

Electronic supporting information for

“Icosahedral Au₇₂: a predicted chiral and spherically aromatic golden fullerene”

by

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Full citation for reference 30

Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

BP86/def2-TZVP optimised cartesian coordinates of the studied gold cages in atomic units

Au18 (C2v)

-4.00150274919485	2.73330982238841	0.62495247908671	au
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-5.17652297134990	0.00000000000000	-3.74757573423715	au
-2.65861029495731	-4.51395366238490	-4.17760710780401	au
-2.65861029495731	4.51395366238490	-4.17760710780401	au
0.00000000000000	0.00000000000000	-5.06857466394461	au
5.17652297134990	0.00000000000000	-3.74757573423715	au
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0.00000000000000	3.30511668832557	4.20436808700176	au
4.00150274919485	-2.73330982238841	0.62495247908671	au
4.00150274919485	2.73330982238841	0.62495247908671	au
-4.15930135762309	0.00000000000000	5.01620263007940	au
0.00000000000000	0.00000000000000	8.25820051271339	au

Au20 (Td)

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2.11667583358231	2.11667583358231	-2.11667583358231	au
-1.78967191122259	1.78967191122259	-5.76900626570761	au
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1.78967191122259	-1.78967191122259	-5.76900626570761	au
-5.41833083216091	5.41833083216091	-5.41833083216091	au
-5.76900626570761	-1.78967191122259	1.78967191122259	au
5.41833083216091	-5.41833083216091	-5.41833083216091	au
1.78967191122259	1.78967191122259	5.76900626570761	au
5.76900626570761	1.78967191122259	1.78967191122259	au
5.41833083216091	5.41833083216091	5.41833083216091	au
-1.78967191122259	-1.78967191122259	5.76900626570761	au

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-5.41833083216091	-5.41833083216091	5.41833083216091	au
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1.78967191122259	-5.76900626570761	-1.78967191122259	au
5.76900626570761	-1.78967191122259	-1.78967191122259	au
1.78967191122259	5.76900626570761	1.78967191122259	au

Au32 (Ih)

6.15939554348443	4.47506280914813	3.80671579602801	au
0.00000000000000	0.00000000000000	8.51207529094085	au
6.15939554348443	-4.47506280914813	3.80671579602801	au
-2.35267974745642	7.24080372699226	3.80671579602801	au
-6.15939554348443	-4.47506280914813	-3.80671579602801	au
-6.15939554348443	4.47506280914813	-3.80671579602801	au
-7.61343159205601	0.00000000000000	3.80671579602801	au
2.27789485159255	-7.01063948416266	1.40781644108259	au
-2.27789485159255	-7.01063948416266	-1.40781644108259	au
-5.96360614426770	-4.33281348408456	1.40781644108259	au
-3.68571129267515	-2.67782600007811	5.96360614426770	au
1.40781644108259	-4.33281348408456	5.96360614426770	au
5.96360614426770	-4.33281348408456	-1.40781644108260	au
3.68571129267515	-2.67782600007811	-5.96360614426770	au
-1.40781644108259	-4.33281348408456	-5.96360614426770	au
7.37142258535029	0.00000000000000	1.40781644108259	au
4.55578970318510	0.00000000000000	5.96360614426770	au
-4.55578970318510	0.00000000000000	-5.96360614426770	au
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-5.96360614426770	4.33281348408456	1.40781644108259	au
-3.68571129267515	2.67782600007811	5.96360614426770	au
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3.68571129267515	2.67782600007811	-5.96360614426770	au
-1.40781644108259	4.33281348408456	-5.96360614426770	au
-2.27789485159255	7.01063948416266	-1.40781644108259	au
2.27789485159255	7.01063948416266	1.40781644108259	au
5.96360614426770	4.33281348408456	-1.40781644108260	au
2.35267974745642	7.24080372699225	-3.80671579602801	au
0.00000000000000	0.00000000000000	-8.51207529094085	au
7.61343159205601	0.00000000000000	-3.80671579602801	au
2.35267974745642	-7.24080372699225	-3.80671579602801	au
-2.35267974745642	-7.24080372699226	3.80671579602801	au

Au42 (Ih)

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7.12443648512815	-5.17620609451863	4.40314389849903	au
0.00000000000000	0.00000000000000	-9.84572907175727	au
0.00000000000000	0.00000000000000	9.84572907175727	au
8.80628779699806	0.00000000000000	-4.40314389849903	au
-8.80628779699806	0.00000000000000	4.40314389849903	au
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-8.23721354318195	2.67643292225626	0.00000000000000	au
-8.23721354318195	-2.67643292225626	0.00000000000000	au
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-7.36758777109469	0.00000000000000	-4.55341965763460	au
7.36758777109469	0.00000000000000	4.55341965763460	au
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-2.72129258662912	-8.37527739370550	4.40314389849903	au
2.72129258662912	8.37527739370550	-4.40314389849903	au
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0.00000000000000	8.66111887363967	0.00000000000000	au
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-2.72129258662912	8.37527739370550	4.40314389849903	au
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-1.40708405673005	4.33055943681983	7.36758777109469	au
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5.96050371436465	4.33055943681983	-4.55341965763460	au
-5.96050371436465	-4.33055943681983	4.55341965763460	au
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5.09087794227739	7.00699235907609	0.00000000000000	au
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-1.40708405673005	-4.33055943681984	7.36758777109469	au
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-4.55341965763460	0.00000000000000	7.36758777109469	au

Au50 (D6d)

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2.23791941634808	8.35202896505592	3.88465398264397	au
6.37999230822453	6.37999230822453	1.26860683591507	au
8.35202896505592	2.23791941634808	3.88465398264397	au
8.71523156898403	-2.33523926075950	1.26860683591507	au
6.11410954870784	-6.11410954870784	3.88465398264397	au
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-2.23791941634808	-8.35202896505592	3.88465398264397	au
-6.37999230822453	-6.37999230822454	1.26860683591507	au
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1.34055895300139	5.00303412314251	8.06585101031132	au
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3.66247517014113	-3.66247517014113	8.06585101031132	au
-1.34055895300139	-5.00303412314251	8.06585101031132	au
0.00000000000000	0.00000000000000	9.16626948302989	au
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6.19191713238496	-6.19191713238495	-6.50095479984630	au
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8.35202896505592	-2.23791941634808	-3.88465398264397	au
5.00303412314251	-1.34055895300139	-8.06585101031132	au
-2.33523926075950	-8.71523156898403	-1.26860683591507	au
-2.26639896858098	-8.45831610096594	-6.50095479984630	au
-3.66247517014113	-3.66247517014113	-8.06585101031132	au
0.00000000000000	0.00000000000000	-9.16626948302989	au
8.71523156898403	2.33523926075950	-1.26860683591507	au
3.66247517014113	3.66247517014113	-8.06585101031132	au
8.45831610096594	2.26639896858099	-6.50095479984630	au
-6.11410954870784	-6.11410954870784	-3.88465398264397	au
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6.11410954870784	6.11410954870784	-3.88465398264397	au
2.26639896858099	8.45831610096594	-6.50095479984630	au
-8.71523156898403	-2.33523926075950	-1.26860683591507	au
-8.35202896505592	2.23791941634808	-3.88465398264397	au
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-2.23791941634808	8.35202896505592	-3.88465398264397	au
2.33523926075950	8.71523156898403	-1.26860683591507	au
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Au72 (I)

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6.13391226592148	9.27613090082026	2.56829829559705	au
-2.51626083129481	11.10997070957474	0.71036791286223	au
-6.92664160705726	8.70017932128745	2.56829829559705	au
-7.48019036098537	1.76699679732270	8.43754198757045	au

Supplementary Material (ESI) for Chemical Communications
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5.01298646488253	-5.82627601656768	8.43754198757045	au
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-9.78864268003922	5.82627601656768	-0.71036791286224	au
-5.76148146823123	6.56805174656452	7.34395451075375	au
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-10.41481220697207	-3.89912437204563	2.56829829559705	au
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5.04032478910479	-9.27613090082027	4.33776000275771	au
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8.02698409939372	-3.44985488425259	-7.34395451075375	au
2.97885618377378	3.44985488425258	-10.46386914216403	au
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-10.71760787140663	-2.96721514048735	-2.56829829559705	au
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-8.52174037349983	-1.92715164452205	-7.34395451075375	au
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-5.04032478910479	-9.27613090082026	-4.33776000275771	au
11.34377739833948	1.04006349596530	-0.71036791286224	au
8.52174037349983	-1.92715164452205	7.34395451075375	au
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-3.57696788811665	-11.00877518226114	5.78765561963967	au
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