Supporting Information

Structural Determination on Yb@C_{78} Reveals an Unexpected Relationship of Yb@C_{2n} (2n=74~80)

Tao Yang,[†] Xiang Zhao,[†,*] and Shigeru Nagase[‡]

[†]Institute for Chemical Physics and Department of Chemistry, State Key Laboratory of Electrical Insulation and Power Equipment, Xi'an Jiaotong University, Xi'an 710049, China.

[‡]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto 606-8103, Japan.

Content

I. Relative energy and corresponding HOMO-LUMO gap of di-anions C_{78}^{2-} and metallofullerenes Yb@C_{78}.

II. Cartesian coordinates of endohedral fullerene Yb@C_{2v}(24107)-C_{78}.

III. Cartesian coordinates of Yb@C_{2v}(24107)-C_{78} with Yb^{2+} locating under the hexagonal ring along the symmetry axis.

I. Relative energy and corresponding HOMO-LUMO gap of di-anions C_{78}^{2-} and metallofullerenes Yb@C_{78}.

Further optimization on these di-anions and corresponding mono-EMFs Yb@C_{78} were carried out at hybrid density functional theory B3LYP level of theory. The split-valence d-polarized 6-31G(d) basis set was used for C and CEP-4G basis with corresponding effective core potential (ECP) for Yb.

Table S1. Optimized relative energy of di-anions C_{78}^{2-} and Yb@C_{78}.

C_{78}			di-annion B3LYP 6-31G(d)		Yb@C_{78} B3LYP 6-31G(d)&CEP-31G	
spiral ID	PA	Sym.	ΔE kcal/mol	Gap eV	ΔE kcal/mol	Gap eV
24107	0	*C2v*	3.24	0.87	0.00	1.18
24109	0	*D3h*	0.00	0.90	0.48	1.20
22595	1	*C1*	15.72	1.27	8.56	1.36
24106	0	*C2v*	15.80	1.13	10.15	1.47
23349	1	*C1*	22.66	0.87	18.26	0.90
24105	0	*D3*	15.63	1.17	19.12	1.18
24060	1	*C1*	23.76	1.54	19.61	1.58
22618	1	*C1*	24.71	1.38	20.02	1.23
23318	1	*C1*	22.91	1.22	20.19	1.18
23474	1	*C1*	26.29	1.41	23.88	1.35
23791	2	*C2*	27.49	1.48	26.81	1.30
22600	2	*C1*	30.75	1.57	29.50	1.21
23788	2	*Cs*	31.67	1.39	30.53	1.24
24108	0	*D3h*	51.39	0.77	48.09	0.90

II. Cartesian coordinates of endohedral fullerene Yb@C_{2v}(24107)-C_{78}.

xyz files:

C	-0.013264	-0.040982	0.131395
C	1.360189	-0.036330	0.118776
C	2.092198	1.221460	0.116325

C	3.271911	1.013487	-0.666871
C	3.810663	2.053987	-1.466554
C	4.411991	1.715115	-2.725689
C	4.345843	2.603624	-3.874935
C	4.348312	1.777262	-5.066227
C	3.537652	2.169937	-6.190432
C	2.737359	1.166065	-6.854910
C	1.470590	1.775060	-7.217835
C	0.265466	1.022611	-7.356619
C	-1.001926	1.665154	-6.986251
C	-2.064478	0.813316	-6.599365
C	-2.972187	1.219486	-5.546693
C	-3.150770	0.127367	-4.622882
C	-3.084837	0.352065	-3.229507
C	-2.477705	-0.707397	-2.410081
C	-1.906044	-0.362494	-1.165246
C	-0.736954	-1.013203	-0.667852
C	-0.737755	1.216961	0.112872
C	-1.906080	1.017741	-0.682608
C	-2.478570	2.063168	-1.440755
C	-3.085990	1.745225	-2.742162
C	-3.151336	2.789043	-3.692277
C	-2.972682	2.510410	-5.095612
C	-2.064508	3.483966	-5.665550
C	-1.001681	3.058554	-6.498220
C	0.265250	3.792573	-6.387115
C	1.470588	3.119143	-6.748623
C	2.737317	3.369033	-6.084848
C	2.773373	4.246147	-4.936677
C	3.591631	3.838140	-3.775636
C	3.177760	4.259028	-2.485443
C	3.232995	3.342381	-1.337256
C	2.086830	3.562953	-0.512373
C	1.415470	2.471734	0.119191
C	-0.056243	2.469879	0.133288
C	-0.752334	3.563000	-0.439786
C	-1.955590	3.368395	-1.199075
C	-2.010201	4.402324	-2.226024
C	-2.561028	4.097156	-3.451306
C	-1.892377	4.525562	-4.678245
C	-0.698659	5.223690	-4.599156
C	0.392656	4.863573	-5.472722
C	1.634450	5.058094	-4.721442
C	1.283824	5.532930	-3.398511

C	2.029323	5.099323	-2.301885
C	1.344749	4.675258	-1.085547
C	-0.035011	4.702321	-1.020444
C	-0.806849	5.208512	-2.137406
C	-0.156235	5.616889	-3.305553
C	2.092516	-1.018103	-0.667495
C	3.272450	-0.367276	-1.149724
C	3.811968	-0.682357	-2.423420
C	4.411405	0.367829	-3.197098
C	4.345048	0.389049	-4.649603
C	3.590595	-0.638302	-5.340646
C	2.773170	-0.235146	-6.503369
C	1.634934	-1.004777	-6.841476
C	0.393144	-0.384855	-7.308422
C	-0.698220	-1.211385	-6.849731
C	-1.892342	-0.616761	-6.476714
C	-2.561113	-1.046148	-5.249710
C	-2.009331	-2.047682	-4.481281
C	-1.954115	-1.878832	-3.034003
C	-0.750855	-2.504035	-2.561345
C	-0.055047	-2.005356	-1.432350
C	1.416477	-1.998028	-1.444119
C	2.088257	-2.457606	-2.617912
C	3.234334	-1.770961	-3.125137
C	3.179077	-1.772497	-4.594443
C	2.030614	-2.544338	-4.974764
C	1.284700	-2.200673	-6.102587
C	-0.155268	-2.324441	-6.082191
C	-0.805902	-2.733076	-4.914441
C	-0.033421	-3.032916	-3.725615
C	1.346194	-2.970351	-3.759420
Yb	1.991323	1.518336	-4.315991

III. Cartesian coordinates of Yb@C_{2v}(24107)-C_{78} with Yb^{2+} locating under the hexagonal ring along the symmetry axis.

xyz files:

C	-0.018557	-0.041377	0.130108
C	1.374264	-0.023412	0.078837
C	2.106250	1.217299	0.087068
C	3.343886	1.004934	-0.642210
C	3.896695	2.066570	-1.440855

C	4.493444	1.727103	-2.705398
C	4.303478	2.595943	-3.852752
C	4.219629	1.761615	-5.024796
C	3.476058	2.150460	-6.136922
C	2.711874	1.158768	-6.848485
C	1.479276	1.776130	-7.258000
C	0.283167	1.027739	-7.377093
C	-0.985564	1.669341	-6.999274
C	-2.041583	0.817918	-6.601060
C	-2.948383	1.220115	-5.553581
C	-3.139996	0.128816	-4.629687
C	-3.083121	0.353426	-3.235209
C	-2.485098	-0.708523	-2.411836
C	-1.920104	-0.355852	-1.162391
C	-0.734791	-1.002874	-0.666945
C	-0.735131	1.207054	0.106361
C	-1.919880	1.009697	-0.684953
C	-2.485625	2.064166	-1.441770
C	-3.084114	1.746943	-2.747687
C	-3.140461	2.791492	-3.698589
C	-2.948680	2.513614	-5.101489
C	-2.041437	3.480794	-5.669757
C	-0.985193	3.062816	-6.511162
C	0.283233	3.800338	-6.406463
C	1.479251	3.141415	-6.779769
C	2.711735	3.369117	-6.075044
C	2.764819	4.230963	-4.937780
C	3.574693	3.821158	-3.777355
C	3.186816	4.259326	-2.478129
C	3.248213	3.344995	-1.355198
C	2.090644	3.572020	-0.511988
C	1.418740	2.468387	0.087915
C	-0.054459	2.462306	0.117541
C	-0.753500	3.557982	-0.444438
C	-1.971498	3.368498	-1.192464
C	-2.010180	4.398393	-2.220943
C	-2.552442	4.096461	-3.450237
C	-1.870453	4.524220	-4.673153
C	-0.689005	5.226681	-4.589318
C	0.413380	4.863663	-5.468090
C	1.633369	5.055362	-4.724400
C	1.283090	5.529744	-3.385418
C	2.029312	5.099352	-2.293390
C	1.350148	4.673362	-1.075639

C	-0.039290	4.700290	-1.014359
C	-0.805398	5.208750	-2.123549
C	-0.152226	5.619168	-3.294921
C	2.106956	-0.999107	-0.687516
C	3.344826	-0.378670	-1.125614
C	3.898785	-0.711055	-2.411734
C	4.494062	0.343089	-3.189337
C	4.304139	0.378941	-4.628419
C	3.573841	-0.625729	-5.332229
C	2.764153	-0.223508	-6.495263
C	1.633215	-1.001640	-6.842508
C	0.413354	-0.388650	-7.305658
C	-0.689111	-1.220610	-6.844613
C	-1.870830	-0.619471	-6.472508
C	-2.552835	-1.046820	-5.248925
C	-2.009730	-2.048423	-4.475422
C	-1.970395	-1.883946	-3.029413
C	-0.752429	-2.498238	-2.562480
C	-0.053648	-1.990636	-1.440598
C	1.419235	-1.977270	-1.466997
C	2.091479	-2.466723	-2.623875
C	3.249634	-1.764212	-3.141460
C	3.187779	-1.778989	-4.589743
C	2.029907	-2.550578	-4.968779
C	1.283249	-2.207066	-6.090978
C	-0.151850	-2.333646	-6.076020
C	-0.805049	-2.742742	-4.904415
C	-0.038334	-3.036147	-3.720351
C	1.351019	-2.976374	-3.751237
Yb	1.995422	1.002240	-2.867642