JP0036036

Supporting information of the manuscript

T. Heine, F. Zerbetto, G. Seifert and P.W. Fowler,

SUPPLEMENTARY MATERIAL

On the isomers of C70 dimer.

Structures in XYZ format

AB TRANS:

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 140
 AB TRANS
 C   -1.56324971101303167309   1.26338226479177118122   2.18817176533340607136
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AB CIS

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C	-3.23069431345802460243	.68564647459586935963	-3.63261064480717310587
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C	-5.67251764395187318968	.70916712870937281821	-3.97067493009208938304
C	-6.85988207786837911328	1.15390862972604746339	-3.27483194555367784773
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C	-8.22930625390459624668	-.01968410198774131481	-1.59912402975483125545
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C	-7.44521576141778673730	-2.30466180298316514197	-1.15841869967292954158
C	-6.61645888690018679767	-3.01924639718872622751	-.21453381471694929483
C	-5.44221185588219480422	-3.45596925583671721327	-.90567829771337626799
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C	-2.99978112775722971506	-3.07687732743811892533	-.95068565366121104976
C	-3.12867126605906875625	-2.57726266340464871263	-2.26380992275875003727
C	-4.40172193580003057178	-2.58580836044680806296	-2.94929726708962203219
C	-4.46398466846391617224	-1.42970144833937706785	-3.81046399079156516976
C	-5.66951113041091669942	-.73781555360764172757	-3.97070195966913397356
C	-6.85501708698188849667	-1.18751337948460400362	-3.27487566289030906930
C	-6.78963092160333570035	-2.31195990603518275464	-2.44519272350826577522
C	-5.54157057993857371514	-3.01873060626571243503	-2.27910924211238663517

Calculated NMR chemical shifts (left: shift with respect to TMS in ppm, right intensity in atoms per shift).

AB TRANS:

141.600	4
147.554	4
146.246	4
139.619	4
141.349	4
153.935	4
67.766	2
67.527	2
144.451	4
155.805	4
147.567	4
147.349	4
140.535	4
134.533	4
134.635	4
141.518	4
142.953	4
133.941	4
134.795	4
146.266	4
149.644	4
139.911	4
134.226	4
138.759	4
140.338	4
149.061	4
147.106	4
146.065	4
149.420	4
147.255	4
144.468	4
146.939	4
147.230	4
150.570	4

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   151.375     4
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   146.188     2
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AB CIS
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   147.355     4
   146.374     4
   139.920     4
   141.252     4
   153.946     4
    67.493     2
    67.532     2
   144.448     4
   155.773     4
   147.535     4
   147.519     4
   140.935     4
   134.606     4
   134.726     4
   141.589     4
   142.781     4
   133.952     4
   134.777     4
   146.476     4
   149.612     4
   140.055     4
   134.256     4
   138.790     4
   140.127     4
   148.876     4
   147.205     4
   146.242     4
   149.469     4
   147.071     4
   144.116     4
   146.927     4
   147.210     4
   150.610     4
   151.437     4
   151.360     2
   146.193     2
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   146.635     1
   154.029     1
   141.933     1
   141.514     1
   144.608     1
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   144.061     1
   141.268     1
   141.679     1
   140.709     1
   133.793     1
   135.573     1
   144.182     1
   144.219     1
   135.226     1
   133.972     1
   140.426     1
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148.130	1
155.790	1
155.712	1
147.425	1
147.490	1
147.355	1
146.515	1
135.061	1
141.440	1
142.253	1
148.854	1
147.210	1
146.546	1
147.282	1
148.893	1
142.037	1
142.219	1
133.918	1
136.377	1
141.160	1
140.387	1
149.319	1
148.874	1
139.178	1
140.804	1
134.365	1
140.173	1
148.769	1
147.388	1
146.228	1
151.398	1
151.400	1
151.474	1
146.371	1
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149.224	1
140.868	1
139.738	1
132.947	1
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139.498	1
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148.014	1
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    147.629     1
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    146.677     1
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    149.701     1
    145.669     1
    147.092     1
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C1:
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    141.252     4
    145.916     4
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141.421	4
134.085	4
134.598	4
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131.994	4
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146.910	4
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144.541	2

C2:

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144.735	4
142.180	4

149.242	4
147.137	4
151.403	4
149.566	4
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144.080	2
