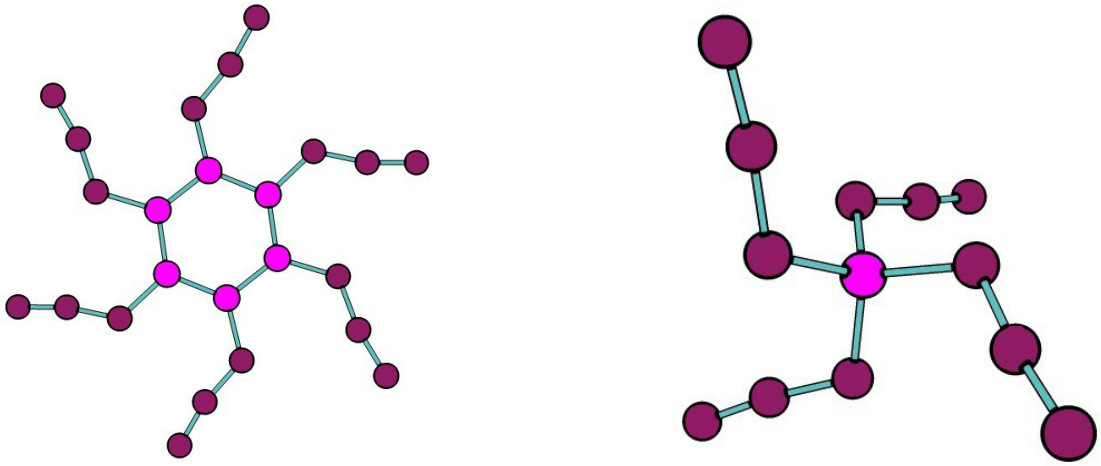
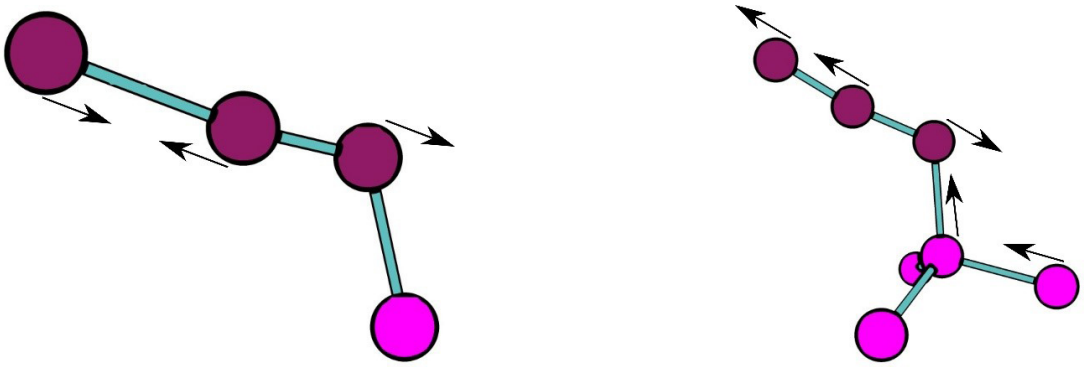
Supplementary material



a b

Fig. S1. (Color online) Optimized geometries of hexaazidobenzene $C_6(N_3)_6$ (a) and tetraazidomethane $C(N_3)_4$ (b) molecules. Nitrogen atoms are depicted in a darker color.



a b

Fig. S2. (Color online) Fragments of the $C_{60}N_{60}$ azidofullerene showing: asymmetric valence vibration of the N_3 azide group (a); symmetric valence vibration of the N_3 azide group, which involves several neighboring carbon atoms (b).

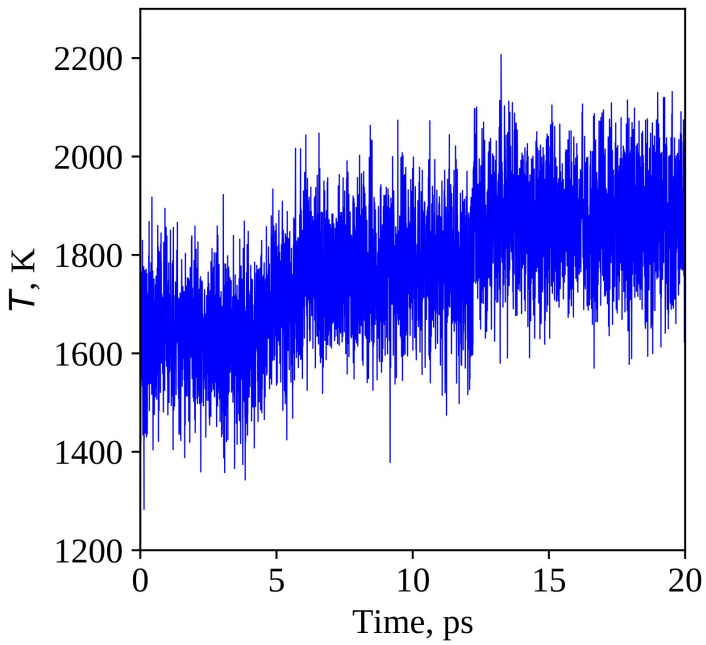


Fig. S3. Dependence temperature on time for the $C_{60}N_{60}$ molecule. The results are obtained using molecular dynamic calculations in the NVE ensemble and the PM3 method.

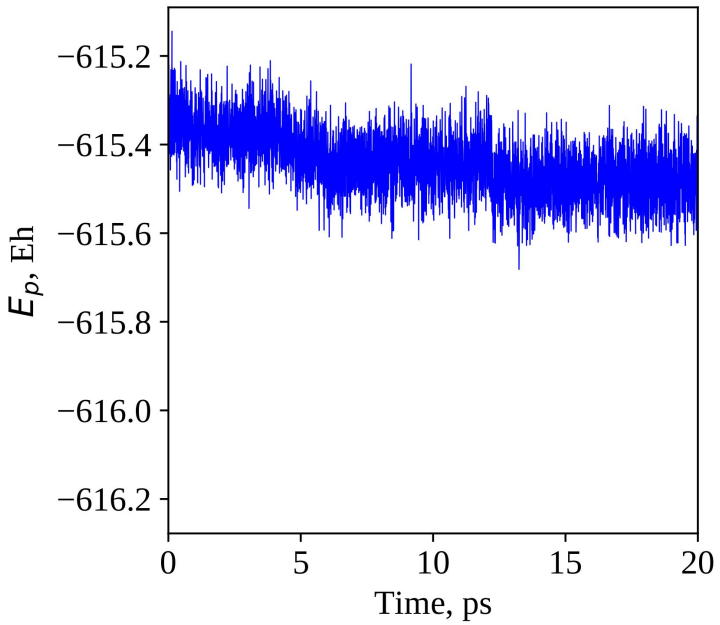


Fig. S4. Dependence of the potential energy on time for the $C_{60}N_{60}$ molecule. The results are obtained using molecular dynamic calculations in the NVE ensemble and the PM3 method.

Table S1. The optimized geometry and vibrational frequencies of the $C_{60}N_{60}$ azidofullerene.

Exchange-correlation functional	Atomic coordinates, Å	Frequency, cm^{-1}
B3LYP	C 0.0974 −0.1884 0.1676	0.00; 0.00; 0.00; 0.00; 0.00; 0.00;
	C 1.5476 −0.3104 −0.0477	19.52; 22.34; 22.78; 28.09; 30.87; 34.73;
	C 2.1079 0.9492 0.0325	35.51; 35.70; 36.46; 36.78; 37.50; 38.63;
	C 1.0234 1.9965 0.2550	39.87; 40.77; 43.03; 46.85; 47.97; 55.12;
	C −0.1797 1.0860 0.5078	56.92; 59.65; 66.74; 69.45; 69.77; 70.47;
	C −1.1128 1.3423 1.5517	70.89; 74.07; 74.28; 75.07; 75.63; 76.37;
	C −0.7674 −1.3929 0.3801	76.70; 78.52; 79.41 83.52; 84.51; 85.63;
	C 2.2264 −1.5178 0.0826	90.14; 93.60; 99.47; 105.92; 151.08; 154.10;
	C 3.5320 1.1518 0.3766	158.10; 165.14; 165.77; 168.08; 169.68;
	C 1.3021 2.8181 1.4825	170.97; 171.80; 173.78; 175.33; 176.73;
	C 3.7075 −1.5547 0.3947	179.10; 180.83; 183.25; 185.71; 187.02;
	C 4.1255 −0.1738 0.8951	189.26; 190.26; 192.47; 193.54; 193.63;
	C 3.5982 2.0265 1.6514	197.60; 199.80; 201.95; 203.30; 204.08;
	C 2.5287 2.8872 2.0492	205.32; 207.32; 208.34; 208.78; 211.72;
	C 0.1907 3.2986 2.4269	212.75; 218.51; 227.68; 229.63; 237.57;
	C −0.9647 2.3248 2.4628	244.13; 248.76; 253.74; 264.33; 275.23;
	C −1.8037 0.1771 2.1514	281.21; 284.27; 288.11; 295.55; 300.85;
	C −1.9247 −1.1608 1.4722	307.52; 312.25; 314.71; 318.88; 323.09;
	C 0.1073 −2.4597 0.9925	329.49; 337.82; 342.60; 351.89; 354.35;
	C 1.4905 −2.7847 0.4563	369.07; 383.80; 388.14; 405.41; 409.52;
	C −0.3822 −2.9555 2.1229	424.36; 428.32; 430.28; 444.93; 446.71;
	C −1.7115 −2.3542 2.5430	449.63; 455.43; 461.52; 465.20; 478.31;
	C 2.3670 −3.2381 1.6086	484.69; 494.01; 500.04; 501.44; 511.32;
	C 3.6179 −2.5073 1.5763	514.51; 517.33; 522.94; 535.45; 539.87;
	C 4.6715 0.0446 2.1049	550.89; 557.10; 558.37; 562.64; 564.94;
	C 4.3750 1.4057 2.5697	565.59; 569.09; 574.93; 575.64; 576.58;
	C 2.4571 3.4185 3.4948	577.16; 577.77; 578.60; 579.27; 579.75;
	C 0.9831 3.2174 3.7266	580.41; 580.90; 581.16; 581.93; 583.74;
	C −1.7114 1.9177 3.7429	583.96; 584.48; 585.41; 586.41; 587.24;
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	C 0.3876 −3.8899 3.0201	594.11; 596.44; 601.80; 603.21; 610.02;
	C 1.8740 −3.7838 2.7327	611.88; 620.65; 626.91; 630.38; 632.11;
	C 4.2771 −2.2878 2.7789	637.08; 645.99; 650.77; 658.21; 662.50;
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C −0.7656 1.9486 4.8908
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C −2.2215 −0.6237 4.4957
C 2.6379 −3.7596 4.0461
C 3.7435 −2.7567 3.9717
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C 4.3762 0.5771 4.8947
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C −0.4329 −1.5305 5.9108
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C 2.7676 −0.3023 6.4877
C 3.0285 −1.5971 6.0412
C 1.8495 −2.5405 6.2932
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N 0.4668 −0.2668 9.2419
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N 6.8456 2.7093 6.2277
N 6.2607 2.6394 5.2682

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PBE	C 0.0995 −0.1925 0.1603 C 1.5450 −0.3133 −0.0570 C 2.1119 0.9596 0.0380 C 1.0272 2.0034 0.2674 C −0.1778 1.0946 0.5138 C −1.1039 1.3380 1.5637 C −0.7675 −1.3955 0.3747 C 2.2265 −1.5209 0.0696 C 3.5356 1.1512 0.3883 C 1.3021 2.8192 1.4995 C 3.7078 −1.5536 0.3953 C 4.1171 −0.1790 0.9026 C 3.6078 2.0262 1.6637 C 2.5432 2.8799 2.0706 C 0.1970 3.2999 2.4499 C −0.9576 2.3271 2.4891 C −1.7902 0.1704 2.1573 C −1.9206 −1.1612 1.4728 C 0.1094 −2.4645 0.9844 C 1.4930 −2.7879 0.4515 C −0.3859 −2.9652 2.1242 C −1.7180 −2.3641 2.5404 C 2.3742 −3.2438 1.6029 C 3.6292 −2.5188 1.5721 C 4.6772 0.0351 2.1220 C 4.3969 1.3938 2.5873 C 2.4728 3.4044 3.5174 C 0.9923 3.2230 3.7483 C −1.7027 1.9085 3.7653 C −2.0574 0.4348 3.4528 C 0.3877 −3.8988 3.0197 C 1.8754 −3.7961 2.7349 C 4.2948 −2.3055 2.7761 C 5.1411 −1.0526 3.0519	0.00; 0.00; 0.00; 0.00; 0.00; 0.00; 13.36; 21.29; 25.86; 26.39; 28.33; 30.58; 31.01; 31.25; 32.92; 34.08; 36.83; 37.66; 38.80; 40.95; 43.48; 45.29; 47.81; 48.87; 53.12; 56.97; 63.02; 65.52; 66.68; 67.36; 67.79; 69.85; 70.44; 70.89; 71.04; 71.62; 73.27; 74.29; 75.45; 77.40; 80.22; 81.85; 84.68; 89.56; 92.70; 100.08; 144.02; 146.72; 151.54; 156.42; 159.32; 160.28; 161.45; 162.27; 163.73; 165.84; 167.59; 169.30; 171.50; 172.41; 174.14; 174.91; 177.99; 180.32; 181.33; 183.90; 184.64; 185.65; 189.30; 193.00; 193.94; 194.44; 196.69; 197.77; 198.91; 199.00; 200.50; 203.44; 203.92; 210.23; 218.04; 220.31; 227.98; 233.56; 237.72; 243.23; 252.68; 263.74; 269.51; 272.54; 275.55; 282.39; 287.47; 292.82; 297.77; 301.81; 306.79; 309.00; 316.75; 324.26; 328.20; 336.35; 340.38; 354.19; 368.76; 372.25; 390.16; 395.36; 408.99; 411.42; 415.19; 427.72; 430.66; 432.87; 437.14; 445.54; 448.41; 460.95; 466.46; 474.65; 480.56; 482.06; 492.31; 494.77; 497.66; 501.89; 516.07; 518.70; 528.77; 535.18; 535.86; 539.16; 541.00; 541.40; 543.18; 543.86; 545.47; 547.62; 548.62; 550.31; 551.02; 551.37; 551.70; 551.96; 553.50; 554.02; 554.49; 555.33; 556.41; 556.76; 557.08; 558.86; 559.15; 559.69; 560.26; 560.98; 562.59; 568.31; 572.50; 572.89; 577.83; 578.51; 585.75; 588.50; 594.22; 602.16; 604.48; 605.49; 612.18; 620.63; 626.14; 633.11; 634.19; 639.43; 643.57; 645.65; 652.33; 655.07; 658.94; 664.66; 668.02; 670.08; 673.52; 675.55; 681.71; 686.93; 688.08; 691.17; 693.04; 697.79; 699.66; 704.24; 707.08; 712.12; 713.84; 718.34; 721.35; 724.42; 724.49; 732.58; 733.26; 738.02; 740.92; 746.69;

	C 4.4941 1.7994 4.0281 C 3.2495 2.5444 4.4460 C −0.7611 1.9344 4.9156 C 0.4846 2.5560 4.8509 C −1.6443 −1.9153 3.9768 C −2.2126 −0.6341 4.5054 C 2.6424 −3.7767 4.0476 C 3.7576 −2.7839 3.9777 C −0.8832 −2.6954 5.0212 C 0.3377 −3.3458 4.4399 C −1.1851 −0.4007 5.5876 C −0.7791 0.9538 6.0646 C 1.3495 1.9686 5.8810 C 2.8320 2.1451 5.8417 C 4.6866 −0.7143 4.4693 C 4.4004 0.5598 4.9085 C 1.5539 −3.2841 5.0082 C −0.4329 −1.5450 5.9180 C 0.6927 0.9582 6.4923 C 3.4480 0.7591 5.9368 C 3.9615 −1.8153 5.0122 C 1.3788 −0.2283 7.1132 C 2.7798 −0.3242 6.5067 C 3.0410 −1.6240 6.0555 C 1.8575 −2.5615 6.3001 C 0.7688 −1.5273 6.5828 N 1.4270 −3.8802 −0.5854 N 1.3005 −3.5214 −1.7609 N −1.2662 −1.9258 −0.9211 N −1.8085 −1.1194 −1.6928 N −3.1996 −1.2444 0.7469 N −4.2293 −0.9364 1.3643 N −2.9070 2.7462 4.0950 N −3.7952 2.7722 3.2312 N −0.3411 4.6845 2.1948 N 0.4159 5.5021 1.6564 N 1.5018 −0.1728 8.6069 N 0.4552 −0.3189 9.2564 N 3.4277 3.0741 6.8863 N 2.6406 3.5917 7.6881 N 6.6190 −1.2530 3.0447 N 7.1278 −1.5073 1.9430 N 2.9518 4.8590 3.4923 N 2.7460 6.1410 5.4828 N 2.8261 5.4789 4.5537 N 4.2869 1.7475 −0.7715 N 6.5461 2.4216 −0.4631 N 5.4589 2.0811 −0.5407 N 0.8213 2.9666 −0.8744 N 0.3134 2.1043 −3.0304 N 0.5585 2.4534 −1.9713 N 2.0701 −3.6046 7.3577 N 3.2954 −3.1034 9.3302 N 2.7186 −3.2726 8.3594 N 3.1192 −5.1770 4.3603 N 4.6912 −5.5441 6.1037 N 3.9367 −5.2953 5.2818 N 5.7452 2.6385 4.1859 N 6.9723 2.5770 6.2203 N 6.3362 2.5607 5.2720	754.86; 755.97; 758.03; 760.11; 768.23; 772.55; 775.38; 781.74; 786.79; 791.62; 793.19; 795.50; 797.54; 803.37; 809.40; 812.87; 818.49; 827.15; 828.61; 837.34; 843.58; 850.40; 852.19; 858.15; 864.30; 868.72; 875.05; 876.97; 887.14; 889.40; 898.85; 900.90; 905.65; 912.30; 916.21; 919.29; 931.20; 939.83; 941.68; 943.22; 962.39; 969.84; 978.67; 989.96; 996.35; 1001.85; 1010.66; 1019.51; 1025.77; 1028.49; 1035.68; 1045.10; 1050.93; 1060.05; 1067.43; 1077.24; 1086.47; 1088.58; 1101.21; 1104.41; 1109.94; 1125.30; 1130.73; 1134.89; 1140.20; 1152.15; 1155.58; 1165.38; 1178.66; 1181.59; 1186.51; 1198.54; 1199.57; 1209.54; 1214.85; 1215.98; 1221.49; 1224.52; 1229.63; 1236.13; 1239.11; 1243.64; 1248.35; 1252.58; 1256.07; 1257.65; 1259.82; 1260.87; 1262.55; 1265.36; 1265.75; 1268.20; 1268.77; 1269.20; 1269.83; 1270.65; 1272.80; 1273.49; 1274.87; 1275.18; 1277.65; 1279.80; 1279.90; 1281.06; 1285.47; 1288.92; 1293.87; 1294.98; 1305.88; 1312.31; 1323.78; 1348.74; 1361.27; 1372.07; 1381.65; 1388.31; 1389.11; 1418.20; 1425.55; 1431.85; 1460.55; 1488.21; 1503.45; 1518.26; 1518.77; 1536.27; 1542.21; 1561.56; 1564.25; 1581.20; 1584.62; 1604.38; 1614.70; 1624.23; 1643.35; 1662.45; 2147.27; 2150.59; 2155.95; 2158.79; 2159.06; 2159.82; 2160.99; 2161.26; 2162.16; 2163.58; 2164.34; 2166.66; 2169.73; 2170.74; 2171.93; 2174.81; 2175.54; 2181.45; 2183.00; 2188.39.

	N 4.6213 −2.1107 −0.6638 N 4.6138 −1.1739 −2.8482 N 4.5720 −1.5747 −1.7788 N −1.7259 −3.6167 5.8719 N −2.7344 −5.5962 5.0385 N −2.2122 −4.6325 5.3583 N −2.8698 −3.3196 2.5067 N −2.9380 −5.0831 0.9160 N −2.8393 −4.2159 1.6496 N −3.6734 −0.6531 4.9313 N −4.3994 −1.9704 6.7708 N −3.9869 −1.3605 5.8975 N −1.5777 1.3649 7.2887 N −3.8963 1.8621 7.1559 N −2.7829 1.6094 7.1427 N 1.2015 −3.3182 −2.8811 N −2.3182 −0.4943 −2.4981 N −5.2499 −0.6762 1.8003 N −4.6776 2.8809 2.5154 N 1.0014 6.3470 1.1590 N −0.4193 −0.4463 9.9780 N 2.0062 4.1253 8.4745 N 7.7252 −1.7400 0.9988 N −0.2046 −5.2787 3.0223 N 0.1900 −6.0405 2.1285 N 0.4794 −6.8413 1.3695	
TPSS	C 0.0959 −0.1883 0.1631 C 1.5422 −0.3100 −0.0535 C 2.1075 0.9615 0.0386 C 1.0241 2.0041 0.2693 C −0.1804 1.0963 0.5148 C −1.1078 1.3414 1.5641 C −0.7713 −1.3906 0.3768 C 2.2227 −1.5176 0.0700 C 3.5299 1.1531 0.3903 C 1.2985 2.8220 1.5005 C 3.7039 −1.5520 0.3943 C 4.1138 −0.1766 0.9020 C 3.6012 2.0256 1.6653 C 2.5362 2.8801 2.0721 C 0.1931 3.3010 2.4502 C −0.9614 2.3279 2.4880 C −1.7975 0.1739 2.1567 C −1.9239 −1.1588 1.4725 C 0.1040 −2.4619 0.9831 C 1.4883 −2.7836 0.4509 C −0.3903 −2.9633 2.1203 C −1.7199 −2.3588 2.5388 C 2.3670 −3.2385 1.6029 C 3.6227 −2.5146 1.5719 C 4.6732 0.0366 2.1187 C 4.3894 1.3954 2.5863 C 2.4667 3.4040 3.5181 C 0.9875 3.2223 3.7479 C −1.7063 1.9105 3.7629 C −2.0640 0.4373 3.4499 C 0.3830 −3.8951 3.0171 C 1.8694 −3.7918 2.7322 C 4.2869 −2.3020 2.7749 C 5.1339 −1.0507 3.0510	0.00; 0.00; 0.00; 0.00; 0.00; 0.00; 21.14; 24.00; 24.39; 26.03; 28.58; 30.10; 30.49; 31.29; 32.82; 35.16; 35.48; 37.74; 39.81; 39.94; 42.07; 49.29; 49.93; 51.32; 52.26; 56.81; 62.11; 64.42; 65.36; 66.16; 66.81; 68.94; 69.84; 70.44; 70.86; 71.44; 71.72; 73.61; 74.12; 77.20; 78.62; 82.39; 83.83; 86.93; 92.68; 98.83; 141.94; 145.21; 150.98; 155.27; 157.29; 157.94; 159.28; 160.80; 162.79; 163.41; 166.06; 168.18; 169.27; 170.16; 171.43; 172.86; 176.43; 178.31; 179.02; 181.71; 182.60; 184.53; 188.64; 192.65; 193.42; 193.78; 196.10; 196.86; 198.05; 198.57; 199.43; 202.54; 203.45; 209.32; 217.40; 220.02; 228.53; 234.16; 238.71; 243.81; 252.83; 263.64; 269.73; 271.57; 275.89; 281.75; 287.22; 292.29; 297.55; 301.21; 306.90; 308.73; 316.31; 323.58; 327.76; 336.42; 339.41; 352.93; 367.70; 371.70; 390.09; 394.18; 408.00; 411.63; 415.76; 427.01; 430.01; 432.26; 437.24; 443.98; 447.09; 460.43; 465.38; 473.79; 479.04; 481.55; 488.54; 492.16; 492.98; 501.37; 511.66; 513.94; 524.86; 532.48; 535.44; 538.51; 539.30; 541.99; 542.76; 544.76; 547.54; 548.32; 549.04; 549.93; 551.40; 551.75; 552.50; 553.45; 553.64; 554.30; 554.99; 555.66; 556.51; 557.04; 557.82; 558.00; 559.70; 560.05; 561.67; 561.80; 562.91; 566.87; 570.46; 571.66; 575.15; 577.25; 583.62; 584.20; 591.07; 598.71; 602.26; 603.17; 610.08; 619.12; 625.46; 632.32; 633.34; 638.30; 642.60; 645.04; 652.89; 655.63; 659.06; 665.30; 667.75; 670.81; 674.07; 675.34; 683.44; 687.46; 688.68; 691.93; 694.29; 697.28; 699.92; 704.65; 709.19; 711.27; 714.78; 717.98; 722.60; 724.60; 725.56; 729.60; 733.43; 739.13; 740.88; 745.96;

	C 4.4848 1.7997 4.0271 C 3.2428 2.5459 4.4466 C −0.7655 1.9360 4.9134 C 0.4796 2.5556 4.8487 C −1.6463 −1.9104 3.9750 C −2.2185 −0.6322 4.5036 C 2.6356 −3.7719 4.0440 C 3.7498 −2.7799 3.9751 C −0.8862 −2.6905 5.0180 C 0.3337 −3.3435 4.4376 C −1.1910 −0.3985 5.5843 C −0.7830 0.9554 6.0603 C 1.3432 1.9684 5.8802 C 2.8254 2.1456 5.8411 C 4.6755 −0.7114 4.4661 C 4.3908 0.5608 4.9057 C 1.5472 −3.2829 5.0061 C −0.4362 −1.5407 5.9131 C 0.6875 0.9598 6.4892 C 3.4397 0.7598 5.9332 C 3.9517 −1.8117 5.0086 C 1.3730 −0.2268 7.1107 C 2.7722 −0.3225 6.5021 C 3.0325 −1.6211 6.0517 C 1.8505 −2.5587 6.2973 C 0.7626 −1.5240 6.5794 N 1.4249 −3.8890 −0.5869 N 1.3071 −3.5262 −1.7647 N −1.2688 −1.9277 −0.9264 N −1.8280 −1.1177 −1.6872 N −3.2033 −1.2515 0.7342 N −4.2361 −0.9419 1.3525 N −2.9151 2.7553 4.1014 N −3.7810 2.8161 3.2131 N −0.3527 4.6946 2.2020 N 0.3998 5.5000 1.6333 N 1.5081 −0.1707 8.6126 N 0.4656 −0.3526 9.2649 N 3.4257 3.0823 6.8930 N 2.6357 3.5486 7.7264 N 6.6209 −1.2511 3.0588 N 7.1317 −1.5224 1.9585 N 2.9519 4.8703 3.4796 N 2.7033 6.1720 5.4514 N 2.8033 5.5007 4.5344 N 4.2823 1.7576 −0.7782 N 6.5273 2.4652 −0.4455 N 5.4492 2.1084 −0.5321 N 0.8116 2.9800 −0.8743 N 0.3994 2.1118 −3.0476 N 0.5983 2.4598 −1.9817 N 2.0608 −3.6109 7.3606 N 3.3520 −3.1199 9.2927 N 2.7458 −3.2820 8.3424 N 3.1137 −5.1861 4.3486 N 4.7284 −5.5468 6.0529 N 3.9548 −5.2992 5.2528 N 5.7458 2.6470 4.1810 N 7.0138 2.5090 6.1856 N 6.3582 2.5280 5.2541	752.65; 754.81; 756.56; 759.63; 764.54; 772.84; 775.04; 776.46; 784.78; 786.98; 793.32; 795.49; 797.94; 800.76; 802.42; 808.66; 811.16; 813.93; 823.72; 826.79; 834.56; 840.04; 844.86; 849.39; 855.34; 856.58; 865.48; 870.48; 878.83; 882.41; 886.83; 891.30; 897.83; 904.76; 910.38; 915.76; 924.99; 935.12; 937.85; 948.72; 957.66; 968.79; 976.86; 988.16; 995.50; 998.98; 1010.00; 1019.35; 1025.55; 1029.12; 1036.40; 1045.57; 1051.88; 1060.39; 1068.44; 1078.07; 1087.99; 1090.47; 1103.13; 1106.40; 1111.72; 1126.17; 1133.04; 1138.16; 1142.47; 1154.12; 1156.84; 1167.05; 1180.49; 1183.41; 1190.71; 1200.87; 1201.59; 1209.68; 1214.69; 1218.62; 1223.03; 1224.57; 1228.01; 1231.74; 1232.60; 1235.04; 1237.10; 1238.22; 1240.62; 1241.75; 1241.95; 1243.22; 1244.97; 1245.57; 1245.64; 1246.37; 1247.58; 1248.49; 1250.17; 1251.18; 1253.52; 1255.06; 1256.03; 1258.04; 1261.51; 1266.02; 1268.44; 1273.34; 1277.28; 1278.73; 1292.38; 1298.62; 1309.95; 1312.61; 1327.21; 1351.29; 1364.22; 1369.05; 1383.56; 1389.13; 1392.99; 1422.02; 1431.54; 1435.56; 1460.27; 1487.26; 1504.00; 1521.63; 1524.28; 1540.93; 1548.46; 1568.85; 1569.73; 1588.15; 1591.42; 1611.12; 1624.00; 1631.33; 1650.98; 1670.48; 2136.34; 2140.15; 2144.92; 2147.57; 2148.33; 2148.88; 2149.93; 2150.85; 2151.82; 2153.23; 2154.16; 2156.93; 2159.54; 2161.86; 2162.41; 2164.51; 2165.87; 2172.48; 2173.99; 2179.31.

	N 4.6241 −2.1253 −0.6636 N 4.6546 −1.1749 −2.8410 N 4.5931 −1.5782 −1.7768 N −1.7368 −3.6071 5.8840 N −2.7134 −5.6119 5.0763 N −2.2061 −4.6385 5.3786 N −2.8816 −3.3183 2.5123 N −2.9530 −5.0611 0.8995 N −2.8500 −4.2051 1.6404 N −3.6911 −0.6455 4.9264 N −4.4188 −1.9623 6.7644 N −4.0037 −1.3560 5.8939 N −1.5758 1.3659 7.3025 N −3.8821 1.9167 7.1889 N −2.7784 1.6379 7.1604 N 1.2178 −3.3260 −2.8832 N −2.3508 −0.4978 −2.4836 N −5.2586 −0.6863 1.7781 N −4.6417 2.9599 2.4823 N 0.9733 6.3344 1.1118 N −0.3966 −0.5107 9.9903 N 2.0023 4.0398 8.5368 N 7.7347 −1.7700 1.0255 N −0.2255 −5.2782 3.0234 N 0.2419 −6.0757 2.1953 N 0.5871 −6.9070 1.4995	

Table S2. The optimized geometry of the C_{60} molecule.

Exchange-correlation functional	Atomic coordinates, Å
B3LYP	C 0.7246 −0.9972 3.3164 C 1.1724 0.3811 3.3164 C 1.4192 −1.9532 2.5852 C 2.2968 0.7463 2.5860 C 2.2968 1.9789 1.8238 C 0.0000 1.2333 3.3175 C 0.0000 2.4152 2.5862 C 1.1726 2.7957 1.8240 C −0.6948 −2.9508 1.8235 C −1.4192 −1.9532 2.5852 C 0.6948 −2.9508 1.8235 C −0.7246 −0.9972 3.3164 C −1.1724 0.3811 3.3164 C −2.5915 −1.5722 1.8235 C −3.0213 −0.2509 1.8239 C −2.2968 0.7463 2.5860 C 0.7246 −3.4116 −0.5910 C −0.7246 −3.4116 −0.5910 C 1.4197 −3.1867 0.5909 C −1.4197 −3.1867 0.5909 C −2.5922 −2.3347 0.5910 C −1.1726 −2.7957 −1.8240 C −2.2968 −1.9789 −1.8238 C −3.0217 −1.7438 −0.5912 C 3.0217 −1.7438 −0.5912 C 2.2968 −1.9789 −1.8238 C 2.5922 −2.3347 0.5910 C 1.1726 −2.7957 −1.8240 C −0.0000 −2.4152 −2.5862 C 2.2968 −0.7463 −2.5860 C 1.1724 −0.3811 −3.3164

	C −0.0000 −1.2333 −3.3175 C 3.0213 −0.2509 1.8239 C 3.4686 0.3653 0.5909 C 2.5915 −1.5722 1.8235 C 3.4686 −0.3653 −0.5909 C 3.0213 0.2509 −1.8239 C 3.0217 1.7438 0.5912 C 2.5922 2.3347 −0.5910 C 2.5915 1.5722 −1.8235 C −0.7246 0.9972 −3.3164 C 0.7246 0.9972 −3.3164 C 1.4192 1.9532 −2.5852 C −1.4192 1.9532 −2.5852 C −3.0213 0.2509 −1.8239 C −2.2968 −0.7463 −2.5860 C −1.1724 −0.3811 −3.3164 C −2.5915 1.5722 −1.8235 C −3.0217 1.7438 0.5912 C −3.4686 0.3653 0.5909 C −3.4686 −0.3653 −0.5909 C −2.5922 2.3347 −0.5910 C −0.7246 3.4116 0.5910 C −1.1726 2.7957 1.8240 C −2.2968 1.9789 1.8238 C −1.4197 3.1867 −0.5909 C 0.6948 2.9508 −1.8235 C 1.4197 3.1867 −0.5909 C 0.7246 3.4116 0.5910 C −0.6948 2.9508 −1.8235
PBE	C 0.7262 −0.9993 3.3297 C 1.1750 0.3821 3.3297 C 1.4251 −1.9614 2.5932 C 2.3064 0.7496 2.5941 C 2.3066 1.9848 1.8304 C −0.0000 1.2359 3.3302 C −0.0000 2.4252 2.5940 C 1.1751 2.8067 1.8304 C −0.6992 −2.9613 1.8301 C −1.4251 −1.9614 2.5932 C 0.6992 −2.9613 1.8301 C −0.7262 −0.9993 3.3297 C −1.1750 0.3821 3.3297 C −2.5997 −1.5796 1.8297 C −3.0323 −0.2498 1.8302 C −2.3064 0.7496 2.5941 C 0.7262 −3.4244 −0.5950 C −0.7262 −3.4244 −0.5950 C 1.4255 −3.1976 0.5946 C −1.4255 −3.1976 0.5946 C −2.6006 −2.3440 0.5947 C −1.1751 −2.8067 −1.8304 C −2.3066 −1.9848 −1.8304 C −3.0330 −1.7493 −0.5950 C 3.0330 −1.7493 −0.5950 C 2.3066 −1.9848 −1.8304 C 2.6006 −2.3440 0.5947 C 1.1751 −2.8067 −1.8304 C −0.0000 −2.4252 −2.5940 C 2.3064 −0.7496 −2.5941 C 1.1750 −0.3821 −3.3297

	C −0.0000 −1.2359 −3.3302 C 3.0323 −0.2498 1.8302 C 3.4810 0.3677 0.5946 C 2.5997 −1.5796 1.8297 C 3.4810 −0.3677 −0.5946 C 3.0323 0.2498 −1.8302 C 3.0330 1.7493 0.5950 C 2.6006 2.3440 −0.5947 C 2.5997 1.5796 −1.8297 C −0.7262 0.9993 −3.3297 C 0.7262 0.9993 −3.3297 C 1.4251 1.9614 −2.5932 C −1.4251 1.9614 −2.5932 C −3.0323 0.2498 −1.8302 C −2.3064 −0.7496 −2.5941 C −1.1750 −0.3821 −3.3297 C −2.5997 1.5796 −1.8297 C −3.0330 1.7493 0.5950 C −3.4810 0.3677 0.5946 C −3.4810 −0.3677 −0.5946 C −2.6006 2.3440 −0.5947 C −0.7262 3.4244 0.5950 C −1.1751 2.8067 1.8304 C −2.3066 1.9848 1.8304 C −1.4255 3.1976 −0.5946 C 0.6992 2.9613 −1.8301 C 1.4255 3.1976 −0.5946 C 0.7262 3.4244 0.5950 C −0.6992 2.9613 −1.8301
TPSS	C 0.7258 −0.9988 3.3271 C 1.1744 0.3819 3.3272 C 1.4239 −1.9598 2.5917 C 2.3045 0.7490 2.5924 C 2.3047 1.9835 1.8291 C −0.0000 1.2354 3.3277 C −0.0000 2.4232 2.5924 C 1.1746 2.8045 1.8292 C −0.6984 −2.9591 1.8287 C −1.4239 −1.9598 2.5917 C 0.6984 −2.9591 1.8287 C −0.7258 −0.9988 3.3271 C −1.1744 0.3819 3.3272 C −2.5980 −1.5782 1.8285 C −3.0301 −0.2500 1.8289 C −2.3045 0.7490 2.5924 C 0.7259 −3.4219 −0.5943 C −0.7259 −3.4219 −0.5943 C 1.4243 −3.1953 0.5939 C −1.4243 −3.1953 0.5939 C −2.5988 −2.3422 0.5941 C −1.1746 −2.8045 −1.8292 C −2.3047 −1.9835 −1.8291 C −3.0308 −1.7482 −0.5943 C 3.0308 −1.7482 −0.5943 C 2.3047 −1.9835 −1.8291 C 2.5988 −2.3422 0.5941 C 1.1746 −2.8045 −1.8292 C 0.0000 −2.4232 −2.5924 C 2.3045 −0.7490 −2.5924 C 1.1744 −0.3819 −3.3272

	C 0.0000 −1.2354 −3.3277 C 3.0301 −0.2500 1.8289 C 3.4785 0.3673 0.5939 C 2.5980 −1.5782 1.8285 C 3.4785 −0.3673 −0.5939 C 3.0301 0.2500 −1.8289 C 3.0308 1.7482 0.5943 C 2.5988 2.3422 −0.5941 C 2.5980 1.5782 −1.8285 C −0.7258 0.9988 −3.3271 C 0.7258 0.9988 −3.3271 C 1.4239 1.9598 −2.5917 C −1.4239 1.9598 −2.5917 C −3.0301 0.2500 −1.8289 C −2.3045 −0.7490 −2.5924 C −1.1744 −0.3819 −3.3272 C −2.5980 1.5782 −1.8285 C −3.0308 1.7482 0.5943 C −3.4785 0.3673 0.5939 C −3.4785 −0.3673 −0.5939 C −2.5988 2.3422 −0.5941 C −0.7259 3.4219 0.5943 C −1.1746 2.8045 1.8292 C −2.3047 1.9835 1.8291 C −1.4243 3.1953 −0.5939 C 0.6984 2.9591 −1.8287 C 1.4243 3.1953 −0.5939 C 0.7259 3.4219 0.5943 C −0.6984 2.9591 −1.8287

Table S3. The optimized geometry of the $C_6(N_3)_6$ molecule.

Exchange-correlation functional	Atomic coordinates, Å
B3LYP	N −2.7943 −0.1362 0.1111 N −1.2757 −2.4917 0.0661 N −1.5222 2.3519 0.0076 N 1.5185 −2.3519 −0.0187 N 1.2750 2.4894 −0.1396 N 2.7938 0.1439 −0.1317 N −3.5051 −1.1359 0.2119 N −0.7757 −3.6059 −0.0871 N −2.7358 2.4666 −0.1638 N 2.7409 −2.4664 0.0687 N 0.7721 3.6094 −0.0500 N 3.5067 1.1300 0.0553 N −4.3213 −1.9055 0.3064 N −0.5225 −4.6968 −0.2017 N −3.8076 2.7824 −0.3008 N 3.8178 −2.7862 0.1414 N 0.5179 4.7046 0.0067 N 4.3212 1.8958 0.1873 C −1.3996 −0.1348 0.0433 C −0.5829 −1.2798 0.0169 C −0.8177 1.1451 −0.0057 C 0.8168 −1.1441 −0.0185 C 0.5811 1.2804 −0.0524 C 1.3984 0.1355 −0.0527

PBE	N −2.8019 −0.1402 0.0115 N −1.2797 −2.4964 0.0373 N −1.5226 2.3563 −0.0278 N 1.5225 −2.3563 0.0265 N 1.2796 2.4963 −0.0365 N 2.8018 0.1402 −0.0097 N −3.5208 −1.1450 −0.0016 N −0.7690 −3.6214 0.0531 N −2.7523 2.4762 −0.0268 N 2.7523 −2.4762 0.0284 N 0.7690 3.6213 −0.0516 N 3.5208 1.1450 −0.0027 N −4.3630 −1.9172 −0.0103 N −0.5217 −4.7368 0.0666 N −3.8422 2.8195 −0.0318 N 3.8422 −2.8193 0.0343 N 0.5216 4.7368 −0.0663 N 4.3632 1.9169 0.0064 C −1.4079 −0.1345 0.0042 C −0.5874 −1.2866 0.0178 C −0.8205 1.1521 −0.0127 C 0.8204 −1.1521 0.0127 C 0.5874 1.2865 −0.0173 C 1.4078 0.1345 −0.0039
TPSS	N −2.8027 −0.1345 0.0313 N −1.2851 −2.4942 0.0530 N −1.5184 2.3600 −0.0240 N 1.5184 −2.3600 0.0237 N 1.2851 2.4941 −0.0542 N 2.8027 0.1346 −0.0292 N −3.5165 −1.1461 −0.0011 N −0.7661 −3.6186 0.0564 N −2.7518 2.4717 −0.0283 N 2.7518 −2.4717 0.0232 N 0.7660 3.6186 −0.0579 N 3.5165 1.1461 0.0068 N −4.3568 −1.9154 −0.0227 N −0.5204 −4.7312 0.0630 N −3.8384 2.8146 −0.0367 N 3.8385 −2.8145 0.0266 N 0.5202 4.7312 −0.0668 N 4.3566 1.9153 0.0367 C −1.4047 −0.1349 0.0119 C −0.5855 −1.2843 0.0227 C −0.8194 1.1493 −0.0101 C 0.8194 −1.1493 0.0098 C 0.5855 1.2843 −0.0228 C 1.4048 0.1349 −0.0112

Table S4. The optimized geometry of the $C(N_3)_4$ molecule.

Exchange-correlation functional	Atomic coordinates, Å
B3LYP	N 1.3922 0.1118 0.4428 N −0.5743 1.3479 −0.0023 N −0.8203 −0.8307 0.8853 N 0.0030 −0.6277 −1.3230 N 2.0715 −0.9130 0.3075 N 0.1174 2.2130 −0.5529 N −1.0829 −0.3290 1.9851 N −1.1083 −0.9717 −1.7434 N 2.7840 −1.7773 0.2411 N 0.6530 3.0798 −1.0231 N −1.3774 0.0157 3.0116 N −2.0582 −1.3191 −2.2293 C 0.0003 0.0003 0.0007
PBE	N 1.3947 0.1088 0.4428 N −0.5754 1.3509 −0.0087 N −0.8278 −0.8288 0.8915 N −0.0001 −0.6396 −1.3231 N 2.0805 −0.9149 0.3010 N 0.1258 2.2209 −0.5480 N −1.0945 −0.3200 1.9914 N −1.1131 −0.9851 −1.7479 N 2.8138 −1.7829 0.2319 N 0.6679 3.1085 −1.0106 N −1.4008 0.0266 3.0315 N −2.0689 −1.3426 −2.2523 C −0.0021 −0.0020 0.0006
TPSS	N 1.3980 0.1160 0.4416 N −0.5777 1.3534 −0.0029 N −0.8302 −0.8317 0.8884 N 0.0055 −0.6416 −1.3244 N 2.0817 −0.9121 0.2899 N 0.1326 2.2216 −0.5409 N −1.1040 −0.3111 1.9848 N −1.1122 −0.9984 −1.7375 N 2.8141 −1.7760 0.2156 N 0.6750 3.1077 −0.9981 N −1.4178 0.0384 3.0181 N −2.0641 −1.3656 −2.2350 C −0.0009 −0.0007 0.0004

Table S5. Bond lengths (l, Å) and bond angles (α) for fullerene C_{60}, hexaazidobenzene $C_6(N_3)_6$, and tetraazidomethane $C(N_3)_4$ obtained in various exchange-correlation functionals.

Molecule	Parameter	Exchange-correlation functional		
		B3LYP	PBE	TPSS
C_{60}	$l_{C\text{-}C(5)}$	1.449	1.452	1.452
	$l_{C\text{-}C(6)}$	1.390	1.398	1.397
$C_6(N_3)_6$	$l_{C\text{-}C}$	1.406	1.414	1.411
	$l_{C\text{-}N}$	1.397	1.394	1.398
	$l_{N=N}$	1.231	1.236	1.239
	$l_{N\text{-}N}$	1.126	1.143	1.140
	$\alpha_{(C\text{-}C\text{-}C)}$	120°	120°	120°
	$\alpha_{(C\text{-}N\text{-}N)}$	125.5°	126°	125°
	$\alpha_{(N\text{-}N\text{-}N)}$	169°	168°	168°
$C(N_3)_4$	$l_{C\text{-}N}$	1.465	1.469	1.472
	$l_{N=N}$	1.237	1.240	1.244
	$l_{N\text{-}N}$	1.122	1.138	1.135
	$\alpha_{(C\text{-}N\text{-}N)}$	115°	115°	115°
	$\alpha_{(N\text{-}N\text{-}N)}$	173.5°	173°	173°

Table S6. Binding energies (E_b), HOMO-LUMO gaps (Δ_{HL}), and Löwdin atomic charges (Q) for fullerene C_{60}, hexaazidobenzene $C_6(N_3)_6$, and tetraazidomethane $C(N_3)_4$ obtained in various exchange-correlation functionals. The following notation for the Löwdin atomic charges has been introduced: Q(C) is the charge of the carbon atoms that are not bound with nitrogen atoms; Q(C1) is the charge of the carbon atoms that are bound with nitrogen atoms; Q(N1) is the charge of the nitrogen atoms that are bound with carbon atoms; Q(N3) is the charge of the nitrogen atoms located at the end of the N_3 radical; Q(N2) is the charge of the nitrogen atoms located between two nitrogen atoms in the N_3 radical.

Molecule	Parameter	Exchange-correlation functional		
		B3LYP	PBE	TPSS
C_{60}	Δ_{HL}, eV	2.72	1.65	1.71
	E_b, eV/atom	8.53	9.21	8.72
$C_6(N_3)_6$	Δ_{HL}, eV	4.08	2.56	2.66
	E_b, eV/atom	5.02	5.60	5.15
	Q(C1)	–0.179	–0.185	–0.179
	Q(N1)	0.062	0.087	0.076
	Q(N2)	0.097	0.086	0.089
	Q(N3)	0.020	0.012	0.014
$C(N_3)_4$	Δ_{HL}, eV	5.71	3.81	3.97
	E_b, eV/atom	4.17	4.73	4.29
	Q(C1)	–0.544	–0.554	–0.536
	Q(N1)	–0.005	0.0189	0.008
	Q(N2)	0.101	0.0886	0.093
	Q(N3)	0.040	0.0309	0.033