

Supplementary Materials

The magnetic response of starphenes

Mesías Orozco-Ic ^{1,2,*} and Gabriel Merino ^{2,*}

¹ Department of Chemistry, Faculty of Science, University of Helsinki, P.O. Box 55, A. I. Virtasen aukio 1, FIN-00014 Helsinki, Finland
² Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados, Unidad Mérida. Km 6 Antigua Carretera a Progreso. Apdo. Postal 73, Cordemex, 97310, Mérida, Yuc., Mexico
* Correspondence: mesiasor@ad.helsinki.fi (M.O.-I.); gmerino@cinvestav.mx (G.M.)
Dedicated to Professor Riccardo Zanasi on the Occasion of His 70th Birthday

Optimized Cartesian coordinates at CAM-B3LYP-D3(BJ)/def2-TZVP level.

Benzene

C	0.000000000	1.393159000	0.000000000
C	1.206511000	0.696580000	0.000000000
C	-1.206511000	0.696580000	0.000000000
C	-1.206511000	-0.696580000	0.000000000
C	0.000000000	-1.393159000	0.000000000
C	1.206511000	-0.696580000	0.000000000
H	0.000000000	2.485233000	0.000000000
H	2.152275000	1.242617000	0.000000000
H	2.152275000	-1.242617000	0.000000000
H	0.000000000	-2.485233000	0.000000000
H	-2.152275000	-1.242617000	0.000000000
H	-2.152275000	1.242617000	0.000000000

[4]starphene

C	0.699011000	3.692065000	0.000000000
C	-0.699011000	3.692065000	0.000000000
C	1.380547000	2.492397000	0.000000000
C	0.706097000	1.255009000	0.000000000
C	-0.706097000	1.255009000	0.000000000
C	1.439918000	-0.016006000	0.000000000
C	0.733821000	-1.239003000	0.000000000
C	-0.733821000	-1.239003000	0.000000000
C	-1.439918000	-0.016006000	0.000000000
C	-1.380547000	2.492397000	0.000000000
C	-1.468206000	-2.441787000	0.000000000
C	-2.848753000	-0.050610000	0.000000000
C	-3.546928000	-1.240671000	0.000000000
C	-2.847916000	-2.451394000	0.000000000
C	2.848753000	-0.050610000	0.000000000
C	3.546928000	-1.240671000	0.000000000
C	2.847916000	-2.451394000	0.000000000
C	1.468206000	-2.441787000	0.000000000
H	2.468443000	2.517165000	0.000000000
H	-2.468443000	2.517165000	0.000000000

H	-0.945708000	-3.396317000	0.000000000
H	-3.414151000	0.879152000	0.000000000
H	3.414151000	0.879152000	0.000000000
H	0.945708000	-3.396317000	0.000000000
H	4.638622000	-1.231872000	0.000000000
H	3.386143000	-3.401228000	0.000000000
H	-4.638622000	-1.231872000	0.000000000
H	-3.386143000	-3.401228000	0.000000000
H	-1.252479000	4.633100000	0.000000000
H	1.252479000	4.633100000	0.000000000

[7]starphene

C	0.710434000	3.718454000	0.000000000
C	-0.710434000	3.718454000	0.000000000
C	1.381146000	2.480064000	0.000000000
C	0.716523000	1.267235000	0.000000000
C	-0.716523000	1.267235000	0.000000000
C	1.455719000	-0.013091000	0.000000000
C	0.739196000	-1.254144000	0.000000000
C	-0.739196000	-1.254144000	0.000000000
C	-1.455719000	-0.013091000	0.000000000
C	-1.381146000	2.480064000	0.000000000
C	-1.457226000	-2.436140000	0.000000000
C	-2.838372000	-0.043925000	0.000000000
C	-3.575493000	-1.243974000	0.000000000
C	-2.865059000	-2.474481000	0.000000000
C	2.838372000	-0.043925000	0.000000000
C	3.575493000	-1.243974000	0.000000000
C	2.865059000	-2.474481000	0.000000000
C	1.457226000	-2.436140000	0.000000000
H	2.469531000	2.510752000	0.000000000
H	-2.469531000	2.510752000	0.000000000
H	-0.939610000	-3.394053000	0.000000000
H	-3.409141000	0.883301000	0.000000000
H	3.409141000	0.883301000	0.000000000
H	0.939610000	-3.394053000	0.000000000
C	3.596727000	-3.694766000	0.000000000
C	4.998124000	-1.267474000	0.000000000
C	-4.998124000	-1.267474000	0.000000000
C	-3.596727000	-3.694766000	0.000000000
C	5.675541000	-2.457374000	0.000000000
C	4.965919000	-3.686475000	0.000000000
H	5.540125000	-0.318885000	0.000000000
H	3.046225000	-4.638447000	0.000000000
C	-4.965919000	-3.686475000	0.000000000
C	-5.675541000	-2.457374000	0.000000000
H	-3.046225000	-4.638447000	0.000000000
H	-5.540125000	-0.318885000	0.000000000
C	-1.401398000	4.962240000	0.000000000

C	1.401398000	4.962240000	0.000000000
C	0.709622000	6.143849000	0.000000000
C	-0.709622000	6.143849000	0.000000000
H	-2.493900000	4.957332000	0.000000000
H	2.493900000	4.957332000	0.000000000
H	5.519472000	-4.627653000	0.000000000
H	6.767401000	-2.466176000	0.000000000
H	1.247929000	7.093829000	0.000000000
H	-1.247929000	7.093829000	0.000000000
H	-6.767401000	-2.466176000	0.000000000
H	-5.519472000	-4.627653000	0.000000000

[10]starphene

C	0.715284000	3.728862000	0.000000000
C	-0.715284000	3.728862000	0.000000000
C	1.384056000	2.476585000	0.000000000
C	0.722712000	1.272059000	0.000000000
C	-0.722712000	1.272059000	0.000000000
C	1.462991000	-0.010142000	0.000000000
C	0.740279000	-1.261917000	0.000000000
C	-0.740279000	-1.261917000	0.000000000
C	-1.462991000	-0.010142000	0.000000000
C	-1.384056000	2.476585000	0.000000000
C	-1.452758000	-2.436920000	0.000000000
C	-2.836814000	-0.039665000	0.000000000
C	-3.586931000	-1.244977000	0.000000000
C	-2.871647000	-2.483885000	0.000000000
C	2.836814000	-0.039665000	0.000000000
C	3.586931000	-1.244977000	0.000000000
C	2.871647000	-2.483885000	0.000000000
C	1.452758000	-2.436920000	0.000000000
H	2.472255000	2.508332000	0.000000000
H	-2.472255000	2.508332000	0.000000000
H	-0.936152000	-3.395201000	0.000000000
H	-3.408406000	0.886870000	0.000000000
H	3.408406000	0.886870000	0.000000000
H	0.936152000	-3.395201000	0.000000000
C	3.584872000	-3.687066000	0.000000000
C	4.985529000	-1.261058000	0.000000000
C	-4.985529000	-1.261058000	0.000000000
C	-3.584872000	-3.687066000	0.000000000
C	5.699225000	-2.459962000	0.000000000
C	4.980002000	-3.705693000	0.000000000
C	7.130631000	-2.495089000	0.000000000
C	5.726126000	-4.927763000	0.000000000
C	7.088914000	-4.917018000	0.000000000
C	7.802720000	-3.680670000	0.000000000
H	5.531397000	-0.314196000	0.000000000
H	3.037800000	-4.633232000	0.000000000
H	5.176868000	-5.872039000	0.000000000

H	7.673769000	-1.547280000	0.000000000
C	-4.980002000	-3.705693000	0.000000000
C	-5.699225000	-2.459962000	0.000000000
C	-7.130631000	-2.495089000	0.000000000
C	-7.802720000	-3.680670000	0.000000000
H	-3.037800000	-4.633232000	0.000000000
H	-5.531397000	-0.314196000	0.000000000
H	-7.673769000	-1.547280000	0.000000000
C	-1.400657000	4.948123000	0.000000000
C	1.400657000	4.948123000	0.000000000
C	0.719223000	6.165655000	0.000000000
C	-0.719223000	6.165655000	0.000000000
C	1.404505000	7.422852000	0.000000000
C	-1.404505000	7.422852000	0.000000000
C	0.713806000	8.597689000	0.000000000
C	-0.713806000	8.597689000	0.000000000
H	-2.493597000	4.947428000	0.000000000
H	2.493597000	4.947428000	0.000000000
H	-2.496901000	7.419319000	0.000000000
H	2.496901000	7.419319000	0.000000000
C	-5.726126000	-4.927763000	0.000000000
C	-7.088914000	-4.917018000	0.000000000
H	-5.176868000	-5.872039000	0.000000000
H	-7.644916000	-5.856761000	0.000000000
H	-8.894562000	-3.692310000	0.000000000
H	7.644916000	-5.856761000	0.000000000
H	8.894562000	-3.692310000	0.000000000
H	1.249646000	9.549072000	0.000000000
H	-1.249646000	9.549072000	0.000000000

[13]starphene

C	0.718943000	3.734254000	0.000000000
C	-0.718943000	3.734254000	0.000000000
C	1.385825000	2.474918000	0.000000000
C	0.726104000	1.274217000	0.000000000
C	-0.726104000	1.274217000	0.000000000
C	1.466556000	-0.008284000	0.000000000
C	0.740452000	-1.265933000	0.000000000
C	-0.740452000	-1.265933000	0.000000000
C	-1.466556000	-0.008284000	0.000000000
C	-1.385825000	2.474918000	0.000000000
C	-1.450430000	-2.437618000	0.000000000
C	-2.836254000	-0.037300000	0.000000000
C	-3.593430000	-1.244505000	0.000000000
C	-2.874488000	-2.489750000	0.000000000
C	2.836254000	-0.037300000	0.000000000
C	3.593430000	-1.244505000	0.000000000
C	2.874488000	-2.489750000	0.000000000
C	1.450430000	-2.437618000	0.000000000
H	2.474050000	2.506626000	0.000000000

H	-2.474050000	2.506626000	0.000000000
H	-0.933777000	-3.395903000	0.000000000
H	-3.407827000	0.889277000	0.000000000
H	3.407827000	0.889277000	0.000000000
H	0.933777000	-3.395903000	0.000000000
C	3.578045000	-3.686352000	0.000000000
C	4.981497000	-1.255502000	0.000000000
C	-4.981497000	-1.255502000	0.000000000
C	-3.578045000	-3.686352000	0.000000000
C	5.707751000	-2.461639000	0.000000000
C	4.985718000	-3.712238000	0.000000000
C	7.116271000	-2.489863000	0.000000000
C	5.714420000	-4.917940000	0.000000000
C	7.101019000	-4.933676000	0.000000000
C	7.823198000	-3.682825000	0.000000000
C	9.258958000	-3.721162000	0.000000000
C	7.852100000	-6.157912000	0.000000000
C	9.927800000	-4.905059000	0.000000000
C	9.211805000	-6.145198000	0.000000000
H	5.527227000	-0.308663000	0.000000000
H	3.030924000	-4.632387000	0.000000000
H	5.168925000	-5.864930000	0.000000000
H	7.663641000	-1.543956000	0.000000000
H	9.802958000	-2.773886000	0.000000000
H	7.303735000	-7.102668000	0.000000000
C	-4.985718000	-3.712238000	0.000000000
C	-5.707751000	-2.461639000	0.000000000
C	-7.116271000	-2.489863000	0.000000000
C	-7.823198000	-3.682825000	0.000000000
H	-3.030924000	-4.632387000	0.000000000
H	-5.527227000	-0.308663000	0.000000000
H	-7.663641000	-1.543956000	0.000000000
C	-1.403452000	4.941854000	0.000000000
C	1.403452000	4.941854000	0.000000000
C	0.722034000	6.173877000	0.000000000
C	-0.722034000	6.173877000	0.000000000
C	1.401851000	7.407803000	0.000000000
C	-1.401851000	7.407803000	0.000000000
C	0.722179000	8.616501000	0.000000000
C	-0.722179000	8.616501000	0.000000000
C	-1.406858000	9.879074000	0.000000000
H	-2.496303000	4.941051000	0.000000000
H	2.496303000	4.941051000	0.000000000
H	-2.494716000	7.408886000	0.000000000
H	2.494716000	7.408886000	0.000000000
H	-2.499223000	9.876554000	0.000000000
C	1.406858000	9.879074000	0.000000000
C	-0.715995000	11.050256000	0.000000000
C	0.715995000	11.050256000	0.000000000
H	2.499223000	9.876554000	0.000000000
C	-5.714420000	-4.917940000	0.000000000

C	-7.101019000	-4.933676000	0.000000000
C	-7.852100000	-6.157912000	0.000000000
C	-9.258958000	-3.721162000	0.000000000
C	-9.211805000	-6.145198000	0.000000000
C	-9.927800000	-4.905059000	0.000000000
H	-5.168925000	-5.864930000	0.000000000
H	-7.303735000	-7.102668000	0.000000000
H	-9.802958000	-2.773886000	0.000000000
H	-11.019753000	-4.917965000	0.000000000
H	-9.768960000	-7.084404000	0.000000000
H	-1.250794000	12.002369000	0.000000000
H	1.250794000	12.002369000	0.000000000
H	11.019753000	-4.917965000	0.000000000
H	9.768960000	-7.084404000	0.000000000

[16]starphene

C	0.720940000	3.736597000	0.000000000
C	-0.720940000	3.736597000	0.000000000
C	1.386868000	2.474275000	0.000000000
C	0.727742000	1.275082000	0.000000000
C	-0.727742000	1.275082000	0.000000000
C	1.468124000	-0.007298000	0.000000000
C	0.740383000	-1.267784000	0.000000000
C	-0.740383000	-1.267784000	0.000000000
C	-1.468124000	-0.007298000	0.000000000
C	-1.386868000	2.474275000	0.000000000
C	-1.449351000	-2.438201000	0.000000000
C	-2.836219000	-0.036075000	0.000000000
C	-3.596458000	-1.243947000	0.000000000
C	-2.875518000	-2.492651000	0.000000000
C	2.836219000	-0.036075000	0.000000000
C	3.596458000	-1.243947000	0.000000000
C	2.875518000	-2.492651000	0.000000000
C	1.449351000	-2.438201000	0.000000000
H	2.475067000	2.505789000	0.000000000
H	-2.475067000	2.505789000	0.000000000
H	-0.932543000	-3.396366000	0.000000000
H	-3.407611000	0.890577000	0.000000000
H	3.407611000	0.890577000	0.000000000
H	0.932543000	-3.396366000	0.000000000
C	3.574574000	-3.686459000	0.000000000
C	4.979854000	-1.252443000	0.000000000
C	-4.979854000	-1.252443000	0.000000000
C	-3.574574000	-3.686459000	0.000000000
C	5.712824000	-2.461550000	0.000000000
C	4.988176000	-3.716676000	0.000000000
C	7.111593000	-2.484801000	0.000000000
C	5.707697000	-4.916420000	0.000000000
C	7.105642000	-4.938384000	0.000000000
C	7.829587000	-3.684474000	0.000000000

C	9.244502000	-3.716381000	0.000000000
C	7.840731000	-6.147783000	0.000000000
C	9.946770000	-4.906169000	0.000000000
C	9.222252000	-6.161071000	0.000000000
C	11.385091000	-4.947051000	0.000000000
C	9.976817000	-7.386252000	0.000000000
C	11.334594000	-7.372853000	0.000000000
C	12.052375000	-6.129620000	0.000000000
H	5.524697000	-0.305143000	0.000000000
H	3.026610000	-4.631956000	0.000000000
H	5.161635000	-5.862925000	0.000000000
H	7.658259000	-1.538645000	0.000000000
H	9.791552000	-2.770319000	0.000000000
H	7.294943000	-7.094573000	0.000000000
H	11.929311000	-3.999835000	0.000000000
H	9.428615000	-8.331169000	0.000000000
C	-4.988176000	-3.716676000	0.000000000
C	-5.712824000	-2.461550000	0.000000000
C	-7.111593000	-2.484801000	0.000000000
C	-7.829587000	-3.684474000	0.000000000
H	-3.026610000	-4.631956000	0.000000000
H	-5.524697000	-0.305143000	0.000000000
H	-7.658259000	-1.538645000	0.000000000
C	-1.405280000	4.938902000	0.000000000
C	1.405280000	4.938902000	0.000000000
C	0.724648000	6.178226000	0.000000000
C	-0.724648000	6.178226000	0.000000000
C	1.403896000	7.401221000	0.000000000
C	-1.403896000	7.401221000	0.000000000
C	0.723945000	8.622858000	0.000000000
C	-0.723945000	8.622858000	0.000000000
C	-1.403771000	9.864164000	0.000000000
H	-2.498087000	4.937100000	0.000000000
H	2.498087000	4.937100000	0.000000000
H	-2.496624000	7.401570000	0.000000000
H	2.496624000	7.401570000	0.000000000
H	-2.496609000	9.864892000	0.000000000
C	1.403771000	9.864164000	0.000000000
C	-0.724518000	11.067240000	0.000000000
C	0.724518000	11.067240000	0.000000000
H	2.496609000	9.864892000	0.000000000
C	1.408274000	12.333303000	0.000000000
C	-1.408274000	12.333303000	0.000000000
C	0.717781000	13.502473000	0.000000000
C	-0.717781000	13.502473000	0.000000000
H	2.500697000	12.331004000	0.000000000
H	1.251223000	14.455211000	0.000000000
H	-1.251223000	14.455211000	0.000000000
H	-2.500697000	12.331004000	0.000000000
C	-5.707697000	-4.916420000	0.000000000
C	-7.105642000	-4.938384000	0.000000000

C	-7.840731000	-6.147783000	0.000000000
C	-9.244502000	-3.716381000	0.000000000
C	-9.222252000	-6.161071000	0.000000000
C	-9.946770000	-4.906169000	0.000000000
C	-11.385091000	-4.947051000	0.000000000
C	-9.976817000	-7.386252000	0.000000000
C	-11.334594000	-7.372853000	0.000000000
C	-12.052375000	-6.129620000	0.000000000
H	-5.161635000	-5.862925000	0.000000000
H	-7.294943000	-7.094573000	0.000000000
H	-9.791552000	-2.770319000	0.000000000
H	-11.929311000	-3.999835000	0.000000000
H	-9.428615000	-8.331169000	0.000000000
H	-11.892969000	-8.311197000	0.000000000
H	-13.144192000	-6.144015000	0.000000000
H	13.144192000	-6.144015000	0.000000000
H	11.892969000	-8.311197000	0.000000000