Supporting Information

1 Cartesian Atomic Coordinates of Eu@C_{74} Minimum Structure

Table 1: Optimized Cartesian coordinates x, y, z (Å) of Eu@C_{74} minimum structure.

Atom	x	y	z
C	2.5905755	−0.7200708	−2.6343136
C	3.0906685	−1.4724019	−1.5089700
C	3.8210814	−0.7264424	−0.5307254
C	3.9019946	−1.1673744	0.8523427
C	3.1769365	−2.3063423	1.2473785
C	1.4406245	−1.1630069	−3.4269831
C	0.7354414	−2.3082143	−2.9744344
C	1.1845328	−3.0614222	−1.8332893
C	2.3647879	−2.6878827	−1.0885413
C	2.4169896	−3.0703320	0.2861331
C	3.2292908	0.0000000	2.9369638
C	2.4572645	−1.1633669	3.3222889
C	3.9417044	0.0000000	1.7092793
C	2.4431083	−2.3044446	2.5070936
C	1.2249849	−3.0660680	2.3263366
C	0.0000000	−2.6829697	2.9699702
C	−1.2249849	−3.0660680	2.3263366
C	0.0000000	−3.5433828	−1.1488916
C	0.0000000	−3.7681604	0.2636691
C	1.2267779	−3.5588533	0.9700713
C	−1.2267779	−3.5588533	0.9700713
C	3.1769365	2.3063423	1.2473785
C	2.4431083	2.3044446	2.5070936
C	3.9019946	1.1673744	0.8523427
C	2.4572645	1.1633669	3.3222889
C	1.2148853	0.7205661	3.9475523
C	0.0000000	1.4683261	3.8111188
C	−1.2148853	0.7205661	3.9475523
C	0.0000000	−1.4683261	3.8111188
C	1.2148853	−0.7205661	3.9475523
C	−1.2148853	−0.7205661	3.9475523
C	1.1845328	3.0614222	−1.8332893
C	2.3647879	2.6878827	−1.0885413
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C	0.0000000	3.7681604	0.2636691
C	0.0000000	3.5433828	−1.1488916
C	0.0000000	2.6829697	2.9699702
C	1.2249849	3.0660680	2.3263366
C	−1.2249849	3.0660680	2.3263366
C	3.0906685	1.4724019	−1.5089700
C	3.8210814	0.7264424	−0.5307254
C	0.7354414	2.3082143	−2.9744344
C	1.4406245	1.1630069	−3.4269831
C	2.5905755	0.7200708	−2.6343136
C	−0.7354414	2.3082143	−2.9744344
C	0.7304507	0.0000000	−3.9418867
C	−0.7304507	0.0000000	−3.9418867
C	−1.4406245	1.1630069	−3.4269831
C	−2.4169896	3.0703320	0.2861331
C	−2.3647879	2.6878827	−1.0885413
C	−1.1845328	3.0614222	−1.8332893
C	−3.1769365	2.3063423	1.2473785
C	−3.9019946	1.1673744	0.8523427
C	−3.8210814	0.7264424	−0.5307254
C	−3.0906685	1.4724019	−1.5089700
C	−2.5905755	0.7200708	−2.6343136
C	−3.2292908	0.0000000	2.9369638
C	−2.4572645	1.1633669	3.3222889
C	−2.4431083	2.3044446	2.5070936
C	−3.9417044	0.0000000	1.7092793
C	−3.1769365	−2.3063423	1.2473785
C	−2.4431083	−2.3044446	2.5070936
C	−2.4572645	−1.1633669	3.3222889
C	−3.9019946	−1.1673744	0.8523427
C	−1.1845328	−3.0614222	−1.8332893
C	−2.3647879	−2.6878827	−1.0885413
C	−2.4169896	−3.0703320	0.2861331
C	−2.5905755	−0.7200708	−2.6343136
C	−1.4406245	−1.1630069	−3.4269831
C	−0.7354414	−2.3082143	−2.9744344
C	−3.8210814	−0.7264424	−0.5307254
C	−3.0906685	−1.4724019	−1.5089700
Eu	0.0000000	0.0000000	−1.5055496

2 Structure of the Interconversion Transition State of Eu@C_{74}

Table 2: Optimized Cartesian coordinates x, y, z (Å) of Eu@C_{74} transition state structure.

Atom	x	y	z
C	−3.7986441	−0.7184205	−0.8214854
C	−3.0771830	−1.4686903	−1.8083792
C	−2.5911175	−0.7215845	−2.9304769
C	−1.4310573	−1.1634892	−3.6978691
C	−0.7288441	−2.3009444	−3.2702763
C	−3.8735666	−1.1588648	0.5738514
C	−3.1595215	−2.3012682	0.9646217
C	−2.3982124	−3.0650924	−0.0010250
C	−2.3480666	−2.6842644	−1.3896535
C	−1.1816824	−3.0631258	−2.1262424
C	0.7111979	0.0000000	−4.1691908
C	1.4310573	−1.1634892	−3.6978691
C	−0.7111979	0.0000000	−4.1691908
C	0.7288441	−2.3009444	−3.2702763
C	1.1816824	−3.0631258	−2.1262424
C	2.3480666	−2.6842644	−1.3896535
C	2.3982124	−3.0650924	−0.0010250
C	−1.2239786	−3.5520503	0.6749313
C	0.0000000	−3.7682674	−0.0319015
C	0.0000000	−3.5565639	−1.4463685
C	1.2239786	−3.5520503	0.6749313
C	−0.7288441	2.3009444	−3.2702763
C	0.7288441	2.3009444	−3.2702763
C	−1.4310573	1.1634892	−3.6978691
C	1.4310573	1.1634892	−3.6978691
C	2.5911175	0.7215845	−2.9304769
C	3.0771830	1.4686903	−1.8083792
C	3.7986441	0.7184205	−0.8214854
C	3.0771830	−1.4686903	−1.8083792
C	2.5911175	−0.7215845	−2.9304769
C	3.7986441	−0.7184205	−0.8214854
C	−2.3982124	3.0650924	−0.0010250
C	−2.3480666	2.6842644	−1.3896535
C	−1.1816824	3.0631258	−2.1262424
C	0.0000000	3.5565639	−1.4463685
C	1.2239786	3.5520503	0.6749313
C	0.0000000	3.7682674	−0.0319015

Atom	x	y	z
C	−1.2239786	3.5520503	0.6749313
C	2.3480666	2.6842644	−1.3896535
C	1.1816824	3.0631258	−2.1262424
C	2.3982124	3.0650924	−0.0010250
C	−3.0771830	1.4686903	−1.8083792
C	−2.5911175	0.7215845	−2.9304769
C	−3.1595215	2.3012682	0.9646217
C	−3.8735666	1.1588648	0.5738514
C	−3.7986441	0.7184205	−0.8214854
C	−2.4289001	2.3014109	2.2284872
C	−3.9320441	0.0000000	1.4350903
C	−3.2096529	0.0000000	2.6696893
C	−2.4499751	1.1624575	3.0683113
C	1.2227580	3.0584250	2.0507057
C	0.0000000	2.6869630	2.7112622
C	−1.2227580	3.0584250	2.0507057
C	2.4289001	2.3014109	2.2284872
C	2.4499751	1.1624575	3.0683113
C	1.2253270	0.7349115	3.7321140
C	0.0000000	1.4928207	3.6060888
C	−1.2253270	0.7349115	3.7321140
C	3.9320441	0.0000000	1.4350903
C	3.8735666	1.1588648	0.5738514
C	3.1595215	2.3012682	0.9646217
C	3.2096529	0.0000000	2.6696893
C	2.4289001	−2.3014109	2.2284872
C	3.1595215	−2.3012682	0.9646217
C	3.8735666	−1.1588648	0.5738514
C	2.4499751	−1.1624575	3.0683113
C	−1.2227580	−3.0584250	2.0507057
C	0.0000000	−2.6869630	2.7112622
C	1.2227580	−3.0584250	2.0507057
C	−1.2253270	−0.7349115	3.7321140
C	−2.4499751	−1.1624575	3.0683113
C	−2.4289001	−2.3014109	2.2284872
C	1.2253270	−0.7349115	3.7321140
C	0.0000000	−1.4928207	3.6060888
Eu	0.0000000	0.0000000	1.4602019