CHE 400 Term Project

Aza fullerenes Heterofullerenes

Science Citation Search 1995-2002

Jimmy Villarreal
December 11, 2008

Annotated Bibliography of references in and after 1995

Topic: Aza fullerene heterofullerene

Years covered by SciFinder Scholar search: 1995-2008

Years covered by Web of Science search: 1995-2002

CA search: Total of 25 references were found by the topic. Removal of duplicates resulted in 0 references being removed. The search was then refined to include only journals, which narrowed it down to 22 references.

Science Citation Search: There was a total of 60 citations found for the key paper. This number was reduced to 36 by limiting the date range from 1995 to 2002. Additionally, 12 non-related papers were found and can be identified by a line through the associated reference.

1. Ewels, C. P.; El Cheikh, H.; Suarez-Martinez, I.; Van Lier, G., Oxidation and reactivity of nitrogen- and phosphorus-doped heterofullerenes. *Physical Chemistry Chemical Physics* **2008,** 10, (16), 2145-2148.

D. functional theory (DFT) calcns. suggest significantly different oxidn. behavior for phosphorus-doped heterofullerenes compared to their pure and nitrogen-doped counterparts, due to formation of a phosphene oxide.

2. Hou, J. Q.; Kang, H. S., DFT Study on the Stabilities of the Heterofullerenes Sc3N@C67B, Sc3N@C67N, and Sc3N@C66BN. *Journal of Physical Chemistry A* **2007,** 111, (6), 1111-1116.

We investigated the relative stabilities of all isomers of Sc3N@C67B and Sc3N@C67N as well as those of stable isomers of Sc3N@C66BN using the DFT-GGA method. Sc3N@C68 can be doped substitutionally with a boron atom much better than C60.

3. Yee, K. A.; Yi, H.; Lee, S.; Kang, S. K.; Song, J. S.; Seong, S., The electronic structure and stability of the heterofullerene: C(60-2x)(BN)x. *Bulletin of the Korean Chemical Society* **2003,** 24, (4), 494-498.

The transition from aroms. to heteroaroms. is very attractive since it provides an extremely large structural variety, the chem. functionality as well as the possibilities for electronic tuning of the fullerene properties.

4. Liang, Y.-X.; Wang, G.-C.; Shang, Z.-F.; Xu, X.-F.; Zhang, C.; Pan, Y.-M.; Zhao, X.-Z., Studies on the structures and stabilities of C59F2nHN (n = 1, 2) isomers. *Jiegou Huaxue* **2003,** 22, (6), 721-728.

The study of the early stages of addn. to C60 forming C60Xn has been extended to X=H, F, Cl, Br, CH3, C4H9, using the AM1 Hamiltonian with the program mopac 6.0 and the d. functional technique B3LYP/6-31G with gaussian 98.

5. Clare, B. W.; Kepert, D. L., Early stages in the addition to C60 to form C60Xn, X=H, F, Cl, Br, CH3, C4H9. *Theochem* **2003,** 621, (3), 211-231.

The study of the early stages of addn. to C60 forming C60Xn has been extended to X=H, F, Cl, Br, CH3, C4H9, using the AM1 Hamiltonian with the program mopac 6.0 and the d. functional technique B3LYP/6-31G with gaussian 98.

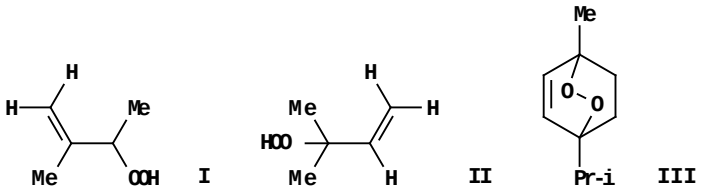
6. Wilke, M., Synthesis of an aza-fullerene with elastic properties. *Naturwissenschaftliche Rundschau* **2002,** 55, (6), 317-319.

A review on prepn. of the C48N12-aza-fullerene with elastic properties and applications.

7. Tagmatarchis, N.; Shinohara, H., Photosensitized oxygenation of alkenes in the presence of bisazafullerene (C59N)2 and hydroazafullerene C59HN. *AIP Conference Proceedings* **2001,** 590, (Nanonetwork Materials), 413-416.

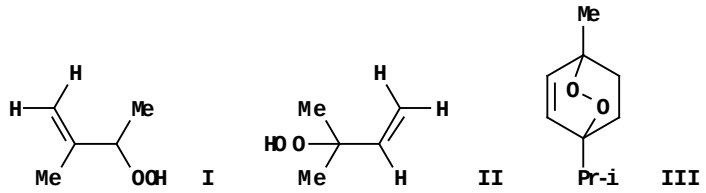
Heterofullerenes (C59N)2 and C59HN sensitize the reaction of olefins with mol. oxygen under photolytic conditions. 2-Methyl-2-butene and □ -terpinene undergo ene and Diels-Alder photooxygenation reactions, resp., in the presence of

minute amts. of these azafullerenes to produce the corresponding peroxides I, II and III, resp.



8. Tagmatarchis, N.; Shinobara, H., Photosensitized oxygenation of alkenes in the presence of heterofullerenes and endohedral metallofullerenes. *Proceedings - Electrochemical Society* **2001,** 2001-11, (Fullerenes--Volume 11: Fullerenes for the New Millennium), 216-222.

Bisazafullerene (C59N)2 and hydroazafullerene C59HN photosensitize the reaction of alkenes with oxygen. 2-Me 2-butene and □ -terpinene undergo ene and Diels-Alder photooxygenation reactions, resp., in the presence of minute amts. of azafullerenes to produce the corresponding peroxides I, II and III.



9. Alder, R. W.; Harvey, J. N.; Schleyer, P. v. R.; Moran, D., Th-Symmetrical N8(C:C)6 and P8(C:C)6; an Extraordinary Contrast in Heterofullerene Stability. *Organic Letters* **2001,** 3, (21), 3233-3236.

Th-sym. P8(C:C)6, 1, is predicted to be a remarkably stable small heterofullerene with carbon atoms less pyramidal than in C60. Th-N8(C:C)6, 2, in sharp contrast, is strongly destabilized relative to Th-(HC)8(C:C)6. The causes of this extraordinarily large difference (nearly 1000 kJ mol-1) between 1 and 2 are explained.

10. Reuther, U.; Hirsch, A., Synthesis, properties and chemistry of Aza[60]fullerene. *Carbon* **2000,** 38, (11-12), 1539-1549.

A review, with 46 refs., is given on the synthesis, properties and chem. of aza[60]fullerene. A general overview of the state of the art in the field of heterofullerene chem. is given.

11. Ren, A.; Feng, J.; Sun, X.; Li, W.; Tian, W.; Sun, C.; Zheng, X.; Zerner, M. C., Theoretical investigation of the heterofullerenes C59N and C69N and their dimers. *International Journal of Quantum Chemistry* **2000,** 78, (6), 422-436.

The heterofullerenes C59N and C69N and their dimers are examd. by the INDO (INDO/1 and INDO/S) models. The results confirm the stability of the (C59N)2 and (C69)2 (C2h) isomers with a 6-6 closure fusion link between the two monomers.

12. Clipston, N. L.; Brown, T.; Vasil'ev, Y. Y.; Barrow, M. P.; Herzschuh, R.; Reuther, U.; Hirsch, A.; Drewello, T., Laser-Induced Formation, Fragmentation, Coalescence, and Delayed Ionization of the C59N Heterofullerene. *Journal of Physical Chemistry A* **2000,** 104, (40), 9171-9179.

The formation of the nitrogen heterofullerene, C59N, following the ablation of a variety of fullerene derivs., all of which possess org. ligands bound to the carbon cage through a nitrogen atom, has been investigated utilizing laser desorption/ionization mass spectrometry.

13. Suzuki, T., Chemistry of fullerene. Heterofullerenes. *Kikan Kagaku Sosetsu* **1999,** 43, (Furaren no Kagaku), 49-51.

A review, with 16 refs., is given on (1) gas phase formation of heterofullerenes and (2) org. syntheses and chem. properties of azafullerene C59NH and (C59N)2.

14.. Ohtsuki, T.; Masumoto, K.; Sueki, K.; Shikano, K.; Shigematsu, T., Observation of radioactive hetero-fullerenes using radiochemical techniques. *Journal of Radioanalytical and Nuclear Chemistry* **1999,** 239, (2), 365-369.

Fullerenes, C60 and C70, were irradiated by 8 and 10 MeV deuterons. The irradiated samples were dissolved in CS2 and filtered to remove insol. byproducts.

15. Hauke, F.; Hirsch, A., Mannich functionalization of C59N. *Chemical Communications (Cambridge)* **1999**, (21), 2199-2200.

The thermal treatment of the heterofullerene dimer (C59N)2 with ketones and aldehydes in the presence of TsOH and air leads to Mannich-type functionalized heterofullerenes RC59N.

16. Gal'pern, E. G.; Stankevich, I. V.; Chistyakov, A. L.; Chernozatonskii, L. A., Molecular and electronic structure of several heterofullerene BNC58 and B2N2C56 oligomers and [B2N2C56]n macromolecule. *Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya)* **1999,** 48, (3), 428-432.

Mol. and electronic structure of heterofullerene BNC58 (C5) and B2N2C56 (C2h) monomers, B2N2C116 and B4N4C112 dimers, and B6N6C168 trimer (the last three mols. with C2h symmetry) was simulated by the MNDO method.

17. Butcher, M. J.; Jones, F. H.; Moriarty, P.; Beton, P. H.; Prassides, K.; Kordatos, K.; Tagmatarchis, N., Room temperature manipulation of the heterofullerene C59N on Si(100)-2*1. *Applied Physics Letters* **1999,** 75, (8), 1074-1076.

The adsorption of the heterofullerene C59N on the Si(100)-2□ 1 surface was studied using scanning tunneling microscopy (STM) under ultrahigh vacuum conditions. The mols. are adsorbed in monomer form in the troughs between Si dimer rows.

18. Mattay, J.; Torres-Garcia, G.; Averdung, J.; Wolff, C.; Schlachter, I.; Luftmann, H.; Siedschlag, C.; Lugerc, P.; Rammc, M., Progress in fullerene chemistry: exohedral

functionalization of first and second generation and a new approach to aza-heterofullerenes. *Journal of Physics and Chemistry of Solids* **1997,** 58, (11), 1929-1937.

A review, with 37 refs., is given in which the methodol. for exohedral functionalization of fullerenes and their monosubstituted derivs. is discussed (functionalization of 1st and 2nd generation).

19. Cao, B.; Zhou, X.; Gu, Z., Studies of carbon-free fullerenes and boron- or nitrogen-doped fullerenes. *Huaxue Tongbao* **1997**, (12), 1-5.

A review, with 35 refs., is given on carbon-free fullerenes, such as B30N30 and inorg. fullerene-like materials, as well as on bora- and aza-heterofullerenes.

20. Esfarjani, K.; Ohno, K.; Kawazoe, Y., Electronic properties of C58BN heterofullerenes. *Surface Review and Letters* **1996,** 3, (1), 747-752.

Recent studies of electronic structure of solid fullerenes have revealed many interesting properties of these systems. Here, we are interested in the effects of substitution of two carbon atoms by nitrogen and boron. We calc. the electronic structure of the C58BN cluster as well as its dispersion relation in the fcc. cryst. phase.

21. Averdung, J.; Torres-Garcia, G.; Luftmann, H.; Schlachter, I.; Mattay, J., Progress in fullerene chemistry: from exohedral functionalization to heterofullerenes. *Fullerene Science and Technology* **1996,** 4, (4), 633-654.

Various types of cycloaddn. such as [2+1], [2+3], and Diels-Alder reactions have been investigated for the purpose of exohedral functionalization of [60]fullerene and also in few cases of [70]fullerene.

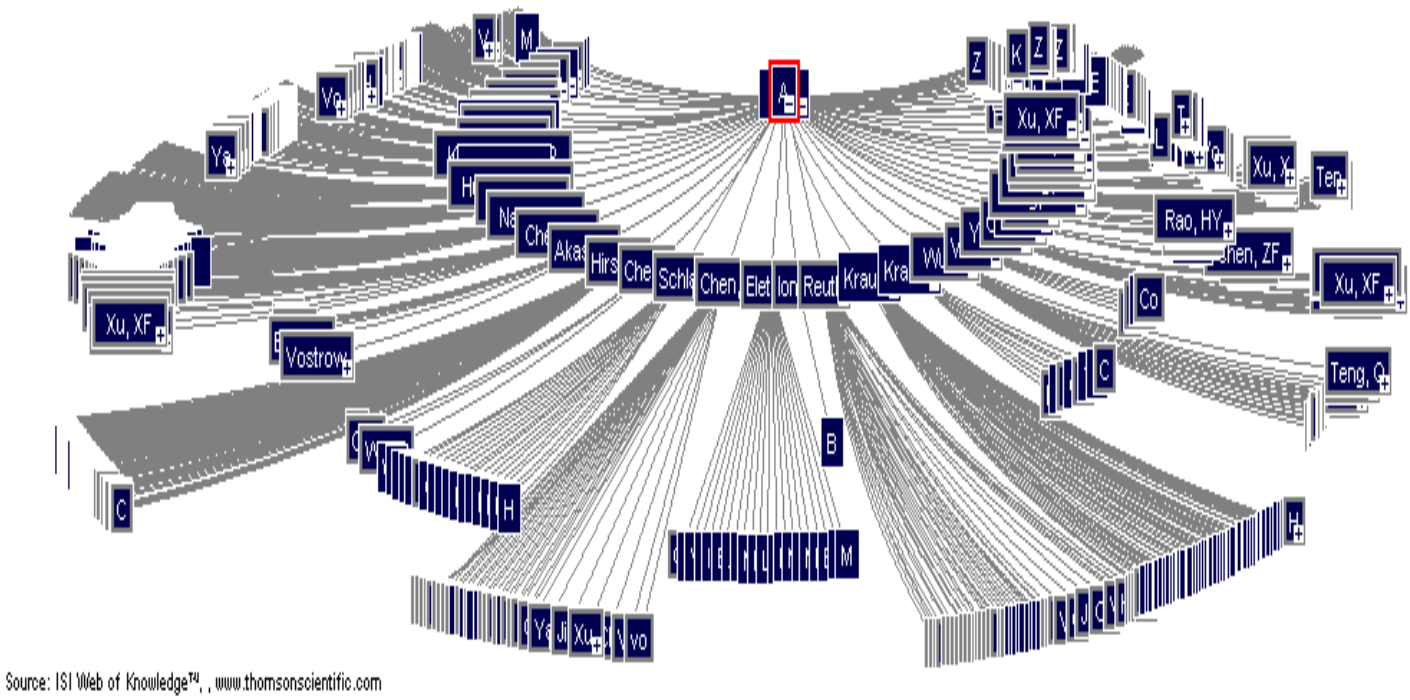
22. Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., Aza-dihydro[60]fullerene in the gas phases. A mass-spectrometric and quantum-chemical study. *Tetrahedron* **1995,** 51, (25), 6977-82.

A new approach to produce heterofullerenes is described. Starting from a fullerene with an intact cage which is activated by suitable exohedral functionalization, the first aza-heterofullerene is generated in the gas phase under DCI mass-spectrometric conditions.

Cycle A

Key Paper:
Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Citation map for key paper:



Citations:

1. ~~Lamparth, I.; Nuber, B.; Schick, G.; Skiebe, A.; Grosser, T.; Hirsch, A., C59N+ AND C69N+ - ISOELECTRONIC HETEROANALOGUES OF C-60 AND C-70. *Angewandte Chemie-International Edition in English* **1995,** 34, (20), 2257-2259.~~
2. ~~Albrecht, K.; Belzner, J., Organic chemistry 1995. *Nachrichten Aus Chemie Technik Und Laboratorium* **1996,** 44, (2), 147-149.~~

3. Averdung, J.; TorresGarcia, G.; Luftmann, H.; Schlachter, I.; Mattay, J., Progress in fullerene chemistry: From exohedral functionalization to heterofullerenes. *Fullerene Science and Technology* **1996,** 4, (4), 633-654.
4. Nuber, B.; Hirsch, A., A new route to nitrogen heterofullerenes and the first synthesis of (C69N)(2). *Chemical Communications* **1996**, (12), 1421-1422.
5. BellaviaLund, C.; KeshavarzK, M.; Collins, T.; Wudl, F., Fullerene carbon resonance assignments through N-15-C-13 coupling constants and location of the sp(3) carbon atoms of (C59N)(2). *Journal of the American Chemical Society* **1997,** 119, (34), 8101-8102.
6. Huczko, A., Heterohedral fullerenes and nanotubes: Formation and characteristics. *Fullerene Science and Technology* **1997,** 5, (6), 1091-1131.
7. Mattay, J.; Torres-Garcia, G.; Averdung, J.; Wolff, C.; Schlachter, I.; Luftmann, H.; Siedschlag, C.; Luger, P.; Ramm, M. In *Progress in fullerene chemistry: Exohedral functionalization of first and second generation and a new approach to aza-heterofullerenes*, 1997; 1997; pp 1929-1937.
8. Prato, M., [60] Fullerene chemistry for materials science applications. *Journal of Materials Chemistry* **1997,** 7, (7), 1097-1109.
9. Shen, C. K. F.; Yu, H. H.; Juo, C. G.; Chien, K. M.; Her, G. R.; Luh, T. Y., Synthesis of 1,2,3,4-bisiminofullerene and 1,2,3,4-bis(triazolino) fullerene - On the mechanism of the addition reactions of organic azides to [60]fullerene. *Chemistry-a European Journal* **1997,** 3, (5), 744-748.
10. Zou, Y.; Wang, Z. J.; Li, W. Z. In *Electronic state studies of a mono-boron-doped giant heterofullerene*, 1997; 1997; pp 1657-1660.
11. Chen, Z. F.; Ma, K. Q.; Chen, L.; Zhao, H. X.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C.; Feng, J. K., Theoretical studies on the substituted fullerenes C60-x-yBxNy (x+y=2). *Theochem-Journal of Molecular Structure* **1998,** 452, 219-225.
12. Chen, Z. F.; Ma, K. Q.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C.; Feng, J. K., Calculations on all possible isomers of the substituted fullerenes C58X2 (X = N,B) using semiempirical methods. *Journal of the Chemical Society-Faraday Transactions* **1998,** 94, (16), 2269-2276.
13. Kanakamma, P. P.; Huang, S. L.; Juo, C. G.; Her, G. R.; Luh, T. Y., Aza-aziridinofullerene: Interconversion between aza-aziridinofullerene and bisazafulleroid. *Chemistry-a European Journal* **1998,** 4, (10), 2037-2042.
14. Rachdi, F.; Hajji, L.; Dollt, H.; Ribet, M.; Yildirim, T.; Fischer, J. E.; Goze, C.; Mehring, M.; Hirsch, A.; Nuber, B. In *NMR investigation of the azafullerene (C59N)(2) and the alkali fullerides NaXC60 with X=2, 4 and 6*, 1998; 1998; pp 607-611.
15. Shang, Z. F.; Pan, Y. M.; Wang, H. X.; Zhao, X. Z.; Tang, A. Q., Theoretical study of C60NH 5/6, 6/6 isomers. *Acta Chimica Sinica* **1998,** 56, (2), 124-128.
16. Akasaka, T.; Okubo, S.; Wakahara, T.; Yamamoto, K.; Kobayashi, K.; Nagase, S.; Kato, T.; Kako, M.; Nakadaira, Y.; Kitayama, Y.; Matsuura, K., Endohedrally metal-doped heterofullerenes: La@C81N and La-2@C79N. *Chemistry Letters* **1999**, (9), 945-946.
17. Chen, Z. F.; Ma, K. Q.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C., Theoretical studies of heterofullerenes C68X2 (X = N, B). *Canadian Journal of Chemistry-Revue Canadienne De Chimie* **1999,** 77, (3), 291-298.

18. Chen, Z. F.; Zhao, X. Z., Recent progress on the theoretical studies of heterofullerenes. *Chinese Journal of Structural Chemistry* **1999,** 18, (6), 463-469.
19. Chen, Z. F.; Zhao, X. Z.; Tang, A. C., Theoretical studies of the substitution patterns in heterofullerenes C60-xNx and C60-xBx (x=2-8). *Journal of Physical Chemistry A* **1999,** 103, (50), 10961-10968.
20. Hirsch, A., Principles of fullerene reactivity. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 1-65.
21. Hirsch, A.; Nuber, B., Nitrogen heterofullerenes. *Accounts of Chemical Research* **1999,** 32, (9), 795-804.
22. Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134.
23. Nagase, S.; Kobayashi, K.; Akasaka, T., Unconventional cage structures of endohedral metallofullerenes. *Journal of Molecular Structure-Theochem* **1999,** 462, 97-104.
24. Schlachter, I.; Howeler, U.; Iwanek, W.; Urbaniak, M.; Mattay, J., Complexation of fullerenes by calix[n]arenes: Molecular dynamic simulations and Benesi-Hildebrand equilibrium constants. *Tetrahedron* **1999,** 55, (52), 14931-14940.
25. Eletskii, A. V., Endohedral structures. *Uspekhi Fizicheskikh Nauk* **2000,** 170, (2), 113-142.
26. Ionov, S. P.; Kuznetsov, N. T.; Alikhanyan, A. S., Modeling of the Heitler-London clusters of the C(x)A(y)L(z) (A = B, N; L = H, F; x, y > 10, z=12 (n+1) and n=0-5) type. *Russian Journal of Coordination Chemistry* **2000,** 26, (6), 388-397.
27. Reuther, U.; Hirsch, A., Synthesis, properties and chemistry of aza[60]fullerene. *Carbon* **2000,** 38, (11-12), 1539-1549.
28. Krause, M.; Baes-Fischlmair, S.; Pfeiffer, R.; Plank, W.; Pichler, T.; Kuzmany, H.; Tagmatarchis, N.; Prassides, K., Thermal stability and high temperature graphitization of bisazafullerene (C59N)(2) as studied by IR and Raman spectroscopy. *Journal of Physical Chemistry B* **2001,** 105, (48), 11964-11969.
29. Krause, M.; Kuzmany, H.; Georgi, P.; Dunsch, L.; Vietze, K.; Seifert, G., Structure and stability of endohedral fullerene Sc3N@C-80: A Raman, infrared, and theoretical analysis. *Journal of Chemical Physics* **2001,** 115, (14), 6596-6605.
30. Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229.
31. Vasil'ev, Y. V.; Abzalimov, R. R.; Tuktarov, R. F.; Nasibullaev, S. K.; Hirsch, A.; Taylor, R.; Drewello, T., In situ hydrogenation of C59N and resonant electron capture of C59NHx (x = 0, 1 and 5). *Chemical Physics Letters* **2002,** 354, (5-6), 361-366.
32. Wu, S.; Teng, Q. W., Studies on electronic structures and spectra of C75N+. *Chemical Journal of Chinese Universities-Chinese* **2002,** 23, (1), 132-134.
33. Yang, X.; Wang, G. C.; Shang, Z. F.; Pan, Y. M.; Cai, Z. S.; Zhao, X. Z., A systematic investigation on the molecular behaviors of boron- or nitrogen-doped C-40 cluster. *Physical Chemistry Chemical Physics* **2002,** 4, (12), 2546-2553.
34. Yang, Z. Y.; Li, R. F.; Yang, X.; Wang, G. C.; Shang, Z. F.; Pan, Y. M.; Wu, B. X.; Zhao, X. Z., The theoretical studies on the structures and relative stability of isomers of C36O. *Chemical Journal of Chinese Universities-Chinese* **2002,** 23, (10), 1926-1929.

35. Yang, Z. Y.; Xu, X. F.; Wang, G. C.; Shang, Z. F.; Cai, Z. S.; Pan, Y. M.; Zhao, X. Z., A systematic investigation on the molecular behaviors of substituted fullerenes C34X2 (X = N, B). *Journal of Molecular Structure-Theochem* **2002,** 618, (3), 191-200.
36. Yang, Z. Y.; Xu, X. F.; Wang, G. C.; Shang, Z. F.; Pan, Y. M.; Zhao, X. Z., Theoretical studies on structures and stabilities of C34BN isomers. *Acta Chimica Sinica* **2002,** 60, (11), 1915-1922.

Cycle B

Key Paper (A):
Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Averdung, J.; TorresGarcia, G.; Luftmann, H.; Schlachter, I.; Mattay, J., Progress in fullerene chemistry: From exohedral functionalization to heterofullerenes. *Fullerene Science and Technology* **1996,** 4, (4), 633-654.
Times Cited: 90

Citations(B):

1. Avent, A. G.; Birkett, P. R.; Darwish, A. D.; Kroto, H. W.; Taylor, R.; Walton, D. R. M., Spontaneous oxidation of C60Ph5X (X=H, Cl) to a benzo[b]furanyl[60]fullerene. *Chemical Communications* **1997**, (16), 1579-1580.
2. Eguchi, S., Synthesis of heterocycle-containing [60]fullerene derivatives .2. Recent progress in [4+2]- and [3+2]- cycloaddition routes. *Fullerene Science and Technology* **1997,** 5, (5), 977-987.
3. Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134.
4. Ohno, M.; Sato, H.; Eguchi, S., Synthesis of fullerotetrahydroquinolines by cycloaddition reaction of C-60 with aza-ortho-xylylenes. *Synlett* **1999**, (2), 207-209.
5. Makurin, Y. N.; Sofronov, A. A.; Ivanovskii, A. L., Electronic structure and conditions for chemical stabilization of fullerene C-28. Exohedral complexes C28M4 (M = H, Cl, Br). *Russian Journal of Coordination Chemistry* **2000,** 26, (7), 464-469.
6. Thilgen, C.; Gosse, I.; Diederich, F., Chirality in fullerene chemistry. In *Topics in Stereochemistry, Vol 23*, 2003; Vol. 23, pp 1-124.
7. Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207.
8. Tovar, A.; Pena, U.; Hernandez, G.; Portillo, R.; Gutierrez, R., Microwave-assisted synthesis of new adducts from the Diels-Alder [4+2]-cycloaddition reaction of chiral alpha-oxo Imines and alpha-diimines with fullerene C-60. *Synthesis-Stuttgart* **2007**, (1), 22-24.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Nuber, B.; Hirsch, A., A new route to nitrogen heterofullerenes and the first synthesis of (C69N)(2). *Chemical Communications* **1996**, (12), 1421-1422.
Times Cited: **70**

The range of the citations was limited from 1997 to 2001 in order to reduce the number of returned citations from 70 to 24.

Citations (B):

1. BellaviaLund, C.; KeshavarzK, M.; Collins, T.; Wudl, F., Fullerene carbon resonance assignments through N-15-C-13 coupling constants and location of the sp(3) carbon atoms of (C59N)(2). *Journal of the American Chemical Society* **1997,** 119, (34), 8101-8102.
2. Huczko, A., Heterohedral fullerenes and nanotubes: Formation and characteristics. *Fullerene Science and Technology* **1997,** 5, (6), 1091-1131.
3. Prassides, K., Fullerenes. *Current Opinion in Solid State & Materials Science* **1997,** 2, (4), 433-439.
4. Prato, M., [60] Fullerene chemistry for materials science applications. *Journal of Materials Chemistry* **1997,** 7, (7), 1097-1109.
5. Thilgen, C.; Herrmann, A.; Diederich, F., The covalent chemistry of higher fullerenes: C-70 and beyond. *Angewandte Chemie-International Edition* **1997,** 36, (21), 2269-2280.
6. Chen, Z. F.; Ma, K. Q.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C.; Feng, J. K., Calculations on all possible isomers of the substituted fullerenes C58X2 (X = N,B) using semiempirical methods. *Journal of the Chemical Society-Faraday Transactions* **1998,** 94, (16), 2269-2276.
7. Nuber, B.; Hirsch, A., Facile synthesis of arylated heterofullerenes ArC59N. *Chemical Communications* **1998**, (3), 405-406.
8. Ren, A. M.; Feng, J. K.; Tian, W. Q.; Sun, X. Y.; Ge, M. F.; Huang, X. R.; Sun, J. Z., Theoretical research on the structures and electronic spectra of free radical C69N and its dimer (C69N)(2). *Chemical Journal of Chinese Universities-Chinese* **1998,** 19, (7), 1131-1135.
9. Chen, Z. F.; Ma, K. Q.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C., Theoretical studies of heterofullerenes C68X2 (X = N, B). *Canadian Journal of Chemistry-Revue Canadienne De Chimie* **1999,** 77, (3), 291-298.
10. Chen, Z. F.; Zhao, X. Z., Recent progress on the theoretical studies of heterofullerenes. *Chinese Journal of Structural Chemistry* **1999,** 18, (6), 463-469.
11. Hauke, F.; Hirsch, A., Mannich functionalization of C59N. *Chemical Communications* **1999**, (21), 2199-2200.

12. Hirsch, A.; Nuber, B., Nitrogen heterofullerenes. *Accounts of Chemical Research* **1999,** 32, (9), 795-804.
13. Jin, H. W.; Feng, J. K.; Ren, A. M.; Fu, W.; Sun, X. Y., Theoretical study on the electronic structure, UV-VIS, NMR spectra and nonlinear second-order optical property of C-59(C6H4CH3)N. *Chinese Journal of Structural Chemistry* **1999,** 18, (6), 451-455.
14. Thilgen, C.; Diederich, F., The higher fullerenes: Covalent chemistry and chirality. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 135-171.
15. Tobe, Y.; Nakanishi, H.; Sonoda, M.; Wakabayashi, T.; Achiba, Y., Pyridine analogue of macrocyclic polyyne C58H4N2 as a precursor to diazafullerene C58N2. *Chemical Communications* **1999**, (17), 1625-1626.
16. Aihara, J., Kinetic instability of azafullerenes. *Journal of Molecular Structure-Theochem* **2000,** 532, 95-102.
17. Clipston, N. L.; Brown, T.; Vasil'ev, Y. Y.; Barrow, M. P.; Herzschuh, R.; Reuther, U.; Hirsch, A.; Drewello, T., Laser-induced formation, fragmentation, coalescence, and delayed ionization of the C59N heterofullerene. *Journal of Physical Chemistry A* **2000,** 104, (40), 9171-9179.
18. Feng, X. D.; Clipston, N.; Brown, T.; Cooper, H.; Reuther, U.; Hirsch, A.; Derrick, P. J.; Drewello, T., Generation and detection of [C59N](+) by laser desorption/ionisation high-field Fourier transform ion cyclotron resonance mass spectrometry. *Rapid Communications in Mass Spectrometry* **2000,** 14, (5), 368-370.
19. Reuther, U.; Hirsch, A., Synthesis, properties and chemistry of aza[60]fullerene. *Carbon* **2000,** 38, (11-12), 1539-1549.
20. Tagmatarchis, N.; Okada, K.; Tomiyama, T.; Shinohara, H., Synthesis and spectroscopic characterization of the second isomer of (C69N)(2) (II) heterofullerene. *Synlett* **2000**, (12), 1761-1764.
21. Xu, J. H.; Li, Y. L.; Guo, Z. X.; Li, F. Y.; Shi, Z. Q.; Pan, C. Y.; Zhu, D. B. In *A novel reaction: [60,70]fullerene reacting with 4,4,5,5-tetramethylimidazoline-2-thione and alpha-aminoacids as carbene reaction*, 2000; 2000; pp 1081-1088.
22. Cases, M.; Duran, M.; Mestres, J.; Martin, N.; Sola, M., Mechanism of the addition reaction of alkyl azides to [60]fullerene and the subsequent N-2 extrusion to form monoimino-[60]fullerenes. *Journal of Organic Chemistry* **2001,** 66, (2), 433-442.
23. Hauke, F.; Hirsch, A., C59N+: A key intermediate in azaheterofullerene chemistry. *Tetrahedron* **2001,** 57, (17), 3697-3708.
24. Murata, Y.; Murata, M.; Komatsu, K., The reaction of fullerene C-60 with 4,6-dimethyl-1,2,3-triazine: Formation of an open-cage fullerene derivative. *Journal of Organic Chemistry* **2001,** 66, (24), 8187-8191.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Huczko, A., Heterohedral fullerenes and nanotubes: Formation and characteristics. *Fullerene Science and Technology* **1997,** 5, (6), 1091-1131.
Times cited: 15

Citations (B):

1. Lange, H.; Huczko, A.; Byszewski, P.; Mizera, E.; Shinohara, H., Influence of boron on carbon arc plasma and formation of fullerenes and nanotubes. *Chemical Physics Letters* **1998,** 289, (1-2), 174-180.
2. Aihara, J., Kinetic instability of boron heterofullerenes. *Fullerene Science and Technology* **1999,** 7, (5), 879-896.
3. Lange, H.; Huczko, A.; Noworyta, K.; Byszewski, P., Carbon-iron arc plasma: Characterization and novel applications. *Czechoslovak Journal of Physics* **1999,** 49, (6), 933-940.
4. Aihara, J., Kinetic instability of azafullerenes. *Journal of Molecular Structure-Theochem* **2000,** 532, 95-102.
5. Aihara, J.; Ishida, T., Kinetic stability of azaborafullerene C58BN as predicted by the bond resonance energy model. *Bulletin of the Chemical Society of Japan* **2000,** 73, (8), 1791-1795.
6. Graja, A., Fullerene research in Poland. *Fullerene Science and Technology* **2000,** 8, (3), 187-223.
7. Lange, H.; Huczko, A., Influence of nitrogen on carbon arc plasma and formation of fullerenes. *Chemical Physics Letters* **2001,** 340, (1-2), 1-6.
8. Makurin, Y. N.; Sofronov, A. A.; Gusev, A. I.; Ivanovsky, A. L., Electronic structure and chemical stabilization of C-28 fullerene. *Chemical Physics* **2001,** 270, (2), 293-308.
9. Lange, H.; Huczko, A.; Sioda, M.; Pacheco, M.; Razafinimanana, M.; Gleizes, A., Influence of gadolinium on carbon arc plasma and formation of fullerenes and nanotubes. *Plasma Chemistry and Plasma Processing* **2002,** 22, (4), 523-536.
10. Stankevich, I. V.; Gal'pern, E. G.; Seto, R., Relations between the total energies of hydrocarbon molecules and carbon clusters and their isostructural analogues with B-N bonds. *Russian Journal of Physical Chemistry* **2003,** 77, (5), 768-773.
11. Song, J.; Vaziri, M., A study of the electronic and structural properties of C-28 and C16N12. *Molecular Physics* **2006,** 104, (2), 319-323.

12. Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207.
13. Bystrzejewski, M.; Huczko, A.; Lange, H.; Cudzilo, S.; Kicinski, W., Combustion synthesis route to carbon-encapsulated iron nanoparticles. *Diamond and Related Materials* **2007,** 16, (2), 225-228.
14. Bystrzejewski, M.; Lange, H.; Huczko, A.; Elim, H. I.; Ji, W., Study of the optical limiting properties of carbon-encapsulated magnetic nanoparticles. *Chemical Physics Letters* **2007,** 444, (1-3), 113-117.
15. Bystrzejewski, M.; Grabias, A.; Borysiuk, J.; Huczko, A.; Lange, H., Mossbauer spectroscopy studies of carbon-encapsulated magnetic nanoparticles obtained by different routes. *Journal of Applied Physics* **2008,** 104, (5).

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Mattay, J.; Torres-Garcia, G.; Averdung, J.; Wolff, C.; Schlachter, I.; Luftmann, H.; Siedschlag, C.; Luger, P.; Ramm, M. In *Progress in fullerene chemistry: Exohedral functionalization of first and second generation and a new approach to aza-heterofullerenes*, 1997; 1997; pp 1929-1937.
Times Cited: 10

Citations (B):

1. Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134.
2. Karaulova, E. N.; Bagrii, E. I., Fullerenes: Functionalisation and the prospects of the use of derivatives. *Uspekhi Khimii* **1999,** 68, (11), 979-998.
3. Ozawa, M.; Deota, P.; Osawa, E., Production of fullerenes by combustion. *Fullerene Science and Technology* **1999,** 7, (3), 387-409.
4. Schlachter, I.; Howeler, U.; Iwanek, W.; Urbaniak, M.; Mattay, J., Complexation of fullerenes by calix[n]arenes: Molecular dynamic simulations and Benesi-Hildebrand equilibrium constants. *Tetrahedron* **1999,** 55, (52), 14931-14940.
5. Makurin, Y. N.; Sofronov, A. A.; Ivanovskii, A. L., Electronic structure and conditions for chemical stabilization of fullerene C-28. Exohedral complexes C28M4 (M = H, Cl, Br). *Russian Journal of Coordination Chemistry* **2000,** 26, (7), 464-469.
6. Bandosz, T. J.; Biggs, M. J.; Gubbins, K. E.; Hattori, Y.; Iiyama, T.; Kaneko, K.; Pikunic, J.; Thomson, K. T., Molecular models of porous carbons. In *Chemistry and Physics of Carbon, Vol 28*, 2003; Vol. 28, pp 41-228.
7. Thilgen, C.; Gosse, I.; Diederich, F., Chirality in fullerene chemistry. In *Topics in Stereochemistry, Vol 23*, 2003; Vol. 23, pp 1-124.
8. Tagmatarchis, N.; Prato, M., Organdullerene materials. In *Fullerene-Based Materials: Structures and Properties*, 2004; Vol. 109, pp 1-39.
9. Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207.
10. Zhang, G. H.; Huang, S. H.; Xiao, Z.; Chen, Q.; Gan, L. B.; Wang, Z. M., Preparation of azafullerene derivatives from fullerene-mixed peroxides and single crystal X-ray structures of azafulleroid and azafullerene. *Journal of the American Chemical Society* **2008,** 130, (38), 12614-+.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Prato, M., [60] Fullerene chemistry for materials science applications. *Journal of Materials Chemistry* **1997,** 7, (7), 1097-1109.
Times Cited: 399

The range of the citations was limited from 1997 to 1998 in order to reduce the number of returned citations from 399 to 28. Increasing the range by even one more year would have resulted in an additional 33 citations.

Citations (B):

1. Avent, A. G.; Benito, A. M.; Birkett, P. R.; Darwish, A. D.; Hitchcock, P. B.; Kroto, H. W.; Locke, I. W.; Meidine, M. F.; O'Donovan, B. F.; Prassides, K.; Taylor, R.; Walton, D. R. M.; van Wijnkoop, M., The structure of fullerene compounds. *Journal of Molecular Structure* **1997,** 437, 1-9.
2. Guldi, D. M.; Maggini, M., Synthesis and photophysical properties of electro- and photoactive fulleropyrrolidines. *Gazzetta Chimica Italiana* **1997,** 127, (12), 779-785.
3. Boudon, C.; Gisselbrecht, J. P.; Gross, M.; Cardullo, F.; Seiler, P.; Isaacs, L.; Nierengarten, J. F.; Haldimann, R. F.; Diederich, F.; Mordasini-Denti, T.; Thiel, W., Redox properties of functionalized fullerenes. *Canadian Journal of Chemical Engineering* **1998,** 76, (6), 1008-1012.
4. Boudon, C.; Gisselbrecht, J. P.; Gross, M.; Herrmann, A.; Ruttimann, M.; Crassous, J.; Cardullo, F.; Echegoyen, L.; Diederich, F., Redox characteristics of covalent derivatives of the higher fullerenes C-70, C-76, and C-78. *Journal of the American Chemical Society* **1998,** 120, (31), 7860-7868.
5. Brustolon, M.; Zoleo, A.; Agostini, G.; Maggini, M., Radical anions of mono- and bis-fulleropyrrolidines: An EPR study. *Journal of Physical Chemistry A* **1998,** 102, (31), 6331-6339.
6. Cardullo, F.; Diederich, F.; Echegoyen, L.; Habicher, T.; Jayaraman, N.; Leblanc, R. M.; Stoddart, J. F.; Wang, S. P., Stable Langmuir and Langmuir-Blodgett films of fullerene-glycodendron conjugates. *Langmuir* **1998,** 14, (8), 1955-1959.

7. Chen, Y.; Zhao, Y.; Cai, R. F.; Huang, Z. E.; Xiao, L. X., Anionic copolymerization of [60]fullerene with styrene initiated by sodium naphthalene. *Journal of Polymer Science Part B-Polymer Physics* **1998,** 36, (14), 2653-2663.
8. Choi, C. H.; Kertesz, M., New interpretation of the valence tautomerism of 1,6-methano[10]annulenes and its application to fullerene derivatives. *Journal of Physical Chemistry A* **1998,** 102, (19), 3429-3437.
9. Chuard, T.; Deschenaux, R., Ferrocene- and Fullerene[60]-containing liquid-crystalline materials. *Chimia* **1998,** 52, (10), 547-550.
10. Dai, L. M.; Lu, J. P.; Matthews, B.; Mau, A. W. H., Doping of conducting polymers by sulfonated fullerene derivatives and dendrimers. *Journal of Physical Chemistry B* **1998,** 102, (21), 4049-4053.
11. Dai, L. M.; Mau, A. W. H.; Zhang, X. Q., Synthesis of fullerene- and fullerol-containing polymers. *Journal of Materials Chemistry* **1998,** 8, (2), 325-330.
12. Deschenaux, R.; Even, M.; Guillon, D., Liquid-crystalline mixed [60]fullerene-ferrocene materials. *Chemical Communications* **1998**, (5), 537-538.
13. Diederich, F.; Gomez-Lopez, M., Supramolecular fullerene materials. *Chimia* **1998,** 52, (10), 551-556.
14. Echegoyen, L.; Echegoyen, L. E., Electrochemistry of fullerenes and their derivatives. *Accounts of Chemical Research* **1998,** 31, (9), 593-601.
15. Ederle, Y.; Mathis, C., Palm-tree architectures derived from C-60-terminated polystyrene. *Macromolecular Rapid Communications* **1998,** 19, (11), 543-547.
16. Gonzalez, B.; Herrera, A.; Illescas, B.; Martin, N.; Martinez, R.; Moreno, F.; Sanchez, L.; Sanchez, A., Diels-Alder cycloadducts of [60]fullerene with pyrimidine o-quinodimethanes. *Journal of Organic Chemistry* **1998,** 63, (20), 6807-6813.
17. Guldi, D. M.; Torres-Garcia, G.; Mattay, J., Intramolecular energy transfer in fullerene pyrazine dyads. *Journal of Physical Chemistry A* **1998,** 102, (48), 9679-9685.
18. Habicher, T.; Nierengarten, J. F.; Gramlich, V.; Diederich, F., Pt-II-directed self-assembly of a dinuclear cyclophane containing two fullerenes. *Angewandte Chemie-International Edition* **1998,** 37, (13-14), 1916-1919.
19. Hsiao, T. Y.; Santhosh, K. C.; Liou, K. F.; Cheng, C. H., Nickel-promoted first ene-diyne cycloaddition reaction on C-60: Synthesis and photochemistry of the fullerene derivatives. *Journal of the American Chemical Society* **1998,** 120, (47), 12232-12236.
20. Llacay, J.; Veciana, J.; Vidal-Gancedo, J.; Bourdelande, J. L.; Gonzalez-Moreno, R.; Rovira, C., Persistent and transient open-shell species derived from C-60-TTF cyclohexene-fused dyads. *Journal of Organic Chemistry* **1998,** 63, (15), 5201-5210.
21. Lu, J.; Dai, L.; Mau, A. W. H., Multi-dimensional doping of polyaniline emeraldine base by hydrogensulfated fullerenol derivatives. *Acta Polymerica* **1998,** 49, (7), 371-375.
22. Maggini, M.; Guldi, D. M.; Mondini, S.; Scorrano, G.; Paolucci, F.; Ceroni, P.; Roffia, S., Photoinduced electron transfer in a tris(2,2 '-bipyridine)-C-60-

ruthenium(II) dyad: Evidence of charge recombination to a fullerene excited state. *Chemistry-a European Journal* **1998,** 4, (10), 1992-2000.
23. Martin, N.; Sanchez, L.; Illescas, B.; Perez, I., C-60-based electroactive organofullerenes. *Chemical Reviews* **1998,** 98, (7), 2527-2547.
24. Nierengarten, J. F.; Schall, C.; Nicoud, J. F.; Heinrich, B.; Guillon, D., Amphiphilic cyclic fullerene bisadducts: Synthesis and Langmuir films at the air-water interface. *Tetrahedron Letters* **1998,** 39, (32), 5747-5750.
25. Prato, M.; Maggini, M., Fulleropyrrolidines: A family of full-fledged fullerene derivatives. *Accounts of Chemical Research* **1998,** 31, (9), 519-526.
26. Song, H.; Lee, K.; Park, J. T.; Choi, M. G., Synthesis, structure, and electrochemical studies of mu(3)-eta(2),eta(2),eta(2)-C-60 triosmium complexes. *Organometallics* **1998,** 17, (20), 4477-4483.
27. Van Lier, G.; Safi, B.; Geerlings, P., Charge delocalisation in hydrofullerenes and substituted hydrofullerenes: effect of deprotonation. *Journal of the Chemical Society-Perkin Transactions 2* **1998**, (2), 349-354.
28. Wang, Z. Y.; Kuang, L.; Meng, X. S.; Gao, J. P., New route to incorporation of [60]fullerene into polymers via the benzocyclobutenone group. *Macromolecules* **1998,** 31, (16), 5556-5558.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Shen, C. K. F.; Yu, H. H.; Juo, C. G.; Chien, K. M.; Her, G. R.; Luh, T. Y., Synthesis of 1,2,3,4-bisiminofullerene and 1,2,3,4-bis(triazolino) fullerene - On the mechanism of the addition reactions of organic azides to [60]fullerene. *Chemistry-a European Journal* **1997,** 3, (5), 744-748.
Times Cited: 32

Citations (B):

1. Nierengarten, J. F.; Habicher, T.; Kessinger, R.; Cardullo, F.; Diederich, F.; Gramlich, V.; Gisselbrecht, J. P.; Boudon, C.; Gross, M., Macrocyclization on the fullerene core: Direct regio- and diastereoselective multi-functionalization of [60]fullerene, and synthesis of fullerene-dendrimer derivatives. *Helvetica Chimica Acta* **1997,** 80, (7), 2238-2276.
2. Bourgeois, J. P.; Echegoyen, L.; Fibbioli, M.; Pretsch, E.; Diederich, F., Regioselective synthesis of trans-1 fullerene bis-adducts directed by a crown ether tether: Alkali metal cation modulated redox properties of fullerene crown ether conjugates. *Angewandte Chemie-International Edition* **1998,** 37, (15), 2118-2121.
3. Kanakamma, P. P.; Huang, S. L.; Juo, C. G.; Her, G. R.; Luh, T. Y., Aza-aziridinofullerene: Interconversion between aza-aziridinofullerene and bisazafulleroid. *Chemistry-a European Journal* **1998,** 4, (10), 2037-2042.
4. Schick, G.; Hirsch, A., Highly diastereoselective formation of stable fulleroids. *Tetrahedron* **1998,** 54, (17), 4283-4296.
5. Ulmer, L.; Torres-Garcia, G.; Luftmann, H.; Mattay, J., Mono- and bisfunctionalization of fullerenes with N-containing reactants. *Journal of Information Recording* **1998,** 24, (3-4), 243-247.
6. Diederich, F.; Kessinger, R., Templated regioselective and stereoselective synthesis in fullerene chemistry. *Accounts of Chemical Research* **1999,** 32, (6), 537-545.
7. Hirsch, A., Principles of fullerene reactivity. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 1-65.
8. Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134.

9. Karaulova, E. N.; Bagrii, E. I., Fullerenes: Functionalisation and the prospects of the use of derivatives. *Uspekhi Khimii* **1999,** 68, (11), 979-998.
10. Rubin, Y., Ring opening reactions of fullerenes: Designed approaches to endohedral metal complexes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 67-91.
11. Rubin, Y.; Ganapathi, P. S.; Franz, A.; An, Y. Z.; Qian, W. Y.; Neier, R., Tandem nucleophilic addition/Diels-Alder reaction of N-butadienyl N,O-ketene silyl acetals with C-60: Stereoselective formation of bicyclic octahydroquinoline-1,2,3,4-tetrahydrobuckminsterfullerenes and combined NMR spectroscopic and computational evaluation of the functionalization reactions. *Chemistry-a European Journal* **1999,** 5, (11), 3162-3184.
12. Schick, G.; Jarrosson, T.; Rubin, Y., Formation of an effective opening within the fullerene core of C-60 by an unusual reaction sequence. *Angewandte Chemie-International Edition* **1999,** 38, (16), 2360-2363.
13. Cases, M.; Duran, M.; Sola, M., The [2+1] cycloaddition of singlet oxycarbonylnitrenes to C-60. *Journal of Molecular Modeling* **2000,** 6, (2), 205-212.
14. Buhl, M.; Hirsch, A., Spherical aromaticity of fullerenes. *Chemical Reviews* **2001,** 101, (5), 1153-1183.
15. Cases, M.; Duran, M.; Mestres, J.; Martin, N.; Sola, M., Mechanism of the addition reaction of alkyl azides to [60]fullerene and the subsequent N-2 extrusion to form monoimino-[60]fullerenes. *Journal of Organic Chemistry* **2001,** 66, (2), 433-442.
16. Haldimann, R. F.; Fokas, C.; Diederich, F., Exploiting the confined reactivity of C-2v-symmetrical pentakis-adducts of [60]fullerene: Regioselective formation of hexakis-, heptakis-, and Octakis-adducts with novel addition patterns by addition of diazomethane followed by dinitrogen extrusion. *Helvetica Chimica Acta* **2001,** 84, (6), 1635-1660.
17. Kabe, Y.; Ohgaki, H.; Yamagaki, T.; Nakanishi, H.; Ando, W., The photochemical reaction of 1,2-digermacyclobutane with C60: possible example of a closed [6,5]-bridged fullerene derivative of germacyclopropane. *Journal of Organometallic Chemistry* **2001,** 636, (1-2), 82-90.
18. Ouchi, A.; Hatsuda, R.; Awen, B. Z. S.; Sakuragi, M.; Ogura, R.; Ishii, T.; Araki, Y.; Ito, O., Large substituent effect on the photochemical rearrangement of 1,6-(N-Aryl)aza-[60]fulleroids to 1,2-(N-Arylaziridino)-[60]fullerenes. *Journal of the American Chemical Society* **2002,** 124, (45), 13364-13365.
19. Romanova, I. P.; Yusupova, G. G.; Nafikova, A. A.; Kovalenko, V. I.; Sinyashin, O. G., Synthesis of a single isomer of the bis-adduct of isocyanurato-substituted azide with [60]fullerene. *Russian Chemical Bulletin* **2002,** 51, (8), 1491-1496.
20. Gonzalez, S.; Martin, N.; Swartz, A.; Guldi, D. M., Addition reaction of azido-exTTFs to C-60: Synthesis of fullerotriazoline and azafulleroid electroactive dyads. *Organic Letters* **2003,** 5, (4), 557-560.
21. Hino, T.; Saigo, K., Unexpected switch in regioselectivity of tether-directed Bingel-type biscyclopropanations depending on the leaving groups at tethered active methylene moieties. *Chemical Communications* **2003**, (3), 402-403.

22. Poater, J.; Fradera, X.; Duran, M.; Sola, M., An insight into the local aromaticities of polycyclic aromatic hydrocarbons and fullerenes. *Chemistry-a European Journal* **2003,** 9, (5), 1113-1122.
23. Ulmer, L.; Mattay, J., Preparation and characterization of sulfonyl-azafulleroid and sulfonylaziridino-fullerene derivatives. *European Journal of Organic Chemistry* **2003**, (15), 2933-2940.
24. Kemner, E.; Hirsch, A.; Zerbetto, F., A Woodward-Hoffmann approach to the C-60 cluster opening leading to homo[6]1fullerenes. *Journal of Physical Chemistry A* **2004,** 108, (35), 7135-7138.
25. Ouchi, A.; Awen, B. Z. S.; Hatsuda, R.; Ogura, R.; Ishii, T.; Araki, Y.; Ito, O., Remote control on the photochemical rearrangement of 1,6-(N-aryl)aza-[60]fulleroids to 1,2-(N-arylaziridino)-[60]fullerenes by N-substituted aryl groups. *Journal of Physical Chemistry A* **2004,** 108, (44), 9584-9592.
26. Tang, G. S.; Chen, X. L.; Zhang, S. Y.; Wang, J., The first trisaza-bridged [60]fulleroid: Drilling a hole on the fullerene. *Organic Letters* **2004,** 6, (22), 3925-3928.
27. Thilgen, C.; Sergeyev, S.; Diederich, F., Spacer-controlled multiple functionalization of fullerenes. In *Templates in Chemistry I*, 2004; Vol. 248, pp 1-61.
28. Chu, C. C.; Hwang, G. L.; Chiou, J. W.; Pong, W. T.; Lin, C. L.; Tsai, C. Y.; Lin, H. M.; Chang, Y. C.; Chang, C. S.; Hsu, A. H.; Huang, W. L.; Guo, J. H.; Chen, P. H.; Luh, T. Y., Polymerization of a confined pi-system: Chemical synthesis of tetrahedral amorphous carbon nanoballs from graphitic carbon nanocapsules. *Advanced Materials* **2005,** 17, (22), 2707-+.
29. Zhou, Z. G.; Wilson, S. R., Tether-directed multiple functionalization of fullerene[60]. *Current Organic Chemistry* **2005,** 9, (8), 789-811.
30. Romanova, I. P.; Yusupova, G. G.; Larionova, O. A.; Nafikova, A. A.; Yakhvarov, D. G.; Zverev, V. V.; Efremov, Y. Y.; Sinyashin, O. G., Synthesis and unusual electrochemical properties of nitropyrimidine-substituted diazadihomo(C-60-I-h)[6,6]fullerene. *Mendeleev Communications* **2006**, (6), 309-311.
31. Greisch, J. F.; De Pauw, E., Mass spectrometric characterization of 3 '-imino[60]fulleryl-3 '-deoxythymidine by collision-induced dissociation. *Journal of Mass Spectrometry* **2007,** 42, (3), 304-311.
32. Reinov, M. V.; Yurovskaya, M. A., The formation of [5,6]- and [6,6]-open fulleroid structures. *Uspekhi Khimii* **2007,** 76, (8), 768-783.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Zou, Y.; Wang, Z. J.; Li, W. Z. In *Electronic state studies of a mono-boron-doped giant heterofullerene*, 1997; 1997; pp 1657-1660.
Times Cited: 2

Citations (B):

1. Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134.
2. ~~Wang, Q.; Chen, H.; Zheng, H., Nonadiabatic approach to dimerization gap and optical absorption coefficient of the Su-Schrieffer-Heeger model. *Physical Review B* **2002,** 66, (17).~~

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Chen, Z. F.; Ma, K. Q.; Chen, L.; Zhao, H. X.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C.; Feng, J. K., Theoretical studies on the substituted fullerenes C60-x-yBxNy (x+y=2). *Theochem-Journal of Molecular Structure* **1998,** 452, 219-225.
Times Cited: 14

Citations (B):

1. Aihara, J., Kinetic instability of boron heterofullerenes. *Fullerene Science and Technology* **1999,** 7, (5), 879-896.
2. Chen, Z.; Ma, K.; Pan, Y.; Zhao, X.; Tang, A., Theoretical studies on the BN substituted fullerenes C70-2x(BN)(x) (x=1-3) - isoelectronic equivalents of C-70. *Journal of Molecular Structure-Theochem* **1999,** 490, 61-68.
3. Chen, Z. F.; Ma, K. Q.; Pan, Y. M.; Zhao, X. Z.; Tang, A. Q., Theoretical studies of P-doped fullerenne C58P2. *Chemical Journal of Chinese Universities-Chinese* **1999,** 20, (12), 1921-1925.
4. Chen, Z. F.; Zhao, X. Z., Recent progress on the theoretical studies of heterofullerenes. *Chinese Journal of Structural Chemistry* **1999,** 18, (6), 463-469.
5. Chen, Z. F.; Zhao, X. Z.; Tang, A. C., Theoretical studies of the substitution patterns in heterofullerenes C60-xNx and C60-xBx (x=2-8). *Journal of Physical Chemistry A* **1999,** 103, (50), 10961-10968.
6. Aihara, J., Kinetic instability of azafullerenes. *Journal of Molecular Structure-Theochem* **2000,** 532, 95-102.
7. Aihara, J.; Ishida, T., Kinetic stability of azaborafullerene C58BN as predicted by the bond resonance energy model. *Bulletin of the Chemical Society of Japan* **2000,** 73, (8), 1791-1795.
8. Pattanayak, J.; Kar, T.; Scheiner, S., Boron-nitrogen (BN) substitution patterns in C/BN hybrid fulterenes: C60-2x(BN)(x) (x=1-7). *Journal of Physical Chemistry A* **2001,** 105, (36), 8376-8384.
9. Pattanayak, J.; Kar, T.; Scheiner, S., Boron-nitrogen (BN) substitution of fullerenes: C-60 to C12B24N24CBN ball. *Journal of Physical Chemistry A* **2002,** 106, (12), 2970-2978.
10. Yang, X.; Wang, G. C.; Shang, Z. F.; Pan, Y. M.; Cai, Z. S.; Zhao, X. Z., A systematic investigation on the molecular behaviors of boron- or nitrogen-doped C-40 cluster. *Physical Chemistry Chemical Physics* **2002,** 4, (12), 2546-2553.
11. Yang, Z. Y.; Xu, X. F.; Wang, G. C.; Shang, Z. F.; Cai, Z. S.; Pan, Y. M.; Zhao, X. Z., A systematic investigation on the molecular behaviors of substituted

fullerenes C34X2 (X = N, B). *Journal of Molecular Structure-Theochem* **2002,** 618, (3), 191-200.
12. Yang, Z. Y.; Xu, X. F.; Wang, G. C.; Shang, Z. F.; Pan, Y. M.; Zhao, X. Z., Theoretical studies on structures and stabilities of C34BN isomers. *Acta Chimica Sinica* **2002,** 60, (11), 1915-1922.
13. Kar, T.; Pattanayak, J.; Scheiner, S., Rules for BN-substitution in BCN-fullerenes. Separation of BN and C domains. *Journal of Physical Chemistry A* **2003,** 107, (41), 8630-8637.
14. Hayashi, A.; Xie, Y. M.; Poblet, J. M.; Campanera, J. M.; Lebrilla, C. B.; Balch, A. L., Mass spectrometric and computational studies of heterofullerenes ([C58Pt](-), [C59Pt](+)) obtained by laser ablation of electrochemically deposited films. *Journal of Physical Chemistry A* **2004,** 108, (12), 2192-2198.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Kanakamma, P. P.; Huang, S. L.; Juo, C. G.; Her, G. R.; Luh, T. Y., Aza-aziridinofullerene: Interconversion between aza-aziridinofullerene and bisazafulleroid. *Chemistry-a European Journal* **1998,** 4, (10), 2037-2042.
Times Cited: 22

Citations (B):

1. Djojo, F.; Hirsch, A.; Grimme, S., The addition patterns of C-60 trisadducts involving the positional relationships e and trans-n (n=2-4): Isolation, properties, and determination of the absolute configuration of tris(malonates) and tris[bis(oxazolines)]. *European Journal of Organic Chemistry* **1999**, (11), 3027-3039.
2. Rubin, Y.; Ganapathi, P. S.; Franz, A.; An, Y. Z.; Qian, W. Y.; Neier, R., Tandem nucleophilic addition/Diels-Alder reaction of N-butadienyl N,O-ketene silyl acetals with C-60: Stereoselective formation of bicyclic octahydroquinoline-1,2,3,4-tetrahydrobuckminsterfullerenes and combined NMR spectroscopic and computational evaluation of the functionalization reactions. *Chemistry-a European Journal* **1999,** 5, (11), 3162-3184.
3. Cases, M.; Duran, M.; Sola, M., The [2+1] cycloaddition of singlet oxycarbonylnitrenes to C-60. *Journal of Molecular Modeling* **2000,** 6, (2), 205-212.
4. Iglesias, M.; Gomez-Lor, B.; Santos, A., New mono- and polyazafulleroids C-60(NR)(n) (n=1, 2, 4, 6) derived from a chiral azide containing N- and O-donor groups, and reactivity with [RhCl(CO)(2)](2). *Journal of Organometallic Chemistry* **2000,** 599, (1), 8-17.
5. Cases, M.; Duran, M.; Mestres, J.; Martin, N.; Sola, M., Mechanism of the addition reaction of alkyl azides to [60]fullerene and the subsequent N-2 extrusion to form monoimino-[60]fullerenes. *Journal of Organic Chemistry* **2001,** 66, (2), 433-442.
6. Kordatos, K.; Bosi, S.; Da Ros, T.; Zambon, A.; Lucchini, V.; Prato, M., Isolation and characterization of all eight bisadducts of fulleropyrrolidine derivatives. *Journal of Organic Chemistry* **2001,** 66, (8), 2802-2808.
7. Ouchi, A.; Hatsuda, R.; Awen, B. Z. S.; Sakuragi, M.; Ogura, R.; Ishii, T.; Araki, Y.; Ito, O., Large substituent effect on the photochemical rearrangement of 1,6-(N-Aryl)aza-[60]fulleroids to 1,2-(N-Arylaziridino)-[60]fullerenes. *Journal of the American Chemical Society* **2002,** 124, (45), 13364-13365.

8. Romanova, I. P.; Yusupova, G. G.; Nafikova, A. A.; Kovalenko, V. I.; Sinyashin, O. G., Synthesis of a single isomer of the bis-adduct of isocyanurato-substituted azide with [60]fullerene. *Russian Chemical Bulletin* **2002,** 51, (8), 1491-1496.
9. Gonzalez, S.; Martin, N.; Swartz, A.; Guldi, D. M., Addition reaction of azido-exTTFs to C-60: Synthesis of fullerotriazoline and azafulleroid electroactive dyads. *Organic Letters* **2003,** 5, (4), 557-560.
10. Thilgen, C.; Gosse, I.; Diederich, F., Chirality in fullerene chemistry. In *Topics in Stereochemistry, Vol 23*, 2003; Vol. 23, pp 1-124.
11. Kemner, E.; Hirsch, A.; Zerbetto, F., A Woodward-Hoffmann approach to the C-60 cluster opening leading to homo[6]1fullerenes. *Journal of Physical Chemistry A* **2004,** 108, (35), 7135-7138.
12. Ouchi, A.; Awen, B. Z. S.; Hatsuda, R.; Ogura, R.; Ishii, T.; Araki, Y.; Ito, O., Remote control on the photochemical rearrangement of 1,6-(N-aryl)aza-[60]fulleroids to 1,2-(N-arylaziridino)-[60]fullerenes by N-substituted aryl groups. *Journal of Physical Chemistry A* **2004,** 108, (44), 9584-9592.
13. Thilgen, C.; Sergeyev, S.; Diederich, F., Spacer-controlled multiple functionalization of fullerenes. In *Templates in Chemistry I*, 2004; Vol. 248, pp 1-61.
14. Zhou, Z. G.; Wilson, S. R., Tether-directed multiple functionalization of fullerene[60]. *Current Organic Chemistry* **2005,** 9, (8), 789-811.
15. Romanova, I. P.; Yusupova, G. G.; Larionova, O. A.; Balandina, A. A.; Latypov, S. K.; Yakhvarov, D. G.; Zverev, V. V.; Sinyashin, O. G., Synthesis and electrochemical properties of individual isomers of isocyanurate-substituted bis-organodiazadihomofullerenes. *Russian Chemical Bulletin* **2006,** 55, (4), 697-702.
16. Zhuang, X. X.; Yang, Z. Y.; Zhang, J. C.; Cao, W. L., Theoretical study on the reaction mechanism of bis-addition of methyl azide to C-60(II). *Journal of Molecular Structure-Theochem* **2006,** 765, (1-3), 53-59.
17. Zhuang, X. X.; Yang, Z. Y.; Zhang, J. C.; Cao, W. L., Theoretical study on the reaction mechanism of bis-addition of methyl azide to C-60. *Journal of Molecular Structure-Theochem* **2006,** 760, (1-3), 45-52.
18. Sander, M.; Jarrosson, T.; Chuang, S. C.; Khan, S. I.; Rubin, Y., Approaches to open fullerenes: Synthesis and thermal stability of cis-1 bis(isobenzofuran) Diels-Alder adducts of C-60. *Journal of Organic Chemistry* **2007,** 72, (8), 2724-2731.
19. Nakahodo, T.; Okada, M.; Morita, H.; Yoshimura, T.; Ishitsuka, M. O.; Tsuchiya, T.; Maeda, Y.; Fujihara, H.; Akasaka, T.; Gao, X.; Nagase, S., [2+1] cycloaddition of nitrene onto C-60 revisited: Interconversion between an aziridinofullerene and an azafulleroid. *Angewandte Chemie-International Edition* **2008,** 47, (7), 1298-1300.
20. Yao, J. Y.; Xiao, Z.; Gan, L. B.; Yang, D. Z.; Wang, Z. M., Towards the rational synthesis of norfullerenes. Controlled deletion of one carbon atom from C-60 and preparation of 2,5,9-trioxo-1-nor(C-60-I-h)[5,6]fullerene C-59(O)(3) derivatives. *Organic Letters* **2008,** 10, (10), 2003-2006.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Rachdi, F.; Hajji, L.; Dollt, H.; Ribet, M.; Yildirim, T.; Fischer, J. E.; Goze, C.; Mehring, M.; Hirsch, A.; Nuber, B. In *NMR investigation of the azafullerene (C59N)(2) and the alkali fullerides NaXC60 with X=2, 4 and 6*, 1998; 1998; pp 607-611.
Times Cited: 7

Citations (B):

1. Chen, Z. F.; Zhao, X. Z., Recent progress on the theoretical studies of heterofullerenes. *Chinese Journal of Structural Chemistry* **1999,** 18, (6), 463-469. dup
2. Reuther, U.; Hirsch, A., Synthesis, properties and chemistry of aza[60]fullerene. *Carbon* **2000,** 38, (11-12), 1539-1549.
3. Pattanayak, J.; Kar, T.; Scheiner, S., Comparison of BN and AlN substitution on the structure and electronic and chemical properties of C-60 fullerene. *Journal of Physical Chemistry A* **2003,** 107, (20), 4056-4065.
4. Schimmelpfennig, B.; Agren, H.; Csillag, S., Theoretical C-13 and N-15 NMR spectra for the C48N12 azafullerene. *Synthetic Metals* **2003,** 132, (3), 265-268.
5. Skadtchenko, B. O.; Trudeau, M.; Schurko, R. W.; Willans, M. J.; Antonelli, D., Structural and spectroscopic studies on mesoporous tantalum oxide-sodium fulleride composites with conducting fulleride columns in the pores. *Advanced Functional Materials* **2003,** 13, (9), 671-681.
6. Teng, Q. W.; Wu, S., Stability and electronic spectroscopy of isomers for C74Si2. *Journal of Molecular Structure-Theochem* **2005,** 756, (1-3), 103-107.
7. Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207. dup

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982. Times Cited: 60

Akasaka, T.; Okubo, S.; Wakahara, T.; Yamamoto, K.; Kobayashi, K.; Nagase, S.; Kato, T.; Kako, M.; Nakadaira, Y.; Kitayama, Y.; Matsuura, K., Endohedrally metal-doped heterofullerenes: La@C81N and La-2@C79N. *Chemistry Letters* **1999**, (9), 945-946. Times Cited: 6

Citations (B):

1. Akasaka, T.; Wakahara, T.; Nagase, S.; Kobayashi, K., Silylfullerenes. *Journal of Synthetic Organic Chemistry Japan* **2000,** 58, (11), 1066-1076.
2. Eletskii, A. V., Endohedral structures. *Uspekhi Fizicheskikh Nauk* **2000,** 170, (2), 113-142.
3. Wakahara, T.; Kako, M.; Maeda, Y.; Akasaka, T.; Kobayashi, K.; Nagase, S., Synthesis and characterization of cyclic silicon compounds of fullerenes. *Current Organic Chemistry* **2003,** 7, (10), 927-943.
4. Yamada, M.; Feng, L.; Wakahara, T.; Tsuchiya, T.; Maeda, Y.; Lian, Y. F.; Kako, M.; Akasaka, T.; Kato, T.; Kobayashi, K.; Nagase, S., Synthesis and characterization of exohedrally silylated M@C-82 (M = Y and La). *Journal of Physical Chemistry B* **2005,** 109, (13), 6049-6051.
5. Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207. dup
6. Zuo, T. M.; Xu, L. S.; Beavers, C. M.; Olmstead, M. M.; Fu, W. J.; Crawford, D.; Balch, A. L.; Dorn, H. C., M-2@C79N (M = Y, Tb): Isolation and characterization of stable endohedral metallofullerenes exhibiting M-M bonding interactions inside aza[80]fullerene cages. *Journal of the American Chemical Society* **2008,** 130, (39), 12992-12997.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Chen, Z. F.; Ma, K. Q.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C., Theoretical studies of heterofullerenes C68X2 (X = N, B). *Canadian Journal of Chemistry-Revue Canadienne De Chimie* **1999,** 77, (3), 291-298.
Times Cited: 16

Citations (B):

1. Chen, Z. F.; Zhao, X. Z., Recent progress on the theoretical studies of heterofullerenes. *Chinese Journal of Structural Chemistry* **1999,** 18, (6), 463-469. dup
2. Chen, Z. F.; Zhao, X. Z.; Tang, A. C., Theoretical studies of the substitution patterns in heterofullerenes C60-xNx and C60-xBx (x=2-8). *Journal of Physical Chemistry A* **1999,** 103, (50), 10961-10968. dup
3. Xie, R. H.; Rao, Q., Third-order optical nonlinearities of higher fullerene and carbon nanotube. *Zeitschrift Fur Naturforschung Section a-a Journal of Physical Sciences* **1999,** 54, (10-11), 645-658.
4. Ivanovskii, A. L., Effect of defects on electronic structure, chemical bonding, and properties of nitrides of group III and IV p elements and materials on their basis. *Russian Journal of Inorganic Chemistry* **2000,** 45, S1-S36.
5. Bergman, J.; Janosik, T.; Wahlstrom, N., Indolocarbazoles. In *Advances in Heterocyclic Chemistry, Vol 80*, 2001; Vol. 80, pp 1-71.
6. Chen, Z. F.; Reuther, U.; Hirsch, A.; Thiel, W., Theoretical studies on the substitution patterns in heterofullerenes C70-xNx and C70-xBx (x=2-10). *Journal of Physical Chemistry A* **2001,** 105, (34), 8105-8110.
7. Ding, C. G.; Yang, Y. L.; Han, R. S.; Wang, K. L., Formation mechanism and structural and electronic properties of metal-substituted fullerenes C69M (M = Co, Rh, and Ir). *Physical Review A* **2001,** 6404, (4).
8. Makurin, Y. N.; Sofronov, A. A.; Gusev, A. I.; Ivanovsky, A. L., Electronic structure and chemical stabilization of C-28 fullerene. *Chemical Physics* **2001,** 270, (2), 293-308.

9. Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229.
10. Chen, Z. F.; Jiao, H. J.; Moran, D.; Hirsch, A.; Thiel, W.; Schleyer, P. V., Aromatic stabilization in heterofullerenes C48X12 (X = N, P, B, Si). *Journal of Physical Organic Chemistry* **2003,** 16, (10), 726-730.
11. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Structures and magnetic properties of mono-doped fullerenes C59Xn and C59X(6-n)- (X = B-, N+, P+, As+, Si): isoelectronic analogues of C-60 and C-60(6-). *Journal of Molecular Modeling* **2003,** 9, (1), 34-38.
12. Pattanayak, J.; Kar, T.; Scheiner, S., Comparison of BN and AlN substitution on the structure and electronic and chemical properties of C-60 fullerene. *Journal of Physical Chemistry A* **2003,** 107, (20), 4056-4065.
13. Gu, F. L.; Chen, Z. F.; Jiao, H. J.; Tian, W. Q.; Aoki, Y.; Thiel, W.; Schleyer, P. V., Study on the optical and magnetic properties of C48N12 azafullerene isomers. *Physical Chemistry Chemical Physics* **2004,** 6, (19), 4566-4570.
14. Chen, Z. F.; King, R. B., Spherical aromaticity: Recent work on fullerenes, polyhedral boranes, and related structures. *Chemical Reviews* **2005,** 105, (10), 3613-3642.
15. Xu, X. F.; Shang, Z. F.; Wang, G. C.; Li, R. F.; Cai, Z. S.; Zhao, X. Z., Theoretical studies of the substitution patterns of boron-nitrogen (BN) fullerenes: From C-50 up to C20B15N15CBN ball. *Journal of Physical Chemistry A* **2005,** 109, (16), 3754-3761.
16. Tang, C.; Deng, K.; Tan, W.; Yuan, Y.; Liu, Y.; Yang, J.; Wang, X. In *Frontier orbitals analysis and density-functional energetics for metal-substituted fullerene C58Fe2*, 2007; 2007; pp 125-128.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Chen, Z. F.; Zhao, X. Z., Recent progress on the theoretical studies of heterofullerenes. *Chinese Journal of Structural Chemistry* **1999,** 18, (6), 463-469.
Times Cited: 3

Citations (B):

1. Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229.
2. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Oxa- and thia-fullerenes (C59O, C59S): Closed or opened cages? *Physical Chemistry Chemical Physics* **2002,** 4, (20), 4916-4920.
3. Wu, S.; Teng, Q. W., Molecular design and studies on electronic spectra for C76Si2. *Chinese Journal of Structural Chemistry* **2004,** 23, (9), 1065-1068.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Chen, Z. F.; Zhao, X. Z.; Tang, A. C., Theoretical studies of the substitution patterns in heterofullerenes C60-xNx and C60-xBx (x=2-8). *Journal of Physical Chemistry A* **1999,** 103, (50), 10961-10968.
Times Cited: 30

Citations (B):

1. Liang, R. S.; Wang, S. F.; Huang, W. T.; Gong, Q. H.; Li, H. B.; Chen, H. Y.; Qiang, D., Measurement of the ultrafast third-order optical nonlinearity of multi-adducts C-70 (NH2CN)(5) and C-70(NH2CNNCNH2)(5). *Journal of Physics D-Applied Physics* **2000,** 33, (18), 2249-2251.
2. Bergman, J.; Janosik, T.; Wahlstrom, N., Indolocarbazoles. In *Advances in Heterocyclic Chemistry, Vol 80*, 2001; Vol. 80, pp 1-71.
3. Chen, Z. F.; Reuther, U.; Hirsch, A.; Thiel, W., Theoretical studies on the substitution patterns in heterofullerenes C70-xNx and C70-xBx (x=2-10). *Journal of Physical Chemistry A* **2001,** 105, (34), 8105-8110.
4. Pattanayak, J.; Kar, T.; Scheiner, S., Boron-nitrogen (BN) substitution patterns in C/BN hybrid fulterenes: C60-2x(BN)(x) (x=1-7). *Journal of Physical Chemistry A* **2001,** 105, (36), 8376-8384.
5. Priyakumar, U. D.; Sastry, G. N., Heterobuckybowls: A theoretical study on the structure, bowl-to-bowl inversion barrier, bond length alternation, structure-inversion barrier relationship, stability, and synthetic feasibility. *Journal of Organic Chemistry* **2001,** 66, (20), 6523-6530.
6. Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229 dup.
7. Mengle-Gaw, L. J.; Schwartz, B. D., Cyclooxygenase-2 inhibitors: promise or peril? *Mediators of Inflammation* **2002,** 11, (5), 275-286.
8. Pattanayak, J.; Kar, T.; Scheiner, S., Boron-nitrogen (BN) substitution of fullerenes: C-60 to C12B24N24CBN ball. *Journal of Physical Chemistry A* **2002,** 106, (12), 2970-2978.

9. Yang, Z. Y.; Xu, X. F.; Wang, G. C.; Shang, Z. F.; Cai, Z. S.; Pan, Y. M.; Zhao, X. Z., A systematic investigation on the molecular behaviors of substituted fullerenes C34X2 (X = N, B). *Journal of Molecular Structure-Theochem* **2002,** 618, (3), 191-200.
10. Brena, B.; Luo, Y., Electronic structures of azafullerene C48N12. *Journal of Chemical Physics* **2003,** 119, (14), 7139-7144.
11. Chen, Z. F.; Jiao, H. J.; Moran, D.; Hirsch, A.; Thiel, W.; Schleyer, P. V., Aromatic stabilization in heterofullerenes C48X12 (X = N, P, B, Si). *Journal of Physical Organic Chemistry* **2003,** 16, (10), 726-730.
12. Han, J. G.; Ren, Z. Y.; Sheng, L. S.; Zhang, Y. W.; Morales, J. A.; Hagelberg, F., The formation of new silicon cages: a semiempirical theoretical investigation. *Journal of Molecular Structure-Theochem* **2003,** 625, 47-58.
13. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Structures and magnetic properties of mono-doped fullerenes C59Xn and C59X(6-n)- (X = B-, N+, P+, As+, Si): isoelectronic analogues of C-60 and C-60(6-). *Journal of Molecular Modeling* **2003,** 9, (1), 34-38.
14. Liang, Y. X.; Shang, Z. F.; Wang, G. C.; Pan, Y. M.; Zhao, X. Z., Studies on the structures and stabilities of C59H3N isomers. *Chemical Journal of Chinese Universities-Chinese* **2003,** 24, (5), 868-871.
15. Pattanayak, J.; Kar, T.; Scheiner, S., Comparison of BN and AlN substitution on the structure and electronic and chemical properties of C-60 fullerene. *Journal of Physical Chemistry A* **2003,** 107, (20), 4056-4065.
16. Gu, F. L.; Chen, Z. F.; Jiao, H. J.; Tian, W. Q.; Aoki, Y.; Thiel, W.; Schleyer, P. V., Study on the optical and magnetic properties of C48N12 azafullerene isomers. *Physical Chemistry Chemical Physics* **2004,** 6, (19), 4566-4570.
17. Hayashi, A.; Xie, Y. M.; Poblet, J. M.; Campanera, J. M.; Lebrilla, C. B.; Balch, A. L., Mass spectrometric and computational studies of heterofullerenes ([C58Pt](-), [C59Pt](+)) obtained by laser ablation of electrochemically deposited films. *Journal of Physical Chemistry A* **2004,** 108, (12), 2192-2198.
18. Xie, R. H.; Bryant, G. W.; Sun, G. Y.; Kar, T.; Chen, Z. F.; Smith, V. H.; Araki, Y.; Tagmatarchis, N.; Shinohara, H.; Ito, O., Tuning spectral properties of fullerenes by substitutional doping. *Physical Review B* **2004,** 69, (20).
19. Campanera, J. M.; Bo, C.; Balch, A. L.; Ferre, J.; Poblet, J. M., Prediction of heterofullerene stabilities: A combined DFT and chemometric study of C56Pt2, C57Pt2 and C81Pt2. *Chemistry-a European Journal* **2005,** 11, (9), 2730-2742.
20. Chen, Z. F.; King, R. B., Spherical aromaticity: Recent work on fullerenes, polyhedral boranes, and related structures. *Chemical Reviews* **2005,** 105, (10), 3613-3642.
21. Liang, Y. X.; Shang, Z. F.; Xu, X. F.; Zhao, X. Z., Structures and stabilities of hydroazafullerenes C60-n(NH)(n) (n=2-3). *Journal of Molecular Structure-Theochem* **2005,** 728, (1-3), 225-229.
22. Pan, X. M.; Fu, Z.; Hong, B.; Zhao, L.; Qiu, Y. Q.; Su, Z. M.; Wang, R. S. In *Theoretical studies of the relative stabilities and electronic properties on B endohedral and exohedral fullerenes*, 2005; 2005; pp 325-328.

23. Xu, X. F.; Shang, Z. F.; Wang, G. C.; Li, R. F.; Cai, Z. S.; Zhao, X. Z., Theoretical studies of the substitution patterns of boron-nitrogen (BN) fullerenes: From C-50 up to C20B15N15CBN ball. *Journal of Physical Chemistry A* **2005,** 109, (16), 3754-3761.
24. Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207. dup
25. Liang, Y. X.; Shui, M.; Li, R. S., Structures and stabilities of boron/nitrogen-doped fullerene C-20. *Acta Physico-Chimica Sinica* **2007,** 23, (10), 1647-1651.
26. Liu, F. L., [5,6]-Heterofulterene-likeC(58)Ge: odd atoms assembling a cage. *Physical Chemistry Chemical Physics* **2007,** 9, (29), 3872-3876.
27. Tarento, R. J.; Joyes, P.; Benlamari, S.; Lahreche, R.; Mekki, D. E. In *C 1s core photoemission of C-60 and C48N12*, 2007; 2007; pp 237-240.
28. Denis, P. A., Theoretical investigation of nitrogen disubstituted corannulenes. *Journal of Molecular Structure-Theochem* **2008,** 865, (1-3), 8-13.
29. Liu, F. L.; Jalbout, A. F., Structural, electronic, and magnetic properties of heterofullerene C58Si with odd number of atoms and a near planar tetracoordinate Si atom. *Journal of Molecular Graphics & Modelling* **2008,** 26, (8), 1327-1332.
30. von Delius, M.; Hauke, F.; Hirsch, A., Evaluation of an intramolecular approach for the synthesis of the elusive C58N2 heterofullerene family. *European Journal of Organic Chemistry* **2008**, (24), 4109-4119.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Hirsch, A.; Nuber, B., Nitrogen heterofullerenes. *Accounts of Chemical Research* **1999,** 32, (9), 795-804.
Times Cited: 93

The range of the citations was limited from 2000 to 2003 in order to reduce the number of returned citations from 93 to 38.

Citations (B):

1. Cases, M.; Duran, M.; Sola, M., The [2+1] cycloaddition of singlet oxycarbonylnitrenes to C-60. *Journal of Molecular Modeling* **2000,** 6, (2), 205-212.
2. Buhl, M.; Hirsch, A., Spherical aromaticity of fullerenes. *Chemical Reviews* **2001,** 101, (5), 1153-1183.
3. Cases, M.; Duran, M.; Mestres, J.; Martin, N.; Sola, M., Mechanism of the addition reaction of alkyl azides to [60]fullerene and the subsequent N-2 extrusion to form monoimino-[60]fullerenes. *Journal of Organic Chemistry* **2001,** 66, (2), 433-442.
4. Chen, Z. F.; Jiao, H. J.; Hirsch, A.; Thiel, W., BN-doped fullerenes: An NICS characterization. *Journal of Organic Chemistry* **2001,** 66, (10), 3380-3383.
5. Chen, Z. F.; Reuther, U.; Hirsch, A.; Thiel, W., Theoretical studies on the substitution patterns in heterofullerenes C70-xNx and C70-xBx (x=2-10). *Journal of Physical Chemistry A* **2001,** 105, (34), 8105-8110.
6. Drechsler, U.; Sandman, D. J.; Foxman, B. M., N-(3-Cyanoprop-2-ynyl)carbazole: synthesis, crystal structure, and solid-state reactivity. *Journal of the Chemical Society-Perkin Transactions 2* **2001**, (4), 581-584.
7. Foley, S.; Bosi, S.; Larroque, C.; Prato, M.; Janot, J. M.; Seta, P., Photophysical properties of novel water soluble fullerene derivatives. *Chemical Physics Letters* **2001,** 350, (3-4), 198-205.
8. Greenwood, N. N., Main group element chemistry at the millennium. *Journal of the Chemical Society-Dalton Transactions* **2001**, (14), 2055-2066.
9. Hirsch, A., New cages and unusual guests: Fullerene chemistry continues to excite. *Angewandte Chemie-International Edition* **2001,** 40, (7), 1195-+.
10. Hirsch, A.; Vostrowsky, O., C-60 hexakisadducts with an octahedral addition pattern - A new structure motif in organic chemistry. *European Journal of Organic Chemistry* **2001**, (5), 829-848.

11. Jie, M.; Cheung, S. W. H.; Ho, J. C. M., Fullerene lipids: Synthesis of novel nitrogen-bridged [60]fullerene fatty ester derivatives. *Lipids* **2001,** 36, (4), 421-426.
12. Lee, K. H.; Park, S. S.; Suh, Y. S.; Yamabe, T.; Osawa, E.; Luthi, H. P.; Gutta, P.; Lee, C. H., Similarities and differences between (C-60)(2)(2-) and (C59N)(2) conformers. *Journal of the American Chemical Society* **2001,** 123, (44), 11085-11086.
13. Murata, Y.; Murata, M.; Komatsu, K., The reaction of fullerene C-60 with 4,6-dimethyl-1,2,3-triazine: Formation of an open-cage fullerene derivative. *Journal of Organic Chemistry* **2001,** 66, (24), 8187-8191.
14. Nakamura, T.; Ishikawa, K.; Goto, A.; Ishihara, M.; Ohana, T.; Koga, Y. In *BN substitution reaction of fullerene using an excimer laser irradiation*, 2001; 2001; pp 1228-1230.
15. Ohno, T.; Moriwaki, K.; Miyata, T., Intramolecular charge-transfer interaction in a new dyad based on C-60 and bis(4 '-tert-butylbiphenyl-4-yl)aniline (BBA) donor. *Journal of Organic Chemistry* **2001,** 66, (10), 3397-3401.
16. Tagmatarchis, N.; Shinohara, H.; Fujitsuka, M.; Ito, O., Photooxidation of olefins sensitized by bisazafullerene (C59N)(2) and hydroazafullerene C59HN: Product analysis, emission of singlet oxygen, and transient absorption spectroscopy. *Journal of Organic Chemistry* **2001,** 66, (24), 8026-8029.
17. Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229.
18. Guldi, D. M.; Luo, C. P.; Da Ros, T.; Bozi, S.; Prato, M., Small reorganisation energy and unique stabilisation of zwitterionic C-60-acceptor moieties. *Chemical Communications* **2002**, (20), 2320-2321.
19. Hauke, F.; Swartz, A.; Guldi, D. M.; Hirsch, A., Supramolecular assembly of a quasi-linear heterofullerene-porphyrin dyad. *Journal of Materials Chemistry* **2002,** 12, (7), 2088-2094.
20. Iwamatsu, S.; Vijayalakshmi, P. S.; Hamajima, M.; Suresh, C. H.; Koga, N.; Suzuki, T.; Murata, S., A novel photorearrangement of a cyclohexadiene derivative of C-60. *Organic Letters* **2002,** 4, (7), 1217-1220.
21. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Oxa- and thia-fullerenes (C59O, C59S): Closed or opened cages? *Physical Chemistry Chemical Physics* **2002,** 4, (20), 4916-4920.
22. Noworyta, K.; Kutner, W.; Deviprasad, G. R.; D'Souza, F., Protonation-induced rearrangements in Langmuir films and redox properties of Langmuir-Blodgett films of 2-(n-alkyl)fulleropyrrolidines. *Synthetic Metals* **2002,** 130, (3), 221-227.
23. Romanova, I. P.; Yusupova, G. G.; Nafikova, A. A.; Kovalenko, V. I.; Sinyashin, O. G., Synthesis of a single isomer of the bis-adduct of isocyanurato-substituted azide with [60]fullerene. *Russian Chemical Bulletin* **2002,** 51, (8), 1491-1496.
24. Sun, N.; Guo, Z. X.; Zhu, D. B., Hexalds-addition reactions of C-60. *Chinese Journal of Organic Chemistry* **2002,** 22, (7), 462-475.

25. Wedig, U.; Brumm, H.; Jansen, M., Synthesis, characterization, and bonding properties of polymeric fullerides AC(70) center dot nNH(3) (A = Ca, Sr, Ba, Eu, Yb). *Chemistry-a European Journal* **2002,** 8, (12), 2769-2774.
26. Bai, J. F.; Virovets, A. V.; Scheer, M., Synthesis of inorganic fullerene-like molecules. *Science* **2003,** 300, (5620), 781-783.
27. Guldi, D. M.; Luo, C. P.; Kotov, N. A.; Da Ros, T.; Bosi, S.; Prato, M., Zwitterionic acceptor moieties: Small reorganization energy and unique stabilization of charge transfer products. *Journal of Physical Chemistry B* **2003,** 107, (30), 7293-7298.
28. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Structures and magnetic properties of mono-doped fullerenes C59Xn and C59X(6-n)- (X = B-, N+, P+, As+, Si): isoelectronic analogues of C-60 and C-60(6-). *Journal of Molecular Modeling* **2003,** 9, (1), 34-38.
29. Kim, K. C.; Hauke, F.; Hirsch, A.; Boyd, P. D. W.; Carter, E.; Armstrong, R. S.; Lay, P. A.; Reed, C. A., Synthesis of the C59N+ carbocation. A monomeric azafullerene isoelectronic to C-60. *Journal of the American Chemical Society* **2003,** 125, (14), 4024-4025.
30. Liang, Y. X.; Shang, Z. F.; Wang, G. C.; Pan, Y. M.; Zhao, X. Z., Studies on the structures and stabilities of C59H3N isomers. *Chemical Journal of Chinese Universities-Chinese* **2003,** 24, (5), 868-871.
31. Liang, Y. X.; Wang, G. C.; Shang, Z. F.; Xu, X. F.; Zhang, C.; Pan, Y. M.; Zhao, X. Z., Studies on the structures and stabilities of C59F2nHN (n=1, 2) isomers. *Chinese Journal of Structural Chemistry* **2003,** 22, (6), 721-728.
32. Liang, Y. X.; Wang, G. C.; Xu, X. F.; Cai, Z. S.; Pan, Y. M.; Zhao, X. Z., Patterns for addition to C59BH. *Physical Chemistry Chemical Physics* **2003,** 5, (9), 1739-1743.
33. Murata, Y.; Murata, M.; Komatsu, K., Synthesis, structure, and properties of novel open-cage fullerenes having heteroatom(s) on the rim of the orifice. *Chemistry-a European Journal* **2003,** 9, (7), 1600-1609.
34. Nakamura, T.; Ishikawa, K.; Goto, A.; Ishihara, A.; Ohana, T.; Koga, Y. In *Synthesis of heterofullerene using a direct BN substitution reaction of fullerene*, 2003; 2003; pp 1908-1911.
35. Schultz, D.; Droppa, R.; Alvarez, F.; dos Santos, M. C., Stability of small carbon-nitride heterofullerenes. *Physical Review Letters* **2003,** 90, (1).
36. Thilgen, C.; Gosse, I.; Diederich, F., Chirality in fullerene chemistry. In *Topics in Stereochemistry, Vol 23*, 2003; Vol. 23, pp 1-124.
37. Vougioukalakis, G. C.; Chronakis, N.; Orfanopoulos, M., Addition of electron-rich aromatics to azafullerenium carbocation. A stepwise electrophilic substitution mechanism. *Organic Letters* **2003,** 5, (24), 4603-4606.
38. Wang, Z. W.; Meier, M. S., Monoalkylation of C-60 and C-70 with Zn and active alkyl bromides. *Journal of Organic Chemistry* **2003,** 68, (8), 3043-3048.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134.
Times Cited: 78

The range of the citations was limited from 1999 to 2002 in order to reduce the number of returned citations from 78 to 25.

Citations (B):

1. Hauke, F.; Hirsch, A., Mannich functionalization of C59N. *Chemical Communications* **1999**, (21), 2199-2200.
2. Hirsch, A.; Nuber, B., Nitrogen heterofullerenes. *Accounts of Chemical Research* **1999,** 32, (9), 795-804.dup
3. Aihara, J., Kinetic instability of azafullerenes. *Journal of Molecular Structure-Theochem* **2000,** 532, 95-102.dup
4. Aihara, J.; Ishida, T., Kinetic stability of azaborafullerene C58BN as predicted by the bond resonance energy model. *Bulletin of the Chemical Society of Japan* **2000,** 73, (8), 1791-1795.
5. Cases, M.; Duran, M.; Sola, M., The [2+1] cycloaddition of singlet oxycarbonylnitrenes to C-60. *Journal of Molecular Modeling* **2000,** 6, (2), 205-212.
6. Ivanovskii, A. L., Effect of defects on electronic structure, chemical bonding, and properties of nitrides of group III and IV p elements and materials on their basis. *Russian Journal of Inorganic Chemistry* **2000,** 45, S1-S36.
7. Ivanovskii, A. L.; Makurin, Y. N.; Sofronov, A. A., Electronic structure and conditions for chemical stabilization of fullerene C-28. Endohedral M@C-28 complexes (M = Sc, Ti, V, Cr, Fe, Cu). *Russian Journal of Coordination Chemistry* **2000,** 26, (10), 714-719.
8. Reed, C. A.; Bolskar, R. D., Discrete fulleride anions and fullerenium cations. *Chemical Reviews* **2000,** 100, (3), 1075-1119.
9. Reuther, U.; Hirsch, A., Synthesis, properties and chemistry of aza[60]fullerene. *Carbon* **2000,** 38, (11-12), 1539-1549.
10. Segura, J. L.; Martin, N., [60]fullerene dimers. *Chemical Society Reviews* **2000,** 29, (1), 13-25.
11. Bagrii, E. I.; Karaulova, E. N., New in fullerene chemistry (a review). *Petroleum Chemistry* **2001,** 41, (5), 295-313.
12. Buhl, M.; Hirsch, A., Spherical aromaticity of fullerenes. *Chemical Reviews* **2001,** 101, (5), 1153-1183.

13. Cases, M.; Duran, M.; Mestres, J.; Martin, N.; Sola, M., Mechanism of the addition reaction of alkyl azides to [60]fullerene and the subsequent N-2 extrusion to form monoimino-[60]fullerenes. *Journal of Organic Chemistry* **2001,** 66, (2), 433-442.
14. Fulop, F.; Rockenbauer, A.; Simon, F.; Pekker, S.; Korecz, L.; Garaj, S.; Janossy, A., Azafullerene C59N, a stable free radical substituent in crystalline C-60. *Chemical Physics Letters* **2001,** 334, (4-6), 233-237.
15. Hirsch, A., New cages and unusual guests: Fullerene chemistry continues to excite. *Angewandte Chemie-International Edition* **2001,** 40, (7), 1195-+.
16. Makurin, Y. N.; Sofronov, A. A.; Gusev, A. I.; Ivanovsky, A. L., Electronic structure and chemical stabilization of C-28 fullerene. *Chemical Physics* **2001,** 270, (2), 293-308.
17. Stafstrom, S.; Hultman, L.; Hellgren, N., Predicted stability of a new aza[60]fullerene molecule, C48N12. *Chemical Physics Letters* **2001,** 340, (3-4), 227-231.
18. Tagmatarchis, N.; Shinohara, H.; Fujitsuka, M.; Ito, O., Photooxidation of olefins sensitized by bisazafullerene (C59N)(2) and hydroazafullerene C59HN: Product analysis, emission of singlet oxygen, and transient absorption spectroscopy. *Journal of Organic Chemistry* **2001,** 66, (24), 8026-8029.
19. Asselberghs, I.; Zhao, Y.; Clays, K.; Persoons, A.; Comito, A.; Rubin, Y., Reversible switching of molecular second-order nonlinear optical polarizability through proton-transfer. *Chemical Physics Letters* **2002,** 364, (3-4), 279-283.
20. Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229.
21. Cheng, F. Y.; Murata, Y.; Komatsu, K., Synthesis, X-ray structure, and properties of the singly bonded C-60 dimer having diethoxyphosphorylmethyl groups utilizing the chemistry of C-60(2-). *Organic Letters* **2002,** 4, (15), 2541-2544.
22. Csanyi, G.; Arias, T. A., Accurate hyperfine couplings for C59N. *Chemical Physics Letters* **2002,** 360, (5-6), 552-556.
23. Guldi, D. M.; Hauke, F.; Hirsch, A., Fullerenes (C-60) versus heteroazafullerenes (C59N); a photophysical comparison of their monoadducts and hexaadducts. *Research on Chemical Intermediates* **2002,** 28, (7-9), 817-830.
24. Hauke, F.; Hirsch, A.; Liu, S. G.; Echegoyen, L.; Swartz, A.; Luo, C. P.; Guldi, D. M., Evidence of pronounced electronic coupling in a directly bonded fullerene-ferrocene dyad. *Chemphyschem* **2002,** 3, (2), 195-+.
25. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Oxa- and thia-fullerenes (C59O, C59S): Closed or opened cages? *Physical Chemistry Chemical Physics* **2002,** 4, (20), 4916-4920.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982. Times Cited: 60

Nagase, S.; Kobayashi, K.; Akasaka, T., Unconventional cage structures of endohedral metallofullerenes. *Journal of Molecular Structure-Theochem* **1999,** 462, 97-104. Times Cited: 34

Citations (B):

1. Kobayashi, K.; Nagase, S., Theoretical study of structures and dynamic properties of Sc-3@C-82. *Chemical Physics Letters* **1999,** 313, (1-2), 45-51.
2. Aihara, J., Kinetic instability of azafullerenes. *Journal of Molecular Structure-Theochem* **2000,** 532, 95-102. dup
3. Aihara, J.; Ishida, T., Kinetic stability of azaborafullerene C58BN as predicted by the bond resonance energy model. *Bulletin of the Chemical Society of Japan* **2000,** 73, (8), 1791-1795.
4. Akasaka, T.; Okubo, S.; Kondo, M.; Maeda, Y.; Wakahara, T.; Kato, T.; Suzuki, T.; Yamamoto, K.; Kobayashi, K.; Nagase, S., Isolation and characterization of two Pr@C-82 isomers. *Chemical Physics Letters* **2000,** 319, (1-2), 153-156.
5. Akasaka, T.; Wakahara, T.; Nagase, S.; Kobayashi, K., Silylfullerenes. *Journal of Synthetic Organic Chemistry Japan* **2000,** 58, (11), 1066-1076.
6. Fujitsuka, M.; Ito, O.; Kobayashi, K.; Nagase, S.; Yamamoto, K.; Kato, T.; Wakahara, T.; Akasaka, T., Transient spectroscopic properties of endohedral metallofullerenes, La@C-82 and La-2@C-80. *Chemistry Letters* **2000**, (8), 902-903.
7. Moriyama, M.; Sato, T.; Yabe, A.; Yamamoto, K.; Kobayashi, K.; Nagase, S.; Wakahara, T.; Akasaka, T., Vibrational spectroscopy of endohedral dimetallofullerene, La-2@C-80. *Chemistry Letters* **2000**, (5), 524-525.
8. Aihara, J., Kinetic stability of carbon cages in non-classical metallofullerenes. *Chemical Physics Letters* **2001,** 343, (5-6), 465-469.
9. Kobayashi, K.; Sano, Y.; Nagase, S., Theoretical study of endohedral metallofullerenes: Sc3-nLanN@C-80 (n=0-3). *Journal of Computational Chemistry* **2001,** 22, (13), 1353-1358.
10. Kobayashi, K.; Nagase, S., A stable unconventional structure of Sc-2@C-66 found by density functional calculations. *Chemical Physics Letters* **2002,** 362, (5-6), 373-379.
11. Slanina, Z.; Kobayashi, K.; Nagase, S., Ca@C-72 IPR and non-IPR structures: computed temperature development of their relative concentrations. *Chemical Physics Letters* **2003,** 372, (5-6), 810-814.

12. Wakahara, T.; Kako, M.; Maeda, Y.; Akasaka, T.; Kobayashi, K.; Nagase, S., Synthesis and characterization of cyclic silicon compounds of fullerenes. *Current Organic Chemistry* **2003,** 7, (10), 927-943.
13. Cheng, H.; Feng, J. K.; Ren, A. M., Theoretical study on the structure, spectra and nonlinear optical susceptibility of Ca @ C-72. *Acta Chimica Sinica* **2004,** 62, (4), 362-368.
14. Ichikawa, T.; Kodama, T.; Suzuki, S.; Fujii, R.; Nishikawa, H.; Ikemoto, I.; Kikuchi, K.; Achiba, Y., Isolation and characterization of a new isomer of Ca@C-72. *Chemistry Letters* **2004,** 33, (8), 1008-1009.
15. Kodama, T.; Fujii, R.; Miyake, Y.; Suzuki, S.; Nishikawa, H.; Ikemoto, I.; Kikuchi, K.; Achiba, Y., C-13 NMR study of Ca@C-74: the cage structure and the site-hopping motion of a Ca atom inside the cage. *Chemical Physics Letters* **2004,** 399, (1-3), 94-97.
16. Matsuoka, H.; Ozawa, N.; Kodama, T.; Nishikawa, H.; Ikemoto, I.; Kikuchi, K.; Furukawa, K.; Sato, K.; Shiomi, D.; Takui, T.; Kato, T., Multifrequency EPR study of metallofullerenes: Eu@C-82 and Eu@C-74. *Journal of Physical Chemistry B* **2004,** 108, (37), 13972-13976.
17. Reich, A.; Panthofer, M.; Modrow, H.; Wedig, U.; Jansen, M., The structure of Ba@C-74. *Journal of the American Chemical Society* **2004,** 126, (44), 14428-14434.
18. Slanina, Z.; Kobayashi, K.; Nagase, S., Ca@C-82 isomers: Computed temperature dependency of relative concentrations. *Journal of Chemical Physics* **2004,** 120, (7), 3397-3400.
19. Campanera, J. M.; Bo, C.; Poblet, J. M., General rule for the stabilization of fullerene cages encapsulating trimetallic nitride templates. *Angewandte Chemie-International Edition* **2005,** 44, (44), 7230-7233.
20. Guha, S.; Nakamoto, K., Electronic structures and spectral properties of endohedral fullerenes. *Coordination Chemistry Reviews* **2005,** 249, (9-10), 1111-1132.
21. Bucher, K.; Epple, L.; Mende, J.; Mehring, M.; Jansen, M. In *Synthesis, isolation and characterization of new endohedral fullerenes M@C-72 (M = Eu, Sr, Yb)*, 2006; 2006; pp 3025-3027.
22. Campanera, J. M.; Bo, C.; Poblet, J. M., Exohedral reactivity of trimetallic nitride template (TNT) endohedral metallofullerenes. *Journal of Organic Chemistry* **2006,** 71, (1), 46-54.
23. Slanina, Z.; Chen, Z. F.; Schleyer, P. V.; Uhlik, F.; Lu, X.; Nagase, S., La-2@C-72 and Sc-2@C-72: Computational characterizations. *Journal of Physical Chemistry A* **2006,** 110, (6), 2231-2234.
24. Slanina, Z.; Nagase, S., Stability computations for Ba@C-74 isomers. *Chemical Physics Letters* **2006,** 422, (1-3), 133-136.
25. Slanina, Z.; Uhlik, F.; Nagase, S., Computed structures of two known Yb@C-74 isomers. *Journal of Physical Chemistry A* **2006,** 110, (47), 12860-12863.
26. Tang, C. M.; Yuan, Y. B.; Deng, K. M.; Yang, J. L., Structural and electronic properties of C-72 and La-2@C-72. *Acta Physica Sinica* **2006,** 55, (7), 3601-3605.

27. Bucher, K.; Mende, J.; Mehring, M.; Jansen, M., Isolation and spectroscopic characterization of Eu@C-72. *Fullerenes Nanotubes and Carbon Nanostructures* **2007,** 15, (1), 29-42.
28. Sato, T.; Kuzumoto, Y.; Tokunaga, K.; Imahori, H.; Tanaka, K., Symmetry of the electronic and geometric structures of metallofullerene M@C-74 (M = Be, Mg, Ca, Sr, and Ba) in terms of vibronic coupling. *Chemical Physics Letters* **2007,** 442, (1-3), 47-52.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Ionov, S. P.; Kuznetsov, N. T.; Alikhanyan, A. S., Modeling of the Heitler-London clusters of the C(x)A(y)L(z) (A = B, N; L = H, F; x, y > 10, z=12 (n+1) and n=0-5) type. *Russian Journal of Coordination Chemistry* **2000,** 26, (6), 388-397.
Times Cited: 1

Citations (B):

~~1. Badalov, A.; Mirsaidov, I. U., System analysis of the thermodynamic properties of binary lanthanide hydrides. *Russian Journal of Physical Chemistry* **2006,** 80, (9), 1521-1524.~~

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Reuther, U.; Hirsch, A., Synthesis, properties and chemistry of aza[60]fullerene. *Carbon* **2000,** 38, (11-12), 1539-1549.
Times Cited: 41

The range of the citations was limited from 2001 to 2005 in order to reduce the number of returned citations from 41 to 22.

Citations (B):

1. Buhl, M.; Hirsch, A., Spherical aromaticity of fullerenes. *Chemical Reviews* **2001,** 101, (5), 1153-1183.
2. Chen, Z. F.; Jiao, H. J.; Hirsch, A.; Thiel, W., BN-doped fullerenes: An NICS characterization. *Journal of Organic Chemistry* **2001,** 66, (10), 3380-3383.
3. Chen, Z. F.; Reuther, U.; Hirsch, A.; Thiel, W., Theoretical studies on the substitution patterns in heterofullerenes C70-xNx and C70-xBx (x=2-10). *Journal of Physical Chemistry A* **2001,** 105, (34), 8105-8110. dup
4. Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229. dup
5. Cheng, W. D.; Wu, D. S.; Zhang, H.; Chen, D. G.; Wang, H. X., Optimization of geometrical structure and simulation of the spectra of third-order nonlinear optical polarizabilities in C59Si and C58Si2 heterofullerenes. *Physical Review B* **2002,** 66, (8).
6. Guldi, D. M.; Hauke, F.; Hirsch, A., Fullerenes (C-60) versus heteroazafullerenes (C59N); a photophysical comparison of their monoadducts and hexaadducts. *Research on Chemical Intermediates* **2002,** 28, (7-9), 817-830.
7. Hauke, F.; Hirsch, A.; Liu, S. G.; Echegoyen, L.; Swartz, A.; Luo, C. P.; Guldi, D. M., Evidence of pronounced electronic coupling in a directly bonded fullerene-ferrocene dyad. *Chemphyschem* **2002,** 3, (2), 195-+.
8. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Oxa- and thia-fullerenes (C59O, C59S): Closed or opened cages? *Physical Chemistry Chemical Physics* **2002,** 4, (20), 4916-4920.
9. Vasil'ev, Y. V.; Abzalimov, R. R.; Tuktarov, R. F.; Nasibullaev, S. K.; Hirsch, A.; Taylor, R.; Drewello, T., In situ hydrogenation of C59N and resonant electron capture of C59NHx (x = 0, 1 and 5). *Chemical Physics Letters* **2002,** 354, (5-6), 361-366.

10. Bandosz, T. J.; Biggs, M. J.; Gubbins, K. E.; Hattori, Y.; Iiyama, T.; Kaneko, K.; Pikunic, J.; Thomson, K. T., Molecular models of porous carbons. In *Chemistry and Physics of Carbon, Vol 28*, 2003; Vol. 28, pp 41-228.
11. Boltalina, O. V.; Goryunkov, A. A.; Markov, V. Y.; Ioffe, I. N.; Sidorov, L. N. In *In situ synthesis and characterization of fullerene derivatives by Knudsen-cell mass spectrometry*, 2003; 2003; pp 807-824.
12. Brena, B.; Luo, Y., Electronic structures of azafullerene C48N12. *Journal of Chemical Physics* **2003,** 119, (14), 7139-7144.
13. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Structures and magnetic properties of mono-doped fullerenes C59Xn and C59X(6-n)- (X = B-, N+, P+, As+, Si): isoelectronic analogues of C-60 and C-60(6-). *Journal of Molecular Modeling* **2003,** 9, (1), 34-38.
14. Murata, Y.; Murata, M.; Komatsu, K., Synthesis, structure, and properties of novel open-cage fullerenes having heteroatom(s) on the rim of the orifice. *Chemistry-a European Journal* **2003,** 9, (7), 1600-1609.
15. Nakamura, T.; Ishikawa, K.; Goto, A.; Ishihara, A.; Ohana, T.; Koga, Y. In *Synthesis of heterofullerene using a direct BN substitution reaction of fullerene*, 2003; 2003; pp 1908-1911.
16. Pattanayak, J.; Kar, T.; Scheiner, S., Comparison of BN and AlN substitution on the structure and electronic and chemical properties of C-60 fullerene. *Journal of Physical Chemistry A* **2003,** 107, (20), 4056-4065.
17. Romanova, I. P.; Yusupova, G. G.; Yakhvarov, D. G.; Larionova, O. A.; Mochul'skaya, N. N.; Sidorova, L. P.; Charushin, V. N.; Zverev, V. V.; Sinyashin, O. G., Reaction of fullerene C-60 with 2-azido-4,6-diphenylpyrimidine. *Russian Chemical Bulletin* **2003,** 52, (10), 2171-2174.
18. Vougioukalakis, G. C.; Chronakis, N.; Orfanopoulos, M., Addition of electron-rich aromatics to azafullerenium carbocation. A stepwise electrophilic substitution mechanism. *Organic Letters* **2003,** 5, (24), 4603-4606.
19. Vougioukalakis, G. C.; Orfanopoulos, M., Photoinduced electron transfer reactivity of aza[60]fullerene: Three discrete functionalization pathways with a single substrate. *Journal of the American Chemical Society* **2004,** 126, (49), 15956-15957.
20. Campanera, J. M.; Bo, C.; Balch, A. L.; Ferre, J.; Poblet, J. M., Prediction of heterofullerene stabilities: A combined DFT and chemometric study of C56Pt2, C57Pt2 and C81Pt2. *Chemistry-a European Journal* **2005,** 11, (9), 2730-2742.
21. Chen, Z. F.; King, R. B., Spherical aromaticity: Recent work on fullerenes, polyhedral boranes, and related structures. *Chemical Reviews* **2005,** 105, (10), 3613-3642.
22. Hauke, F.; Hirsch, A.; Atalick, S.; Guldi, D., Quantitative transduction of excited-state energy in fluorophore-heterofullerene conjugates. *European Journal of Organic Chemistry* **2005**, (9), 1741-1751.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Krause, M.; Baes-Fischlmair, S.; Pfeiffer, R.; Plank, W.; Pichler, T.; Kuzmany, H.; Tagmatarchis, N.; Prassides, K., Thermal stability and high temperature graphitization of bisazafullerene (C59N)(2) as studied by IR and Raman spectroscopy. *Journal of Physical Chemistry B* **2001,** 105, (48), 11964-11969.
Times Cited: 54

The range of the citations was limited from 2002 to 2005 in order to reduce the number of returned citations from 54 to 24.

Citations (B):

1. Alvarez, L.; Pichler, T.; Georgi, P.; Schwieger, T.; Peisert, H.; Dunsch, L.; Hu, Z.; Knupfer, M.; Fink, J.; Bressler, P.; Mast, M.; Golden, M. S., Electronic structure of pristine and intercalated Sc3N@C-80 metallofullerene. *Physical Review B* **2002,** 66, (3).
2. Iezzi, E. B.; Cromer, F.; Stevenson, P.; Dorn, H. C., Synthesis of the first water-soluble trimetallic nitride endohedral metallofullerols. *Synthetic Metals* **2002,** 128, (3), 289-291.
3. Dunsch, L.; Georgi, P.; Krause, M.; Wang, C. R. In *New clusters in endohedral fullerenes: The metalnitrides*, 2003; 2003; pp 761-762.
4. Dunsch, L.; Krause, M.; Noack, J.; Georgi, P. In *Endohedral nitride cluster fullerenes - Formation and spectroscopic analysis of L3-xMxN@C-2n (0 <= x <= 3; N=39,40)*, 2004; 2004; pp 309-315.
5. Gluch, K.; Feil, S.; Matt-Leubner, S.; Echt, O.; Scheier, P.; Mark, T. D., On the stabilization of fullerenes by caged atoms: Singly and multiply charged Sc3N@C-78 and Sc3N@C-80 ions. *Journal of Physical Chemistry A* **2004,** 108, (34), 6990-6995.
6. Golden, M. S.; Pichler, T.; Rudolf, P., Charge transfer and bonding in endohedral fullerenes from high-energy spectroscopy. In *Fullerene-Based Materials: Structures and Properties*, 2004; Vol. 109, pp 201-229.
7. Heine, T.; Vietze, K.; Seifert, G., C-13 NMR fingerprint characterizes long time-scale structure of SC3N@C-80 endohedral fullerene. *Magnetic Resonance in Chemistry* **2004,** 42, S199-S201.
8. Krause, M.; Dunsch, L., Isolation and characterisation of two Sc3N@C-80 isomers. *Chemphyschem* **2004,** 5, (9), 1445-1449.
9. Krause, M.; Popov, V. N.; Inakuma, M.; Tagmatarchis, N.; Shinohara, H.; Georgi, P.; Dunsch, L.; Kuzmany, H., Multipole induced splitting of metal-cage

vibrations in crystalline endohedral D-2d-M-2@C-84 dimetallofullerenes. *Journal of Chemical Physics* **2004,** 120, (4), 1873-1880.
10. Cardona, C. M.; Kitaygorodskiy, A.; Echegoyen, L., Trimetallic nitride endohedral metallofullerenes: Reactivity dictated by the encapsulated metal cluster. *Journal of the American Chemical Society* **2005,** 127, (29), 10448-10453.
11. Cardona, C. M.; Kitaygorodskiy, A.; Ortiz, A.; Herranz, M. A.; Echegoyen, L., The first fulleropyrrolidine derivative of Sc3N@C-80: Pronounced chemical shift differences of the geminal protons on the pyrrolidine ring. *Journal of Organic Chemistry* **2005,** 70, (13), 5092-5097.
12. Elliott, B.; Yu, L.; Echegoyen, L., A simple isomeric separation of D-5h and I-h Sc3N@C-80 by selective chemical oxidation. *Journal of the American Chemical Society* **2005,** 127, (31), 10885-10888.
13. Guha, S.; Nakamoto, K., Electronic structures and spectral properties of endohedral fullerenes. *Coordination Chemistry Reviews* **2005,** 249, (9-10), 1111-1132.
14. Krause, M.; Dunsch, L., Gadolinium nitride Gd3N in carbon cages: The influence of cluster size and bond strength. *Angewandte Chemie-International Edition* **2005,** 44, (10), 1557-1560.
15. Krause, M.; Liu, X. J.; Wong, J.; Pichler, T.; Knupfer, M.; Dunsch, L., The electronic and vibrational structure of endohedral Tm3N@C-80 (I) fullerene - Proof of an encaged Tm3+. *Journal of Physical Chemistry A* **2005,** 109, (32), 7088-7093.
16. Krause, M.; Wong, J.; Dunsch, L., Expanding the world of endohedral fullerenes - The Tm3N@C-2n (39 <= n <= 43) clusterfullerene family. *Chemistry-a European Journal* **2005,** 11, (2), 706-711.
17. Lu, X.; Shi, Z. J.; Sun, B. Y.; He, X. R.; Gu, Z. N., Isolation and spectroscopic study of a series of monogadolinium endohedral metallofullerenes. *Fullerenes Nanotubes and Carbon Nanostructures* **2005,** 13, (1), 13-20.
18. Reveles, J. U.; Heine, T.; Koster, A. M., C-13 NMR pattern of SC3N@C-68. Structural assignment of the first fullerene with adjacent pentagons. *Journal of Physical Chemistry A* **2005,** 109, (32), 7068-7072.
19. Slanina, Z.; Nagase, S., Sc3N@C-80: Computations on the two-isomer equilibrium at high temperatures. *Chemphyschem* **2005,** 6, (10), 2060-2063.
20. Stevenson, S.; Stephen, R. R.; Amos, T. M.; Cadorette, V. R.; Reid, J. E.; Phillips, J. P., Synthesis and purification of a metallic nitride fullerene BisAdduct: Exploring the reactivity of Gd3N@C-80. *Journal of the American Chemical Society* **2005,** 127, (37), 12776-12777.
21. Wolf, M.; Muller, K. H.; Eckert, D.; Skourski, Y.; Georgi, P.; Marczak, R.; Krause, M.; Dunsch, L. In *Magnetic moments in Ho3N@C-80 and Tb3N@C-80*, 2005; 2005; pp 290-293.
22. Wolf, M.; Muller, K. H.; Skourski, Y.; Eckert, D.; Georgi, P.; Krause, M.; Dunsch, L., Magnetic moments of the endohedral cluster fullerenes Ho3N@C-80 and Tb3N@C-80: The role of ligand fields. *Angewandte Chemie-International Edition* **2005,** 44, (21), 3306-3309.

23. Yang, S. F.; Dunsch, L., A large family of dysprosium-based trimetallic nitride endohedral fullerenes: Dy3N@C-2n (39 <= n <= 44). *Journal of Physical Chemistry B* **2005,** 109, (25), 12320-12328.
24. Yumura, T.; Sato, Y.; Suenaga, K.; Iijima, S., Which do endohedral Ti2C80 metallofullerenes prefer energetically: Ti-2@C-80 or Ti2C2@C-78? A theoretical study. *Journal of Physical Chemistry B* **2005,** 109, (43), 20251-20255.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982. Times Cited: 60

Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229. Times Cited: 4

Citations (B):

1. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Oxa- and thia-fullerenes (C59O, C59S): Closed or opened cages? *Physical Chemistry Chemical Physics* **2002,** 4, (20), 4916-4920.
2. Chen, Z. F.; Jiao, H. J.; Moran, D.; Hirsch, A.; Thiel, W.; Schleyer, P. V., Aromatic stabilization in heterofullerenes C48X12 (X = N, P, B, Si). *Journal of Physical Organic Chemistry* **2003,** 16, (10), 726-730.
3. Gu, F. L.; Chen, Z. F.; Jiao, H. J.; Tian, W. Q.; Aoki, Y.; Thiel, W.; Schleyer, P. V., Study on the optical and magnetic properties of C48N12 azafullerene isomers. *Physical Chemistry Chemical Physics* **2004,** 6, (19), 4566-4570.
4. Chen, Z. F.; King, R. B., Spherical aromaticity: Recent work on fullerenes, polyhedral boranes, and related structures. *Chemical Reviews* **2005,** 105, (10), 3613-3642.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Vasil'ev, Y. V.; Abzalimov, R. R.; Tuktarov, R. F.; Nasibullaev, S. K.; Hirsch, A.; Taylor, R.; Drewello, T., In situ hydrogenation of C59N and resonant electron capture of C59NHx (x = 0, 1 and 5). *Chemical Physics Letters* **2002,** 354, (5-6), 361-366.
Times Cited: 5

Citations (B):

1. Cheng, W. D.; Wu, D. S.; Zhang, H.; Chen, D. G.; Wang, H. X., Optimization of geometrical structure and simulation of the spectra of third-order nonlinear optical polarizabilities in C59Si and C58Si2 heterofullerenes. *Physical Review B* **2002,** 66, (8).
2. Liang, Y. X.; Wang, G. C.; Xu, M. F.; Zhang, C.; Cai, Z. S.; Pan, Y. M.; Zhao, X. Z., Structures and stabilities of hydroazafullerenes C59H2n+1N (n=1-5). *Journal of Molecular Structure-Theochem* **2003,** 622, (3), 203-210.
3. Vasil'ev, Y. V.; Hirsch, A.; Taylor, R.; Drewello, T., Hydrogen storage on fullerenes: hydrogenation of C59N center dot using C60H36 as the source of hydrogen. *Chemical Communications* **2004**, (15), 1752-1753.
4. Darwish, A. D.; Abdul-Sada, A. K.; Taylor, R., Pyrolytic trifluoromethylation of [76]-, [78]-, [84]-, and aza[60]fullerenes with silver trifluoroacetate; evidence for coordination of fullerenes to silver. *Fullerenes Nanotubes and Carbon Nanostructures* **2006,** 14, (1), 111-124.
5. Contreras-Torres, F. F.; Basiuk, V. A.; Basiuk, E. V., Regioselectivity in azahydro[60]fullerene derivatives: Application of general-purpose reactivity indicators. *Journal of Physical Chemistry A* **2008,** 112, (35), 8154-8163.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Yang, Z. Y.; Xu, X. F.; Wang, G. C.; Shang, Z. F.; Cai, Z. S.; Pan, Y. M.; Zhao, X. Z., A systematic investigation on the molecular behaviors of substituted fullerenes C34X2 (X = N, B). *Journal of Molecular Structure-Theochem* **2002,** 618, (3), 191-200.
Times Cited: 8

Citations (B):

1. Xu, X. F.; Xing, Y. M.; Shang, Z. F.; Wang, G. C.; Cai, Z. S.; Pan, Y. M.; Zhao, X. Z., Systematic investigation of heterofullerenes the molecular behaviors of C48X2 (X = B, N). *Chemical Physics* **2003,** 287, (3), 317-333.
2. Li, X. D.; Cheng, W. D.; Wu, D. S.; Lan, Y. Z.; Zhang, H.; Gong, Y. J.; Li, F. F.; Shen, J., Modeling of configurations and third-order nonlinear optical properties of C-36 and C34X2 (X = B,N). *Journal of Chemical Physics* **2004,** 121, (12), 5885-5892.
3. Pattanayak, J.; Kar, T.; Scheiner, S., Substitution patterns in mono-BN-fullerenes: C-n (n=20, 24, 28, 32, 36, and 40). *Journal of Physical Chemistry A* **2004,** 108, (38), 7681-7685.
4. Chen, Z. F.; King, R. B., Spherical aromaticity: Recent work on fullerenes, polyhedral boranes, and related structures. *Chemical Reviews* **2005,** 105, (10), 3613-3642.
5. Xu, X. F.; Shang, Z. F.; Wang, G. C.; Li, R. F.; Cai, Z. S.; Zhao, X. Z., Theoretical studies of the substitution patterns of boron-nitrogen (BN) fullerenes: From C-50 up to C20B15N15CBN ball. *Journal of Physical Chemistry A* **2005,** 109, (16), 3754-3761.
6. Dang, H. V.; Stadlbauer, W., Amination of pyrido[3,2,1-jk]carbazol-6-ones. *Journal of Heterocyclic Chemistry* **2006,** 43, (1), 65-70.
7. Liang, Y. X.; Shui, M.; Li, R. S., Structures and stabilities of boron/nitrogen-doped fullerene C-20. *Acta Physico-Chimica Sinica* **2007,** 23, (10), 1647-1651.
8. Liang, C.; Yang, J.; Hao, C.; Li, S. M.; Li, Y.; Jin, Y. F., The interaction between oxygen atom and C-36 (D-6h). *Journal of Molecular Structure-Theochem* **2008,** 851, (1-3), 342-347.

Cycle B

Key Paper (A):

Averdung, J.; Luftmann, H.; Schlachter, I.; Mattay, J., AZA-DIHYDRO[60]FULLERENE IN THE GAS-PHASE - A MASS-SPECTROMETRIC AND QUANTUMCHEMICAL STUDY. *Tetrahedron* **1995,** 51, (25), 6977-6982.
Times Cited: 60

Yang, Z. Y.; Xu, X. F.; Wang, G. C.; Shang, Z. F.; Pan, Y. M.; Zhao, X. Z., Theoretical studies on structures and stabilities of C34BN isomers. *Acta Chimica Sinica* **2002,** 60, (11), 1915-1922.
Times Cited: 3

Citations (B):

1. Rao, H. Y.; Le, Z. G., Theoretical studies on stabilities of C26BN isomers. *Chinese Chemical Letters* **2004,** 15, (2), 246-249.
2. Liang, Y. X.; Shang, Z. F.; Zhao, X. Z., Theoretical studies on the regioselectivity of radical addition to C59XH (X=N, B). *Acta Chimica Sinica* **2005,** 63, (13), 1161-1166.
3. Liang, Y. X.; Shui, M.; Li, R. S., Structures and stabilities of boron/nitrogen-doped fullerene C-20. *Acta Physico-Chimica Sinica* **2007,** 23, (10), 1647-1651.

Cycle C

Key Paper(B)

Averdung, J.; TorresGarcia, G.; Luftmann, H.; Schlachter, I.; Mattay, J., Progress in fullerene chemistry: From exohedral functionalization to heterofullerenes. *Fullerene Science and Technology* **1996,** 4, (4), 633-654.
Times Cited: 90

Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134.
Times cited: 10

Citations:
1. Hauke, F.; Chen, Z. F.; Hirsch, A., Complete assignment of All C-13 NMR signals of C-s symmetric monoazafullerene derivatives by comparison of experimental and calculated spectra. *Polish Journal of Chemistry* **2007,** 81, (5-6), 971-983.
2. Liu, F. L., [5,6]-Heterofulterene-likeC(58)Ge: odd atoms assembling a cage. *Physical Chemistry Chemical Physics* **2007,** 9, (29), 3872-3876.
3. Wang, F. D.; Xiao, Z.; Gan, L. B.; Jia, Z. S.; Jiang, Z. P.; Zhang, S. W.; Zheng, B.; Gu, Y., From fullerene-mixed peroxide to open-cage oxafulleroid C-59(O)(3)(OH)(2)((OOBu)-Bu-t)(2) embedded with furan and lactone motifs. *Organic Letters* **2007,** 9, (9), 1741-1743.
4. Xiao, Z.; Yao, J. Y.; Yang, D. Z.; Wang, F. D.; Huang, S. H.; Gan, L. B.; Jia, Z. S.; Jiang, Z. P.; Yang, X. B.; Zheng, B.; Yuan, G.; Zhang, S. W.; Wang, Z. M., Synthesis of [59]fullerenones through peroxide-mediated stepwise cleavage of fullerene skeleton bonds and x-ray structures of their water-encapsulated open-cage complexes. *Journal of the American Chemical Society* **2007,** 129, (51), 16149-16162.
5. Contreras-Torres, F. F.; Basiuk, V. A.; Basiuk, E. V., Regioselectivity in azahydro[60]fullerene derivatives: Application of general-purpose reactivity indicators. *Journal of Physical Chemistry A* **2008,** 112, (35), 8154-8163.
6. Hoffmann, N., Photochemical reactions as key steps in organic synthesis. *Chemical Reviews* **2008,** 108, (3), 1052-1103.
7. Liang, Y. X.; Shang, Z. F.; Xu, X. F.; Zhao, X. Z., Regioselectivity of 1,3-Butadiene Diels-Alder Cycloaddition to C59XH (X=N, B). *Acta Physico-Chimica Sinica* **2008,** 24, (10), 1811-1816.
8. Liu, F. L.; Jalbout, A. F., Structural, electronic, and magnetic properties of heterofullerene C58Si with odd number of atoms and a near planar tetracoordinate Si atom. *Journal of Molecular Graphics & Modelling* **2008,** 26, (8), 1327-1332.
9. von Delius, M.; Hauke, F.; Hirsch, A., Evaluation of an intramolecular approach for the synthesis of the elusive C58N2 heterofullerene family. *European Journal of Organic Chemistry* **2008**, (24), 4109-4119.

10. Yao, J. Y.; Xiao, Z.; Gan, L. B.; Yang, D. Z.; Wang, Z. M., Towards the rational synthesis of norfullerenes. Controlled deletion of one carbon atom from C-60 and preparation of 2,5,9-trioxo-1-nor(C-60-I-h)[5,6]fullerene C-59(O)(3) derivatives. *Organic Letters* **2008,** 10, (10), 2003-2006.

Key Paper(B)

Nuber, B.; Hirsch, A., A new route to nitrogen heterofullerenes and the first synthesis of (C69N)(2). *Chemical Communications* **1996**, (12), 1421-1422.
Times Cited: **70**

Huczko, A., Heterohedral fullerenes and nanotubes: Formation and characteristics. *Fullerene Science and Technology* **1997,** 5, (6), 1091-1131.Times cited: 5

Citations:
1. Song, J.; Vaziri, M., A study of the electronic and structural properties of C-28 and C16N12. *Molecular Physics* **2006,** 104, (2), 319-323.
2. Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207.
3. Bystrzejewski, M.; Huczko, A.; Lange, H.; Cudzilo, S.; Kicinski, W., Combustion synthesis route to carbon-encapsulated iron nanoparticles. *Diamond and Related Materials* **2007,** 16, (2), 225-228.
4. Bystrzejewski, M.; Lange, H.; Huczko, A.; Elim, H. I.; Ji, W., Study of the optical limiting properties of carbon-encapsulated magnetic nanoparticles. *Chemical Physics Letters* **2007,** 444, (1-3), 113-117.
5. Bystrzejewski, M.; Grabias, A.; Borysiuk, J.; Huczko, A.; Lange, H., Mossbauer spectroscopy studies of carbon-encapsulated magnetic nanoparticles obtained by different routes. *Journal of Applied Physics* **2008,** 104, (5).

Key Paper(B)

Nuber, B.; Hirsch, A., A new route to nitrogen heterofullerenes and the first synthesis of (C69N)(2). *Chemical Communications* **1996**, (12), 1421-1422.
Times Cited: **70**

Reuther, U.; Hirsch, A., Synthesis, properties and chemistry of aza[60]fullerene. *Carbon* **2000,** 38, (11-12), 1539-1549.
Times cited: 8

Citations:

1. Romanova, I. P.; Yusupova, G. G.; Balandina, A. A.; Latypov, S. K.; Yakhvarov, D. G.; Nifant'ev, N. E.; Yashunskii, D. V.; Sinyashin, O. G., Synthesis of the individual regioisomer of the bisadduct of fullerene C-60 with tert-butyl 11-azido-3,6,9-trioxaundecanoate. *Russian Chemical Bulletin* **2007,** 56, (8), 1495-1500.
2. Boudou, J. P.; Schimmelmann, A.; Ader, M.; Mastalerz, M.; Sebilo, M.; Gengembre, L., Organic nitrogen chemistry during low-grade metamorphism. *Geochimica Et Cosmochimica Acta* **2008,** 72, (4), 1199-1221.
3. Contreras-Torres, F. F.; Basiuk, V. A.; Basiuk, E. V., Regioselectivity in azahydro[60]fullerene derivatives: Application of general-purpose reactivity indicators. *Journal of Physical Chemistry A* **2008,** 112, (35), 8154-8163.
4. Hoffmann, N., Photochemical reactions as key steps in organic synthesis. *Chemical Reviews* **2008,** 108, (3), 1052-1103.
5. Kaneko, T.; Li, Y. F.; Nishigaki, S.; Hatakeyama, R., Azafullerene encapsulated single-walled carbon nanotubes with n-type electrical transport property. *Journal of the American Chemical Society* **2008,** 130, (9), 2714-+.
6. Liang, Y. X.; Shang, Z. F.; Xu, X. F.; Zhao, X. Z., Regioselectivity of 1,3-Butadiene Diels-Alder Cycloaddition to C59XH (X=N, B). *Acta Physico-Chimica Sinica* **2008,** 24, (10), 1811-1816.
7. Romanova, I. P.; Larionova, O. A.; Balandina, A. A.; Latypov, S. K.; Mustarina, A. R.; Skripacheva, V. V.; Zverev, V. V.; Sinyashin, O. G., Proton-acceptor properties of azahomofullerene and fullerenoaziridine containing a cyanuric acid fragment. *Russian Journal of General Chemistry* **2008,** 78, (3), 451-456.
8. von Delius, M.; Hauke, F.; Hirsch, A., Evaluation of an intramolecular approach for the synthesis of the elusive C58N2 heterofullerene family. *European Journal of Organic Chemistry* **2008**, (24), 4109-4119.

Key Paper(B)

Huczko, A., Heterohedral fullerenes and nanotubes: Formation and characteristics. *Fullerene Science and Technology* **1997,** 5, (6), 1091-1131.
Times cited: 15

Aihara, J., Kinetic instability of azafullerenes. *Journal of Molecular Structure-Theochem* **2000,** 532, 95-102.
Times cited: 0

Key Paper(B)

Huczko, A., Heterohedral fullerenes and nanotubes: Formation and characteristics. *Fullerene Science and Technology* **1997,** 5, (6), 1091-1131.
Times cited: 15

Aihara, J.; Ishida, T., Kinetic stability of azaborafullerene C58BN as predicted by the bond resonance energy model. *Bulletin of the Chemical Society of Japan* **2000,** 73, (8), 1791-1795.
Times cited: 0

Key Paper(B)

Huczko, A., Heterohedral fullerenes and nanotubes: Formation and characteristics. *Fullerene Science and Technology* **1997,** 5, (6), 1091-1131.
Times cited: 15

Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207.
Times cited: 0

Key Paper(B)

Mattay, J.; Torres-Garcia, G.; Averdung, J.; Wolff, C.; Schlachter, I.; Luftmann, H.; Siedschlag, C.; Luger, P.; Ramm, M. In *Progress in fullerene chemistry: Exohedral functionalization of first and second generation and a new approach to aza-heterofullerenes*, 1997; 1997; pp 1929-1937.
Times Cited: 10

Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134..
Times cited: 11

Citations:

1. Nierengarten, J. F.; Solladie, N. In *Self-assembly of a C-60 derivative bearing an ammonium unit with porphyrin-crown ether conjugates*, 2005; 2005; pp 760-768.
2. Jikeii, M.; Kouketsu, T.; Kakimoto, M. A.; Yamane, Y.; Ando, I., Preparation and properties of polyamide dendrons-poly(4-vinylpyridine) complexes via multiple hydrogen bonding. *High Performance Polymers* **2006,** 18, (4), 421-436.
3. Nierengarten, J. F.; Hahn, U.; Duarte, T. M. F.; Cardinali, F.; Solladie, N.; Walther, M. E.; Van Dorsselaer, A.; Herschbach, H.; Leize, E.; Albrecht-Gary, A. M.; Trabolsi, A.; Elhabiri, M., Ammonium-crown ether interactions for the construction of fullerene-containing photoactive supramolecular devices. *Comptes Rendus Chimie* **2006,** 9, (7-8), 1022-1030.
4. Alexander, A. M.; Bria, M.; Brunklaus, G.; Caldwell, S.; Cooke, G.; Garety, J. F.; Hewage, S. G.; Hocquel, Y.; McDonald, N.; Rabani, G.; Rosair, G.; Smith, B. O.; Spiess, H. W.; Rotello, V. M.; Woisel, P., Probing the solvent-induced tautomerism of a redox-active ureidopyrimidinone. *Chemical Communications* **2007**, (22), 2246-2248.
5. Figueira-Duarte, T. M.; Gegout, A.; Nierengarten, J. F., Molecular and supramolecular C-60-oligophenylenevinylene conjugates. *Chemical Communications* **2007**, (2), 109-119.
6. Imahori, H.; Ueda, M.; Kang, S.; Hayashi, H.; Hayashi, S.; Kaji, H.; Seki, S.; Saeki, A.; Tagawa, S.; Umeyama, T.; Matano, Y.; Yoshida, K.; Isoda, S.; Shiro, M.; Tkachenko, N. V.; Lemmetyinen, H., Effects of porphyrin substituents on film structure and photoelectrochemical properties of porphyrin/fullerene composite clusters electrophoretically deposited on nanostructured SnO2 electrodes. *Chemistry-a European Journal* **2007,** 13, (36), 10182-10193.
7. Langa, F.; de la Cruz, P., Microwave irradiation: An important tool to functionalize fullerenes and carbon nanotubes. *Combinatorial Chemistry & High Throughput Screening* **2007,** 10, (9), 766-782.
8. Wei, X. L.; Luo, W.; Wei, X. W., Supramolecular architectures of fullerenes assembled by hydrogen bonding. *Chinese Journal of Organic Chemistry* **2007,** 27, (2), 153-165.
9. Wessendorf, F.; Gnichwitz, J. F.; Sarova, G. H.; Hager, K.; Hartnagel, U.; Guldi, D. M.; Hirsch, A., Implementation of a hamiliton-receptor-based hydrogen-bonding motif toward a new electron donor-acceptor prototype: Electron versus energy transfer. *Journal of the American Chemical Society* **2007,** 129, (51), 16057-16071.
10. Gnichwitz, J. F.; Wielopolski, M.; Hartnagel, K.; Hartnagel, U.; Guldi, D. M.; Hirsch, A., Cooperativity and tunable excited state deactivation: Modular self-assembly of depsipeptide dendrons on a Hamilton receptor modified porphyrin platform. *Journal of the American Chemical Society* **2008,** 130, (26), 8491-8501.
11. Trabolsi, A.; Urbani, M.; Delgado, J. L.; Ajamaa, F.; Elhabiri, M.; Solladie, N.; Nierengarten, J. F.; Albrecht-Gary, A. M., Large photoactive supramolecular ensembles prepared from C-60-pyridine substrates and multi-Zn(II)-porphyrin receptors. *New Journal of Chemistry* **2008,** 32, (1), 159-165.

Key Paper(B)

Mattay, J.; Torres-Garcia, G.; Averdung, J.; Wolff, C.; Schlachter, I.; Luftmann, H.; Siedschlag, C.; Luger, P.; Ramm, M. In *Progress in fullerene chemistry: Exohedral functionalization of first and second generation and a new approach to aza-heterofullerenes*, 1997; 1997; pp 1929-1937.
Times Cited: 10

Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207.
Times cited: 0

Key Paper(B)

Prato, M., [60] Fullerene chemistry for materials science applications. *Journal of Materials Chemistry* **1997,** 7, (7), 1097-1109.
Times Cited: 399

No topical references found.

Key Paper(B)

Shen, C. K. F.; Yu, H. H.; Juo, C. G.; Chien, K. M.; Her, G. R.; Luh, T. Y., Synthesis of 1,2,3,4-bisiminofullerene and 1,2,3,4-bis(triazolino) fullerene - On the mechanism of the addition reactions of organic azides to [60]fullerene. *Chemistry-a European Journal* **1997,** 3, (5), 744-748.

Times Cited: 32

Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134.
Times cited: 0

This is the only topical reference and it is a duplicate.

Key Paper(B)

Zou, Y.; Wang, Z. J.; Li, W. Z. In *Electronic state studies of a mono-boron-doped giant heterofullerene*, 1997; 1997; pp 1657-1660.
Times Cited: 2

Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134.
Times cited: 0

This is the only topical reference and it is a duplicate.

Key Paper(B)

Chen, Z. F.; Ma, K. Q.; Chen, L.; Zhao, H. X.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C.; Feng, J. K., Theoretical studies on the substituted fullerenes C60-x-yBxNy (x+y=2). *Theochem-Journal of Molecular Structure* **1998,** 452, 219-225.

Times Cited: 14

Aihara, J., Kinetic instability of boron heterofullerenes. *Fullerene Science and Technology* **1999,** 7, (5), 879-896.
Times cited: 0

Key Paper(B)

Chen, Z. F.; Ma, K. Q.; Chen, L.; Zhao, H. X.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C.; Feng, J. K., Theoretical studies on the substituted fullerenes C60-x-yBxNy (x+y=2). *Theochem-Journal of Molecular Structure* **1998,** 452, 219-225.
Times Cited: 14

Chen, Z. F.; Zhao, X. Z., Recent progress on the theoretical studies of heterofullerenes. *Chinese Journal of Structural Chemistry* **1999,** 18, (6), 463-469.
Times cited: 3

Citations:
1. Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229.
2. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Oxa- and thia-fullerenes (C59O, C59S): Closed or opened cages? *Physical Chemistry Chemical Physics* **2002,** 4, (20), 4916-4920.
3. Wu, S.; Teng, Q. W., Molecular design and studies on electronic spectra for C76Si2. *Chinese Journal of Structural Chemistry* **2004,** 23, (9), 1065-1068.

Key Paper(B)

Chen, Z. F.; Ma, K. Q.; Chen, L.; Zhao, H. X.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C.; Feng, J. K., Theoretical studies on the substituted fullerenes C60-x-yBxNy (x+y=2). *Theochem-Journal of Molecular Structure* **1998,** 452, 219-225.
Times Cited: 14

Chen, Z. F.; Zhao, X. Z.; Tang, A. C., Theoretical studies of the substitution patterns in heterofullerenes C60-xNx and C60-xBx (x=2-8). *Journal of Physical Chemistry A* **1999,** 103, (50), 10961-10968.
Times cited: 6

Citations:
1. Liang, Y. X.; Shui, M.; Li, R. S., Structures and stabilities of boron/nitrogen-doped fullerene C-20. *Acta Physico-Chimica Sinica* **2007,** 23, (10), 1647-1651.
2. Liu, F. L., [5,6]-Heterofulterene-likeC(58)Ge: odd atoms assembling a cage. *Physical Chemistry Chemical Physics* **2007,** 9, (29), 3872-3876.
3. Tarento, R. J.; Joyes, P.; Benlamari, S.; Lahreche, R.; Mekki, D. E. In *C 1s core photoemission of C-60 and C48N12*, 2007; 2007; pp 237-240.
4. Denis, P. A., Theoretical investigation of nitrogen disubstituted corannulenes. *Journal of Molecular Structure-Theochem* **2008,** 865, (1-3), 8-13.
5. Liu, F. L.; Jalbout, A. F., Structural, electronic, and magnetic properties of heterofullerene C58Si with odd number of atoms and a near planar tetracoordinate Si atom. *Journal of Molecular Graphics & Modelling* **2008,** 26, (8), 1327-1332.
6. von Delius, M.; Hauke, F.; Hirsch, A., Evaluation of an intramolecular approach for the synthesis of the elusive C58N2 heterofullerene family. *European Journal of Organic Chemistry* **2008**, (24), 4109-4119.

Key Paper(B)

Chen, Z. F.; Ma, K. Q.; Chen, L.; Zhao, H. X.; Pan, Y. M.; Zhao, X. Z.; Tang, A. C.; Feng, J. K., Theoretical studies on the substituted fullerenes C60-x-yBxNy (x+y=2). *Theochem-Journal of Molecular Structure* **1998,** 452, 219-225.
Times Cited: 14

Aihara, J., Kinetic instability of azafullerenes. *Journal of Molecular Structure-Theochem* **2000,** 532, 95-102.
Times cited: 4

Citations:
1. Ionov, S. P.; Kuznetsov, N. T.; Sevast'yanov, V. G., Thermodynamics of coordination bonds in metal closo heteroclusters of the endofullerene type MNk, Br, Csn, m = k+r+s = 12, 24, or 28; n = 0-4, where M = Li, Mg, Al, Ti, Zr, Hf, V, Nb, Mo, Ru, Rh, Ir, Ta, Pt, Pd, and Au. *Russian Journal of Coordination Chemistry* **2003,** 29, (11), 766-772.

2. Balaban, A. T.; Oniciu, D. C.; Katritzky, A. R., Aromaticity as a cornerstone of heterocyclic chemistry. *Chemical Reviews* **2004,** 104, (5), 2777-2812.
3. Dang, H. V.; Stadlbauer, W., Amination of pyrido[3,2,1-jk]carbazol-6-ones. *Journal of Heterocyclic Chemistry* **2006,** 43, (1), 65-70.
4. Ewels, C. P., Nitrogen violation of the isolated pentagon rule. *Nano Letters* **2006,** 6, (5), 890-895.

Key Paper(B)

Kanakamma, P. P.; Huang, S. L.; Juo, C. G.; Her, G. R.; Luh, T. Y., Aza-aziridinofullerene: Interconversion between aza-aziridinofullerene and bisazafulleroid. *Chemistry-a European Journal* **1998,** 4, (10), 2037-2042.
Times Cited: 22

No topical references found.

Key Paper(B)

Chen, Z. F.; Zhao, X. Z., Recent progress on the theoretical studies of heterofullerenes. *Chinese Journal of Structural Chemistry* **1999,** 18, (6), 463-469.
Times cited: 3

Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229.
Times cited: 4

Citations:

1. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Oxa- and thia-fullerenes (C59O, C59S): Closed or opened cages? *Physical Chemistry Chemical Physics* **2002,** 4, (20), 4916-4920.
2. Chen, Z. F.; Jiao, H. J.; Moran, D.; Hirsch, A.; Thiel, W.; Schleyer, P. V., Aromatic stabilization in heterofullerenes C48X12 (X = N, P, B, Si). *Journal of Physical Organic Chemistry* **2003,** 16, (10), 726-730.
3. Gu, F. L.; Chen, Z. F.; Jiao, H. J.; Tian, W. Q.; Aoki, Y.; Thiel, W.; Schleyer, P. V., Study on the optical and magnetic properties of C48N12

azafullerene isomers. *Physical Chemistry Chemical Physics* **2004,** 6, (19), 4566-4570.
4. Chen, Z. F.; King, R. B., Spherical aromaticity: Recent work on fullerenes, polyhedral boranes, and related structures. *Chemical Reviews* **2005,** 105, (10), 3613-3642.

Key Paper(B)

Chen, Z. F.; Zhao, X. Z.; Tang, A. C., Theoretical studies of the substitution patterns in heterofullerenes C60-xNx and C60-xBx (x=2-8). *Journal of Physical Chemistry A* **1999,** 103, (50), 10961-10968.
Times Cited: 30

Brena, B.; Luo, Y., Electronic structures of azafullerene C48N12. *Journal of Chemical Physics* **2003,** 119, (14), 7139-7144.
Times cited: 0

Key Paper(B)

Hirsch, A.; Nuber, B., Nitrogen heterofullerenes. *Accounts of Chemical Research* **1999,** 32, (9), 795-804.
Times Cited: 93

No topical references found.

Key Paper(B)

Hummelen, J. C.; Bellavia-Lund, C.; Wudl, F., Heterofullerenes. In *Fullerenes and Related Structures*, 1999; Vol. 199, pp 93-134.
Times Cited: 78

Bagrii, E. I.; Karaulova, E. N., New in fullerene chemistry (a review). *Petroleum Chemistry* **2001,** 41, (5), 295-313.
Times cited: 4

Citations:
1. Nekhaev, A. I.; Bagrii, E. I., Transformations of saturated hydrocarbons at room temperature in the presence of the fullerene C-60-aluminum bromide-hydrochloric acid system. *Petroleum Chemistry* **2003,** 43, (6), 383-386.
2. Lyon, D. Y.; Fortner, J. D.; Sayes, C. M.; Colvin, V. L.; Hughes, J. B., Bacterial cell association and antimicrobial activity of a C-60 water suspension. *Environmental Toxicology and Chemistry* **2005,** 24, (11), 2757-2762.
3. Lee, J.; Fortner, J. D.; Hughes, J. B.; Kim, J. H., Photochemical production of reactive oxygen species by C-60 in the aqueous phase during UV irradiation. *Environmental Science & Technology* **2007,** 41, (7), 2529-2535.
4. Klaine, S. J.; Alvarez, P. J. J.; Batley, G. E.; Fernandes, T. F.; Handy, R. D.; Lyon, D. Y.; Mahendra, S.; McLaughlin, M. J.; Lead, J. R., Nanomaterials in the environment: Behavior, fate, bioavailability, and effects. *Environmental Toxicology and Chemistry* **2008,** 27, (9), 1825-1851.

Key Paper(B)

Nagase, S.; Kobayashi, K.; Akasaka, T., Unconventional cage structures of endohedral metallofullerenes. *Journal of Molecular Structure-Theochem* **1999,** 462, 97-104.
Times Cited: 34

Aihara, J.; Ishida, T., Kinetic stability of azaborafullerene C58BN as predicted by the bond resonance energy model. *Bulletin of the Chemical Society of Japan* **2000,** 73, (8), 1791-1795.
Times cited: 2

Citations:
1. Dang, H. V.; Stadlbauer, W., Amination of pyrido[3,2,1-jk]carbazol-6-ones. *Journal of Heterocyclic Chemistry* **2006,** 43, (1), 65-70.
2. Kerim, A., Study on the aromaticity of all possible C36CH2 isomers. *Acta Chimica Sinica* **2007,** 65, (9), 841-846.

Key Paper(B)

Ionov, S. P.; Kuznetsov, N. T.; Alikhanyan, A. S., Modeling of the Heitler-London clusters of the C(x)A(y)L(z) (A = B, N; L = H, F; x, y > 10, z=12 (n+1) and n=0-5) type. *Russian Journal of Coordination Chemistry* **2000,** 26, (6), 388-397.
Times Cited: 1

No topical references found.

Key Paper(B)

Krause, M.; Baes-Fischlmair, S.; Pfeiffer, R.; Plank, W.; Pichler, T.; Kuzmany, H.; Tagmatarchis, N.; Prassides, K., Thermal stability and high temperature graphitization of bisazafullerene (C59N)(2) as studied by IR and Raman spectroscopy. *Journal of Physical Chemistry B* **2001,** 105, (48), 11964-11969.
Times Cited: 54

No topical references found.

Key Paper(B)

Chen, Z. F.; Wang, G. C.; Zhao, X. Z.; Tang, A. C., Isomerism and aromaticity of heterofullerene C70-nPn (n=2-10). *Journal of Molecular Modeling* **2002,** 8, (7), 223-229.
Times Cited: 4

Chen, Z. F.; Jiao, H. J.; Moran, D.; Hirsch, A.; Thiel, W.; Schleyer, P. V., Aromatic stabilization in heterofullerenes C48X12 (X = N, P, B, Si). *Journal of Physical Organic Chemistry* **2003,** 16, (10), 726-730.
Times cited: 6

Citations:

1. Chen, Z. F.; King, R. B., Spherical aromaticity: Recent work on fullerenes, polyhedral boranes, and related structures. *Chemical Reviews* **2005,** 105, (10), 3613-3642.

2. Cyranski, M. K., Energetic aspects of cyclic Pi-electron delocalization: Evaluation of the methods of estimating aromatic stabilization energies. *Chemical Reviews* **2005,** 105, (10), 3773-3811.
3. Lu, X.; Chen, Z. F., Curved Pi-conjugation, aromaticity, and the related chemistry of small fullerenes (< C-60) and single-walled carbon nanotubes. *Chemical Reviews* **2005,** 105, (10), 3643-3696.
4. Shainyan, B. A., Rules for counting electrons and three-dimensional aromaticity. *Russian Journal of Organic Chemistry* **2006,** 42, (2), 304-306.
5. Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207.
6. Emanuele, E.; Negri, F.; Orlandi, G., Structure, stability and spectroscopic properties of isomers Of C48B6N6 heterofullerene with isolated and sequential BN substitutional patterns. *Inorganica Chimica Acta* **2007,** 360, (3), 1052-1062.

Key Paper(B)

Vasil'ev, Y. V.; Abzalimov, R. R.; Tuktarov, R. F.; Nasibullaev, S. K.; Hirsch, A.; Taylor, R.; Drewello, T., In situ hydrogenation of C59N and resonant electron capture of C59NHx (x = 0, 1 and 5). *Chemical Physics Letters* **2002,** 354, (5-6), 361-366.
Times Cited: 5

Cheng, W. D.; Wu, D. S.; Zhang, H.; Chen, D. G.; Wang, H. X., Optimization of geometrical structure and simulation of the spectra of third-order nonlinear optical polarizabilities in C59Si and C58Si2 heterofullerenes. *Physical Review B* **2002,** 66, (8).
Times cited: 7

Citations:

1. Jiao, H. J.; Chen, Z. F.; Hirsch, A.; Thiel, W., Structures and magnetic properties of mono-doped fullerenes C59Xn and C59X(6-n)- (X = B-, N+, P+, As+, Si): isoelectronic analogues of C-60 and C-60(6-). *Journal of Molecular Modeling* **2003,** 9, (1), 34-38.
2. Pattanayak, J.; Kar, T.; Scheiner, S., Comparison of BN and AlN substitution on the structure and electronic and chemical properties of C-60 fullerene. *Journal of Physical Chemistry A* **2003,** 107, (20), 4056-4065.
3. Chen, Z. F.; King, R. B., Spherical aromaticity: Recent work on fullerenes, polyhedral boranes, and related structures. *Chemical Reviews* **2005,** 105, (10), 3613-3642.

4. Simeon, T. M.; Yanov, I.; Leszczynski, J. In *Ab initio quantum chemical studies of fullerene molecules with substitutes C59X [X=Si, Ge, Sn], C59X- [X=B, Al, Ga, In], and C59X+ [X=N, P, As, Sb]*, 2005; 2005; pp 429-436.
5. Papadopoulos, M. G.; Reis, H.; Avramopoulos, A.; Erkoc, S.; Amirouche, L., Polarizabilities and second hyperpolarizabilities of ZnmCdn clusters. *Molecular Physics* **2006,** 104, (13-14), 2027-2036.
6. Ray, A. K.; Huda, M. N., Silicon-carbide nano-clusters: A pathway to future nano-electronics. *Journal of Computational and Theoretical Nanoscience* **2006,** 3, (3), 315-341.
7. Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207.

Key Paper(B)

Yang, Z. Y.; Xu, X. F.; Wang, G. C.; Shang, Z. F.; Cai, Z. S.; Pan, Y. M.; Zhao, X. Z., A systematic investigation on the molecular behaviors of substituted fullerenes C34X2 (X = N, B). *Journal of Molecular Structure-Theochem* **2002,** 618, (3), 191-200.
Times Cited: 8

Xu, X. F.; Xing, Y. M.; Shang, Z. F.; Wang, G. C.; Cai, Z. S.; Pan, Y. M.; Zhao, X. Z., Systematic investigation of heterofullerenes the molecular behaviors of C48X2 (X = B, N). *Chemical Physics* **2003,** 287, (3), 317-333.
Times cited: 9

Citations:

1. Chen, Z. F.; King, R. B., Spherical aromaticity: Recent work on fullerenes, polyhedral boranes, and related structures. *Chemical Reviews* **2005,** 105, (10), 3613-3642.
2. Lu, X.; Chen, Z. F., Curved Pi-conjugation, aromaticity, and the related chemistry of small fullerenes (< C-60) and single-walled carbon nanotubes. *Chemical Reviews* **2005,** 105, (10), 3643-3696.
3. Dang, H. V.; Stadlbauer, W., Amination of pyrido[3,2,1-jk]carbazol-6-ones. *Journal of Heterocyclic Chemistry* **2006,** 43, (1), 65-70.
4. Vostrowsky, O.; Hirsch, A., Heterofullerenes. *Chemical Reviews* **2006,** 106, (12), 5191-5207.
5. Wu, S.; Teng, Q. W., UV and IR studies on heterofullerene C76BN. *Chinese Journal of Chemical Physics* **2006,** 19, (4), 301-304.

6. Xu, X. F.; Shang, Z. F.; Li, R. F.; Cai, Z. S.; Zhao, X. Z., Comparative theoretical study of methano- and imino-[50] fullerenes: C50CH2 and C50NH. *Journal of Molecular Structure-Theochem* **2006,** 760, (1-3), 99-107.
7. Liang, Y. X.; Shui, M.; Li, R. S., Structures and stabilities of boron/nitrogen-doped fullerene C-20. *Acta Physico-Chimica Sinica* **2007,** 23, (10), 1647-1651.
8. Kassaee, M. Z.; Arefrad, H.; Ghambarian, M., Novel silicon nanorings: Persilacyclacenes at DFT. *International Journal of Quantum Chemistry* **2008,** 108, (4), 696-707.
9. von Delius, M.; Hauke, F.; Hirsch, A., Evaluation of an intramolecular approach for the synthesis of the elusive C58N2 heterofullerene family. *European Journal of Organic Chemistry* **2008**, (24), 4109-4119.

Key paper (B)

Yang, Z. Y.; Xu, X. F.; Wang, G. C.; Shang, Z. F.; Pan, Y. M.; Zhao, X. Z., Theoretical studies on structures and stabilities of C34BN isomers. *Acta Chimica Sinica* **2002,** 60, (11), 1915-1922.
Times Cited: 3

No topical references found.