Supporting Information

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Theoretical Study of Structure, Vibrational Frequencies and Electronic Spectra of Dibenzofuran and its Polychlorinated Derivatives

Figure 1. The Active Orbitals of Dibenzofuran at the CASSCF(14,13)/cc-pVDZ Level

Figure 2. Kohn-Sham (B3P86/6-31G(d,p)) Molecular Orbitals of Dibenzofuran

Table 1. CASSCF(14,13)/cc-pVDZ Harmonic Vibrational Wave-numbers of the 1^1B_2 states of DF, TCDF and OCDF (Unscaled)

Table 2. CASSCF(14,13)/cc-pVDZ Harmonic Vibrational Wave-numbers of the 1^3A_1 and 1^3B_2 states of DF (Unscaled)

Figure 1

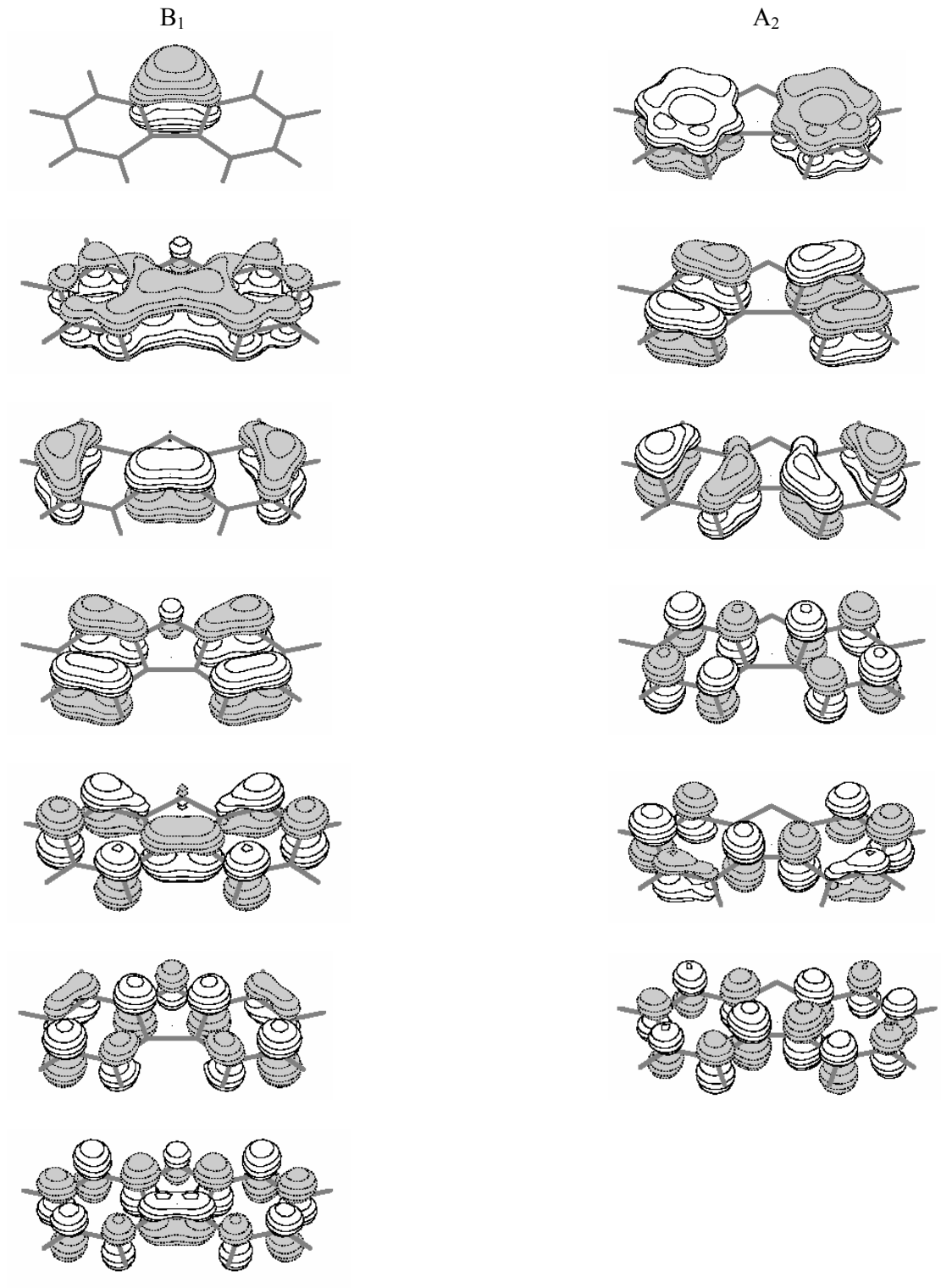
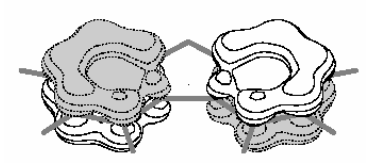


Figure 2.



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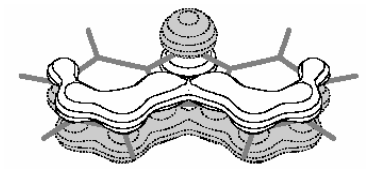

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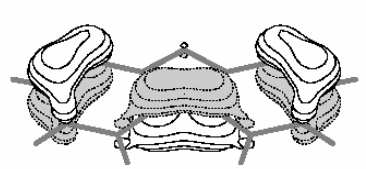

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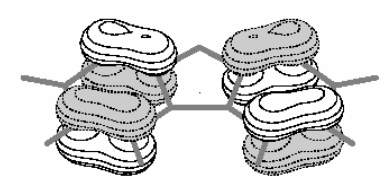

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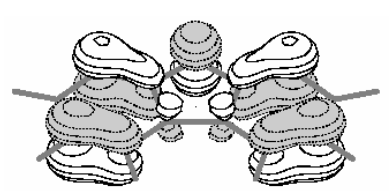

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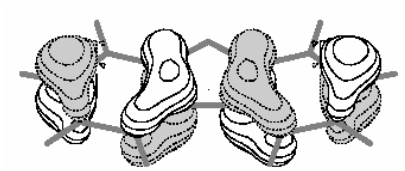
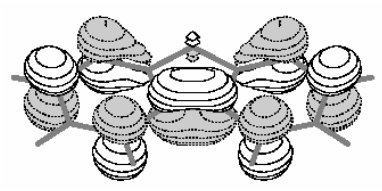
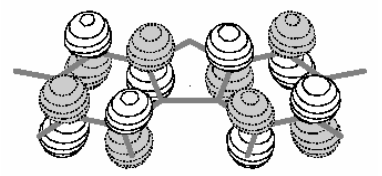


44 (HOMO)



45 (LUMO)



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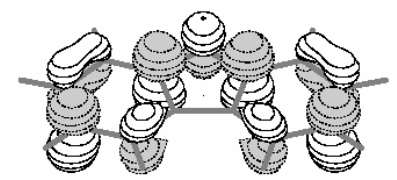

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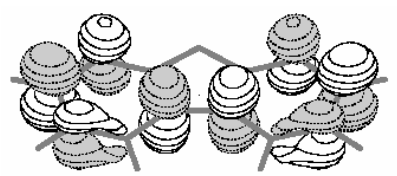

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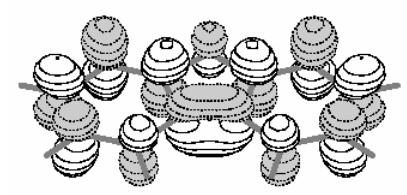

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Table 1.

	1^1B_2 (DF)
a_1	223 428 678 764 894 1020 1136 1234 1278 1353 1404 1530 1552 1631 1702 1730 3347 3363 3380 3390
b_1	93 292 383 503 650 673 724 801 871
a_2	152 257 439 508 664 701 720 798 871
b_2	551 569 628 918 1054 1109 1188 1235 1341 1444 1528 1553 1586 1642 1761 3347 3363 3381 3406

	1^1B_2 (TCDF)
a_1	106 205 262 357 515 674 764 832 999 1155 1246 1299 1372 1435 1526 1597 1699 1724 3405 3413
b_1	42 116 223 352 395 540 644 691 741
a_2	53 130 224 354 432 545 672 695 737
b_2	216 263 415 473 624 721 736 991 1111 1185 1297 1407 1498 1514 1556 1622 1768 3406 3422

	1^1B_2 (OCDF)
a_1	109 182 234 266 278 362 377 505 695 782 863 1008 1037 1266 1305 1410 1455 1574 1637 1707
b_1	30 64 89 195 263 346 457 525 631
a_2	26*i* 42 70 166 299 347 490 532 676
b_2	184 218 238 255 345 368 502 617 757 836 898 1084 1205 1359 1421 1482 1562 1589 1713

Table 2.

	1^3A_1 (DF)
a_1	219 426 681 773 923 1012 1056 1196 1234 1330 1382 1489 1503 1585 1591 1705 3340 3359 3379 3393
b_1	97 317 382 545 611 629 706 780 936
a_2	159 238 403 538 608 628 738 780 935
b_2	532 547 635 904 960 1075 1091 1254 1284 1372 1420 1457 1517 1587 2347 3340 3359 3381 3417

	1^3B_2 (DF)
a_1	231 449 681 752 889 1015 1141 1151 1262 1310 1415 1483 1506 1568 1696 1738 3340 3363 3371 3382
b_1	94 294 360 524 647 667 748 843 946
a_2	145 264 428 521 651 702 751 840 945
b_2	533 562 615 813 974 1053 1105 1161 1223 1362 1398 1508 1543 1551 1670 3340 3362 3369 3380