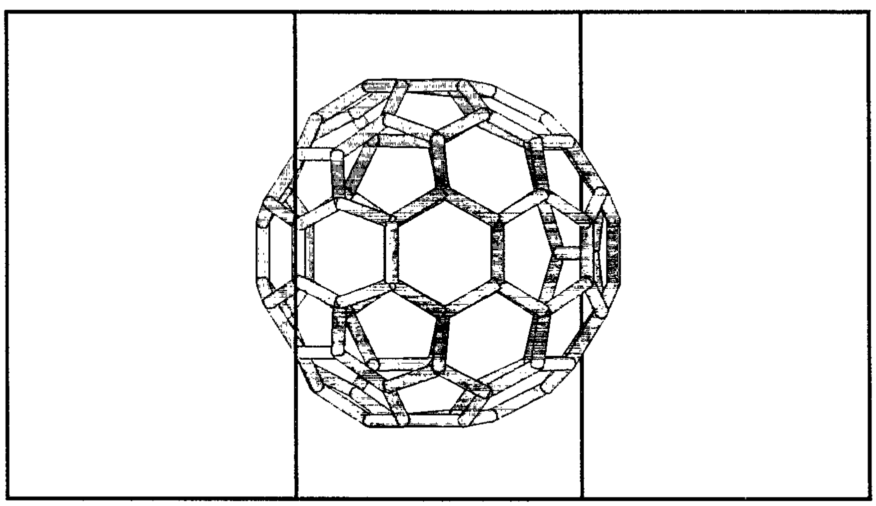


Figure 7 iv