Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Application of MCD Spectroscopy and TD-DFT to Endohedral Metallofullerenes for Characterization of Their Electronic Transitions

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Atomic coordinate data of La@C_{2v}-C_{82}

Energy: -2234172.7141493 Hartree

La	0.00000	0.00000	1.66951
C	0.00000	3.08693	2.62571
C	-2.68094	0.00000	2.98829
C	-3.11636	1.16709	2.24325
C	-2.35959	2.37386	2.26375
C	-1.16169	2.37787	3.07034
C	-0.73732	1.23439	3.85014
C	-1.50665	0.00000	3.81102
C	-3.76859	0.71874	1.05014
C	-2.38716	3.18432	1.10510
C	0.00000	3.86728	1.41580
C	-3.69410	1.46497	-0.16404
C	-1.21718	3.94132	0.68565
C	-1.21285	4.01326	-0.74278
C	-2.39618	3.32213	-1.20180
C	0.00000	3.96271	-1.49180
C	-3.08651	2.75197	-0.07652
C	-2.40233	2.66066	-2.41112
C	0.00000	3.25887	-2.78208
C	-1.20557	2.64790	-3.23561
C	-3.66630	0.73392	-1.43435
C	-3.09104	1.40398	-2.55127
C	-1.20287	1.42385	-3.96997
C	0.00000	0.73716	-4.28728

C	-2.39712	0.68608	-3.58583
C	0.00000	-3.08693	2.62571
C	2.68094	0.00000	2.98829
C	-3.11636	-1.16709	2.24325
C	3.11636	1.16709	2.24325
C	3.11636	-1.16709	2.24325
C	-2.35959	-2.37386	2.26375
C	2.35959	2.37386	2.26375
C	2.35959	-2.37386	2.26375
C	-1.16169	-2.37787	3.07034
C	1.16169	2.37787	3.07034
C	1.16169	-2.37787	3.07034
C	-0.73732	-1.23439	3.85014
C	0.73732	1.23439	3.85014
C	0.73732	-1.23439	3.85014
C	1.50665	0.00000	3.81102
C	-3.76859	-0.71874	1.05014
C	3.76859	0.71874	1.05014
C	3.76859	-0.71874	1.05014
C	-2.38716	-3.18432	1.10510
C	2.38716	3.18432	1.10510
C	2.38716	-3.18432	1.10510
C	0.00000	-3.86728	1.41580
C	-3.69410	-1.46497	-0.16404
C	3.69410	1.46497	-0.16404
C	3.69410	-1.46497	-0.16404
C	-1.21718	-3.94132	0.68565
C	1.21718	3.94132	0.68565
C	1.21718	-3.94132	0.68565
C	-1.21285	-4.01326	-0.74278
C	1.21285	4.01326	-0.74278
C	1.21285	-4.01326	-0.74278
C	-2.39618	-3.32213	-1.20180

C	2.39618	3.32213	-1.20180
C	2.39618	-3.32213	-1.20180
C	0.00000	-3.96271	-1.49180
C	-3.08651	-2.75197	-0.07652
C	3.08651	2.75197	-0.07652
C	3.08651	-2.75197	-0.07652
C	-2.40233	-2.66066	-2.41112
C	2.40233	2.66066	-2.41112
C	2.40233	-2.66066	-2.41112
C	0.00000	-3.25887	-2.78208
C	-1.20557	-2.64790	-3.23561
C	1.20557	2.64790	-3.23561
C	1.20557	-2.64790	-3.23561
C	-3.66630	-0.73392	-1.43435
C	3.66630	0.73392	-1.43435
C	3.66630	-0.73392	-1.43435
C	-3.09104	-1.40398	-2.55127
C	3.09104	1.40398	-2.55127
C	3.09104	-1.40398	-2.55127
C	-1.20287	-1.42385	-3.96997
C	1.20287	1.42385	-3.96997
C	1.20287	-1.42385	-3.96997
C	0.00000	-0.73716	-4.28728
C	-2.39712	-0.68608	-3.58583
C	2.39712	0.68608	-3.58583
C	2.39712	-0.68608	-3.58583

Atomic coordinate data of $La_2@I_h$-C_{80}

Energy: -2459755.8244025 Hartree

La	-1.86782	0.00000	0.00000
La	1.86782	0.00000	0.00000
C	-3.97193	0.74320	1.23874
C	-3.15171	1.16596	2.36391

C	-2.67946	0.00000	3.05254
C	-3.95247	1.51881	0.00000
C	-3.12441	2.69576	0.00000
C	-2.38662	3.15153	1.16675
C	-2.35466	2.37024	2.35798
C	-1.16658	2.39355	3.14249
C	-0.71893	1.22243	3.85482
C	-1.44420	0.00000	3.79854
C	-1.22599	3.86269	0.72067
C	0.00000	3.81982	1.46073
C	0.00000	3.11216	2.69795
C	-3.97193	-0.74320	1.23874
C	3.97193	0.74320	1.23874
C	3.97193	-0.74320	1.23874
C	-3.97193	0.74320	-1.23874
C	-3.97193	-0.74320	-1.23874
C	3.97193	0.74320	-1.23874
C	3.97193	-0.74320	-1.23874
C	-3.15171	-1.16596	2.36391
C	3.15171	1.16596	2.36391
C	3.15171	-1.16596	2.36391
C	-3.15171	1.16596	-2.36391
C	-3.15171	-1.16596	-2.36391
C	3.15171	1.16596	-2.36391
C	3.15171	-1.16596	-2.36391
C	2.67946	0.00000	3.05254
C	-2.67946	0.00000	-3.05254
C	2.67946	0.00000	-3.05254
C	-3.95247	-1.51881	0.00000
C	3.95247	1.51881	0.00000
C	3.95247	-1.51881	0.00000
C	-3.12441	-2.69576	0.00000
C	3.12441	2.69576	0.00000

C	3.12441	-2.69576	0.00000
C	-2.38662	-3.15153	1.16675
C	2.38662	3.15153	1.16675
C	2.38662	-3.15153	1.16675
C	-2.38662	3.15153	-1.16675
C	-2.38662	-3.15153	-1.16675
C	2.38662	3.15153	-1.16675
C	2.38662	-3.15153	-1.16675
C	-2.35466	-2.37024	2.35798
C	2.35466	2.37024	2.35798
C	2.35466	-2.37024	2.35798
C	-2.35466	2.37024	-2.35798
C	-2.35466	-2.37024	-2.35798
C	2.35466	2.37024	-2.35798
C	2.35466	-2.37024	-2.35798
C	-1.16658	-2.39355	3.14249
C	1.16658	2.39355	3.14249
C	1.16658	-2.39355	3.14249
C	-1.16658	2.39355	-3.14249
C	-1.16658	-2.39355	-3.14249
C	1.16658	2.39355	-3.14249
C	1.16658	-2.39355	-3.14249
C	-0.71893	-1.22243	3.85482
C	0.71893	1.22243	3.85482
C	0.71893	-1.22243	3.85482
C	-0.71893	1.22243	-3.85482
C	-0.71893	-1.22243	-3.85482
C	0.71893	1.22243	-3.85482
C	0.71893	-1.22243	-3.85482
C	1.44420	0.00000	3.79854
C	-1.44420	0.00000	-3.79854
C	1.44420	0.00000	-3.79854
C	-1.22599	-3.86269	0.72067

C	1.22599	3.86269	0.72067
C	1.22599	-3.86269	0.72067
C	-1.22599	3.86269	-0.72067
C	-1.22599	-3.86269	-0.72067
C	1.22599	3.86269	-0.72067
C	1.22599	-3.86269	-0.72067
C	0.00000	-3.81982	1.46073
C	0.00000	3.81982	-1.46073
C	0.00000	-3.81982	-1.46073
C	0.00000	-3.11216	2.69795
C	0.00000	3.11216	-2.69795
C	0.00000	-3.11216	-2.69795

Atomic coordinate data of $Sc_3N@I_h$-C_{80}

Energy: -2035484.7047463 Hartree

Sc	-0.16122	2.01528	0.00000
Sc	-0.02705	-1.14722	1.66623
Sc	-0.02705	-1.14722	-1.66623
N	-0.05579	-0.01915	0.00000
C	3.81714	0.41187	1.45755
C	-3.79564	-0.38988	1.45417
C	3.73994	1.63234	0.71935
C	3.98737	-0.79534	0.71982
C	-3.71168	-1.60997	0.71932
C	-3.97677	0.81975	0.71908
C	3.10878	0.33850	2.70222
C	-3.07742	-0.31404	2.69200
C	2.26990	1.41638	3.15294
C	2.51586	-0.88907	3.13591
C	-2.24446	-1.39641	3.13775
C	-2.48478	0.91179	3.14299
C	1.15230	0.85613	3.86019
C	1.29392	-0.58441	3.86532

C	-1.12374	-0.84269	3.88584
C	-1.27757	0.59579	3.85815
C	0.17065	-1.48318	3.93987
C	-0.13891	1.45345	3.80790
C	2.89174	2.69892	1.16573
C	3.40514	-2.03216	1.16773
C	-2.88328	-2.69749	1.16883
C	-3.37158	2.04331	1.16537
C	2.36015	3.37141	0.00000
C	3.03826	-2.79348	0.00000
C	-2.37121	-3.37053	0.00000
C	-2.99516	2.81023	0.00000
C	1.08875	4.03250	0.00000
C	1.86987	-3.58808	0.00000
C	-1.06350	-3.90496	0.00000
C	-1.87526	3.70465	0.00000
C	1.11655	-3.67825	1.21635
C	-0.30921	-3.83825	1.22098
C	-1.12579	3.82386	1.22879
C	0.33004	3.98464	1.23064
C	0.30022	-2.75035	3.22554
C	-0.26964	2.67396	3.07228
C	0.83956	3.24122	2.36230
C	1.49445	-2.98172	2.41362
C	-0.82890	-3.26418	2.43659
C	-1.47282	2.99764	2.36282
C	2.12019	2.59105	2.35601
C	2.61953	-2.07742	2.35655
C	-2.10879	-2.59335	2.36742
C	-2.58893	2.09639	2.35100
C	3.81714	0.41187	-1.45755
C	-3.79564	-0.38988	-1.45417
C	3.73994	1.63234	-0.71935

C	3.98737	-0.79534	-0.71982
C	-3.71168	-1.60997	-0.71932
C	-3.97677	0.81975	-0.71908
C	3.10878	0.33850	-2.70222
C	-3.07742	-0.31404	-2.69200
C	2.26990	1.41638	-3.15294
C	2.51586	-0.88907	-3.13591
C	-2.24446	-1.39641	-3.13775
C	-2.48478	0.91179	-3.14299
C	1.15230	0.85613	-3.86019
C	1.29392	-0.58441	-3.86532
C	-1.12374	-0.84269	-3.88584
C	-1.27757	0.59579	-3.85815
C	0.17065	-1.48318	-3.93987
C	-0.13891	1.45345	-3.80790
C	2.89174	2.69892	-1.16573
C	3.40514	-2.03216	-1.16773
C	-2.88328	-2.69749	-1.16883
C	-3.37158	2.04331	-1.16537
C	1.11655	-3.67825	-1.21635
C	-0.30921	-3.83825	-1.22098
C	-1.12579	3.82386	-1.22879
C	0.33004	3.98464	-1.23064
C	0.30022	-2.75035	-3.22554
C	-0.26964	2.67396	-3.07228
C	0.83956	3.24122	-2.36230
C	1.49445	-2.98172	-2.41362
C	-0.82890	-3.26418	-2.43659
C	-1.47282	2.99764	-2.36282
C	2.12019	2.59105	-2.35601
C	2.61953	-2.07742	-2.35655
C	-2.10879	-2.59335	-2.36742
C	-2.58893	2.09639	-2.35100