

Supporting Information

Evaluating the Impact of Hartree-Fock Exact Exchange on the Performance of Global Hybrid Functionals for the Vertical Excited-State Energies of Fused-Ring Electron Acceptors using TD-DFT

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Table S1 Experimental excitation energies ($E_{\text{max-exp}}$ in eV) and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed with PCM-TD-DFT/6-31G(d,p) and exchange-correlation functionals in chloroform solvent

| Molecule | $E_{\text{ver-theo}}$ | | | | | | $E_{\text{max-exp}}$ | |
|-----------|-----------------------|---------|------|------|----------|---------|----------------------|------------|
| | B3PW91 | mPW3PBE | B971 | B972 | mPW1PW91 | mPW1LYP | mPW1PBE | Experiment |
| F(DPP)2B2 | 1.88 | 1.88 | 1.90 | 1.91 | 1.97 | 1.96 | 1.97 | 2.02 |
| Cz-RH | 2.28 | 2.28 | 2.30 | 2.31 | 2.38 | 2.37 | 2.38 | 2.48 |
| Flu-RH | 2.20 | 2.20 | 2.22 | 2.23 | 2.30 | 2.28 | 2.30 | 2.48 |
| FRd2 | 2.12 | 2.12 | 2.14 | 2.15 | 2.23 | 2.21 | 2.23 | 2.44 |
| ITDI | 1.74 | 1.74 | 1.76 | 1.77 | 1.83 | 1.82 | 1.83 | 1.92 |
| SiIDT-IC | 1.97 | 1.97 | 1.99 | 2.00 | 2.05 | 2.04 | 2.05 | 1.94 |
| IDIDT-C8 | 1.74 | 1.74 | 1.76 | 1.77 | 1.85 | 1.85 | 1.85 | 1.89 |
| IDT-BOC6 | 1.72 | 1.72 | 1.74 | 1.75 | 1.84 | 1.83 | 1.84 | 1.80 |
| ATT1 | 1.67 | 1.67 | 1.68 | 1.69 | 1.75 | 1.74 | 1.75 | 1.80 |
| DC-IDT2T | 1.66 | 1.66 | 1.68 | 1.68 | 1.75 | 1.74 | 1.75 | 1.77 |
| BZIC | 1.79 | 1.79 | 1.80 | 1.81 | 1.85 | 1.84 | 1.85 | 1.75 |
| ITOIC | 1.66 | 1.66 | 1.67 | 1.68 | 1.74 | 1.73 | 1.74 | 1.72 |
| IDTOT2F | 1.63 | 1.63 | 1.64 | 1.65 | 1.71 | 1.70 | 1.71 | 1.72 |
| ITOIC-F | 1.66 | 1.66 | 1.67 | 1.68 | 1.74 | 1.73 | 1.74 | 1.69 |
| ITOIC-2F | 1.63 | 1.63 | 1.65 | 1.66 | 1.72 | 1.71 | 1.72 | 1.68 |
| IEICO | 1.45 | 1.45 | 1.46 | 1.47 | 1.53 | 1.52 | 1.53 | 1.58 |
| ATT2 | 1.49 | 1.49 | 1.50 | 1.50 | 1.56 | 1.55 | 1.56 | 1.57 |
| IEICO-4F | 1.43 | 1.43 | 1.44 | 1.44 | 1.50 | 1.49 | 1.50 | 1.54 |
| m-ITIC | 1.81 | 1.81 | 1.82 | 1.83 | 1.89 | 1.88 | 1.89 | 1.88 |
| IT-DM | 1.82 | 1.82 | 1.83 | 1.84 | 1.90 | 1.89 | 1.90 | 1.86 |
| IT-M | 1.82 | 1.82 | 1.83 | 1.84 | 1.90 | 1.88 | 1.90 | 1.86 |
| ITCPTC | 1.78 | 1.78 | 1.79 | 1.80 | 1.85 | 1.84 | 1.85 | 1.83 |
| Cl-ITIC | 1.78 | 1.78 | 1.79 | 1.80 | 1.86 | 1.85 | 1.86 | 1.79 |
| Br-ITIC | 1.78 | 1.78 | 1.79 | 1.80 | 1.86 | 1.85 | 1.86 | 1.79 |
| NFBDT | 1.74 | 1.74 | 1.75 | 1.76 | 1.82 | 1.81 | 1.82 | 1.76 |
| ITIC2 | 1.68 | 1.68 | 1.70 | 1.71 | 1.77 | 1.76 | 1.77 | 1.74 |
| ITVFFIC | 1.64 | 1.64 | 1.66 | 1.66 | 1.72 | 1.71 | 1.72 | 1.65 |
| INIC | 1.73 | 1.73 | 1.75 | 1.75 | 1.82 | 1.81 | 1.82 | 1.79 |
| INIC2 | 1.70 | 1.70 | 1.71 | 1.72 | 1.79 | 1.78 | 1.79 | 1.76 |
| INIC1 | 1.71 | 1.71 | 1.72 | 1.73 | 1.80 | 1.78 | 1.80 | 1.75 |
| INIC3 | 1.71 | 1.71 | 1.72 | 1.73 | 1.79 | 1.78 | 1.80 | 1.75 |
| IPIC | 1.69 | 1.69 | 1.70 | 1.71 | 1.77 | 1.76 | 1.77 | 1.63 |
| IPIC-4F | 1.67 | 1.67 | 1.68 | 1.69 | 1.75 | 1.74 | 1.75 | 1.60 |
| IPIC-4Cl | 1.65 | 1.65 | 1.66 | 1.67 | 1.73 | 1.72 | 1.73 | 1.57 |

Table S2 Experimental λ_{\max} (in nm) and theoretical $\lambda_{\text{ver-theo}}$ (in nm) of all FREAs computed with PCM-TD-DFT/6-31G(d,p) and exchange-correlation functionals in chloroform solvent

| Molecule | $\lambda_{\text{ver-theo}}$ | | | | | | | λ_{\max} |
|-----------|-----------------------------|--------|---------|-------|------|------|-----|------------------|
| | B3LYP | B3PW91 | mPW3PBE | X3LYP | B971 | B972 | B98 | Experiment |
| F(DPP)2B2 | 660 | 658 | 658 | 649 | 654 | 650 | 654 | 615 |
| Cz-RH | 547 | 544 | 544 | 538 | 540 | 537 | 541 | 500 |
| Flu-RH | 566 | 563 | 563 | 557 | 559 | 556 | 560 | 500 |
| FRd2 | 587 | 584 | 584 | 577 | 580 | 577 | 581 | 509 |
| ITDI | 715 | 711 | 711 | 702 | 706 | 702 | 707 | 647 |
| SiIDT-IC | 631 | 628 | 628 | 623 | 624 | 621 | 625 | 639 |
| IDIDT-C8 | 714 | 712 | 711 | 698 | 703 | 700 | 705 | 655 |
| IDT-BOC6 | 724 | 720 | 720 | 707 | 712 | 708 | 713 | 688 |
| ATT1 | 745 | 741 | 741 | 734 | 737 | 732 | 738 | 690 |
| DC-IDT2T | 749 | 745 | 745 | 735 | 739 | 736 | 741 | 700 |
| BZIC | 696 | 692 | 692 | 688 | 689 | 686 | 690 | 710 |
| ITOIC | 752 | 748 | 748 | 739 | 742 | 739 | 744 | 722 |
| IDTOT2F | 766 | 762 | 762 | 752 | 755 | 752 | 757 | 723 |
| ITOIC-F | 751 | 747 | 747 | 738 | 741 | 738 | 742 | 732 |
| ITOIC-2F | 763 | 759 | 759 | 749 | 752 | 749 | 754 | 737 |
| IEICO | 858 | 853 | 853 | 843 | 847 | 843 | 849 | 785 |
| ATT2 | 839 | 833 | 833 | 824 | 828 | 824 | 829 | 791 |
| IEICO-4F | 875 | 870 | 870 | 860 | 863 | 860 | 865 | 805 |
| m-ITIC | 688 | 686 | 685 | 678 | 681 | 678 | 682 | 660 |
| IT-DM | 685 | 683 | 682 | 675 | 678 | 675 | 679 | 665 |
| IT-M | 686 | 683 | 683 | 675 | 678 | 675 | 679 | 668 |
| ITCPTC | 701 | 698 | 697 | 690 | 693 | 690 | 694 | 678 |
| Cl-ITIC | 699 | 696 | 696 | 688 | 691 | 688 | 692 | 691 |
| Br-ITIC | 700 | 697 | 697 | 689 | 692 | 689 | 693 | 692 |
| NFBDT | 715 | 712 | 712 | 703 | 707 | 704 | 708 | 703 |
| ITIC2 | 739 | 736 | 736 | 726 | 730 | 727 | 731 | 714 |
| ITVFFIC | 758 | 755 | 754 | 745 | 748 | 746 | 749 | 750 |
| INIC | 720 | 716 | 715 | 706 | 710 | 707 | 711 | 692 |
| INIC2 | 734 | 730 | 730 | 720 | 724 | 720 | 725 | 704 |
| INIC1 | 730 | 726 | 726 | 717 | 720 | 717 | 721 | 710 |
| INIC3 | 730 | 727 | 726 | 717 | 720 | 717 | 721 | 710 |
| IPIC | 737 | 734 | 734 | 725 | 728 | 725 | 729 | 761 |
| IPIC-4F | 747 | 744 | 743 | 734 | 737 | 735 | 738 | 776 |
| IPIC-4Cl | 760 | 751 | 751 | 741 | 745 | 742 | 746 | 790 |

Table S3 Experimental λ_{\max} (in nm) and theoretical $\lambda_{\text{ver-theo}}$ (in nm) of all FREAs computed with PCM-TD-DFT/6-31G(d,p) and exchange-correlation functionals in chloroform solvent

| Molecule | $\lambda_{\text{ver-theo}}$ | λ_{\max} |
|----------|-----------------------------|------------------|
|----------|-----------------------------|------------------|

| | APF/ APFD | PBE0 | mPW1PW91 | mPW1LYP | mPW1PBE | M06 | M05 | M062X | Experiment |
|-----------|-----------|------|----------|---------|---------|-----|-----|-------|------------|
| F(DPP)2B2 | 640 | 628 | 629 | 632 | 629 | 627 | 617 | 555 | 615 |
| Cz-RH | 529 | 520 | 520 | 524 | 520 | 523 | 515 | 452 | 500 |
| Flu-RH | 548 | 538 | 539 | 543 | 539 | 542 | 534 | 466 | 500 |
| FRd2 | 567 | 556 | 556 | 561 | 556 | 560 | 553 | 470 | 509 |
| ITDI | 690 | 676 | 677 | 681 | 677 | 670 | 655 | 568 | 647 |
| SiIDT-IC | 614 | 605 | 605 | 609 | 605 | 605 | 591 | 532 | 639 |
| IDIDT-C8 | 685 | 668 | 669 | 672 | 669 | 659 | 644 | 536 | 655 |
| IDT-BOC6 | 692 | 674 | 675 | 679 | 675 | 668 | 650 | 535 | 688 |
| ATT1 | 721 | 708 | 708 | 714 | 708 | 708 | 694 | 598 | 690 |
| DC-IDT2T | 722 | 707 | 708 | 713 | 708 | 700 | 682 | 586 | 700 |
| BZIC | 678 | 669 | 670 | 674 | 669 | 669 | 652 | 594 | 710 |
| ITOIC | 726 | 711 | 712 | 717 | 712 | 704 | 687 | 596 | 722 |
| IDTOT2F | 738 | 723 | 724 | 729 | 724 | 717 | 698 | 603 | 723 |
| ITOIC-F | 725 | 710 | 711 | 716 | 711 | 704 | 687 | 596 | 732 |
| ITOIC-2F | 736 | 721 | 722 | 727 | 721 | 714 | 696 | 602 | 737 |
| IEICO | 828 | 811 | 813 | 818 | 812 | 807 | 787 | 671 | 785 |
| ATT2 | 808 | 792 | 794 | 801 | 793 | 786 | 766 | 664 | 791 |
| IEICO-4F | 844 | 827 | 829 | 835 | 828 | 825 | 804 | 555 | 805 |
| m-ITIC | 667 | 656 | 657 | 660 | 656 | 653 | 637 | 452 | 660 |
| IT-DM | 664 | 652 | 653 | 657 | 653 | 650 | 633 | 466 | 665 |
| IT-M | 665 | 653 | 654 | 658 | 654 | 651 | 634 | 470 | 668 |
| ITCPTC | 680 | 668 | 669 | 673 | 669 | 666 | 648 | 568 | 678 |
| Cl-ITIC | 677 | 665 | 666 | 670 | 666 | 663 | 647 | 532 | 691 |
| Br-ITIC | 678 | 666 | 667 | 671 | 667 | 665 | 648 | 536 | 692 |
| NFBDT | 693 | 681 | 682 | 684 | 681 | 680 | 665 | 535 | 703 |
| ITIC2 | 715 | 701 | 702 | 705 | 702 | 700 | 683 | 598 | 714 |
| ITVFFIC | 733 | 719 | 720 | 724 | 720 | 715 | 694 | 586 | 750 |
| INIC | 694 | 679 | 680 | 685 | 680 | 674 | 655 | 594 | 692 |
| INIC2 | 707 | 692 | 693 | 698 | 693 | 686 | 667 | 596 | 704 |
| INIC1 | 704 | 689 | 690 | 695 | 690 | 683 | 664 | 603 | 710 |
| INIC3 | 704 | 689 | 691 | 695 | 690 | 684 | 665 | 596 | 710 |
| IPIC | 713 | 700 | 701 | 705 | 700 | 696 | 679 | 602 | 761 |
| IPIC-4F | 722 | 708 | 710 | 713 | 709 | 705 | 688 | 671 | 776 |
| IPIC-4Cl | 729 | 721 | 716 | 720 | 716 | 711 | 694 | 664 | 790 |

Table S4 Deviation ($E_{\text{max-exp}} - E_{\text{ver-theo}}$) of theoretical value from experimental one for all FREAs^a

| Molecule | Deviation ($E_{\text{max-exp}} - E_{\text{ver-theo}}$) (eV) |
|----------|---|
|----------|---|

| | B3LYP | B3PW91 | mPW3PBE | X3LYP | B971 | B972 | B98 |
|-----------|-------|--------|---------|-------|-------|-------|-------|
| F(DPP)2B2 | 0.14 | 0.14 | 0.14 | 0.11 | 0.12 | 0.11 | 0.12 |
| Cz-RH | 0.21 | 0.2 | 0.2 | 0.18 | 0.18 | 0.17 | 0.19 |
| Flu-RH | 0.29 | 0.28 | 0.28 | 0.25 | 0.26 | 0.25 | 0.27 |
| FRd2 | 0.33 | 0.32 | 0.32 | 0.29 | 0.3 | 0.29 | 0.31 |
| ITDI | 0.19 | 0.18 | 0.18 | 0.15 | 0.16 | 0.15 | 0.17 |
| SiIDT-IC | -0.03 | -0.03 | -0.03 | -0.05 | -0.05 | -0.06 | -0.04 |
| IDIDT-C8 | 0.15 | 0.15 | 0.15 | 0.11 | 0.13 | 0.12 | 0.13 |
| IDT-BOC6 | 0.09 | 0.08 | 0.08 | 0.05 | 0.06 | 0.05 | 0.06 |
| ATT1 | 0.14 | 0.13 | 0.13 | 0.11 | 0.12 | 0.11 | 0.12 |
| DC-IDT2T | 0.11 | 0.11 | 0.11 | 0.08 | 0.09 | 0.09 | 0.1 |
| BZIC | -0.03 | -0.04 | -0.04 | -0.05 | -0.05 | -0.06 | -0.05 |
| ITOIC | 0.07 | 0.06 | 0.06 | 0.04 | 0.05 | 0.04 | 0.05 |
| IDTOT2F | 0.1 | 0.09 | 0.09 | 0.07 | 0.08 | 0.07 | 0.08 |
| ITOIC-F | 0.04 | 0.03 | 0.03 | 0.01 | 0.02 | 0.01 | 0.02 |
| ITOIC-2F | 0.05 | 0.05 | 0.05 | 0.02 | 0.03 | 0.02 | 0.04 |
| IEICO | 0.13 | 0.13 | 0.13 | 0.11 | 0.12 | 0.11 | 0.12 |
| ATT2 | 0.09 | 0.08 | 0.08 | 0.07 | 0.07 | 0.07 | 0.07 |
| IEICO-4F | 0.12 | 0.11 | 0.11 | 0.1 | 0.1 | 0.1 | 0.11 |
| m-ITIC | 0.08 | 0.07 | 0.07 | 0.05 | 0.06 | 0.05 | 0.06 |
| IT-DM | 0.05 | 0.04 | 0.04 | 0.02 | 0.03 | 0.02 | 0.03 |
| IT-M | 0.05 | 0.04 | 0.04 | 0.02 | 0.03 | 0.02 | 0.03 |
| ITCPTC | 0.06 | 0.05 | 0.05 | 0.03 | 0.04 | 0.03 | 0.04 |
| Cl-ITIC | 0.02 | 0.01 | 0.01 | -0.01 | 0 | -0.01 | 0 |
| Br-ITIC | 0.02 | 0.01 | 0.01 | -0.01 | 0 | -0.01 | 0 |
| NFBDT | 0.03 | 0.02 | 0.02 | 0 | 0.01 | 0 | 0.01 |
| ITIC2 | 0.06 | 0.06 | 0.06 | 0.03 | 0.04 | 0.03 | 0.04 |
| ITVFFIC | 0.01 | 0.01 | 0.01 | -0.01 | -0.01 | -0.01 | -0.01 |
| INIC | 0.07 | 0.06 | 0.06 | 0.03 | 0.04 | 0.04 | 0.05 |
| INIC2 | 0.07 | 0.06 | 0.06 | 0.04 | 0.05 | 0.04 | 0.05 |
| INIC1 | 0.05 | 0.04 | 0.04 | 0.02 | 0.03 | 0.02 | 0.03 |
| INIC3 | 0.05 | 0.04 | 0.04 | 0.02 | 0.03 | 0.02 | 0.03 |
| IPIC | -0.05 | -0.06 | -0.06 | -0.08 | -0.07 | -0.08 | -0.07 |
| IPIC-4F | -0.06 | -0.07 | -0.07 | -0.09 | -0.08 | -0.09 | -0.08 |
| IPIC-4Cl | -0.06 | -0.08 | -0.08 | -0.1 | -0.09 | -0.1 | -0.09 |

^a $E_{\text{ver-theo}}$ and $E_{\text{max-exp}}$ are the theoretical vertical and experimental maximum excitation energies, respectively.

Table S5 Deviation ($E_{\text{max-exp}} - E_{\text{ver-theo}}$) of theoretical value from experimental one for all FREAs^a

| Molecule | Deviation ($E_{\text{max-exp}} - E_{\text{ver-theo}}$) (eV) |
|----------|---|
|----------|---|

| | APF /APFD | PBE0 | mPW1PW91 | mPW1LYP | mPW1PBE | M06 | M05 | M06-2X |
|-----------|-----------|-------|----------|---------|---------|-------|-------|--------|
| F(DPP)2B2 | 0.08 | 0.05 | 0.05 | 0.06 | 0.05 | 0.04 | 0.01 | -0.22 |
| Cz-RH | 0.14 | 0.10 | 0.1 | 0.11 | 0.1 | 0.11 | 0.07 | -0.26 |
| Flu-RH | 0.22 | 0.18 | 0.18 | 0.2 | 0.18 | 0.19 | 0.16 | -0.18 |
| FRd2 | 0.25 | 0.21 | 0.21 | 0.23 | 0.21 | 0.23 | 0.2 | -0.2 |
| ITDI | 0.12 | 0.09 | 0.09 | 0.1 | 0.09 | 0.07 | 0.03 | -0.26 |
| SiIDT-IC | -0.08 | -0.11 | -0.11 | -0.1 | -0.11 | -0.11 | -0.16 | -0.39 |
| IDIDT-C8 | 0.08 | 0.03 | 0.04 | 0.04 | 0.04 | 0.01 | -0.04 | -0.42 |
| IDT-BOC6 | 0.01 | -0.04 | -0.04 | -0.03 | -0.04 | -0.06 | -0.11 | -0.52 |
| ATT1 | 0.08 | 0.05 | 0.05 | 0.06 | 0.05 | 0.05 | 0.01 | -0.27 |
| DC-IDT2T | 0.05 | 0.02 | 0.02 | 0.03 | 0.02 | 0 | -0.05 | -0.35 |
| BZIC | -0.08 | -0.10 | -0.1 | -0.09 | -0.1 | -0.1 | -0.15 | -0.34 |
| ITOIC | 0.01 | -0.02 | -0.02 | -0.01 | -0.02 | -0.04 | -0.08 | -0.36 |
| IDTOT2F | 0.04 | 0.00 | 0.01 | 0.02 | 0.01 | -0.01 | -0.06 | -0.34 |
| ITOIC-F | -0.02 | -0.06 | -0.05 | -0.04 | -0.05 | -0.07 | -0.11 | -0.39 |
| ITOIC-2F | 0 | -0.04 | -0.04 | -0.03 | -0.04 | -0.06 | -0.1 | -0.38 |
| IEICO | 0.08 | 0.05 | 0.05 | 0.06 | 0.05 | 0.04 | 0 | -0.27 |
| ATT2 | 0.04 | 0.00 | 0.01 | 0.02 | 0.01 | -0.01 | -0.05 | -0.3 |
| IEICO-4F | 0.07 | 0.04 | 0.04 | 0.05 | 0.04 | 0.04 | 0 | -0.27 |
| m-ITIC | 0.02 | -0.01 | -0.01 | 0 | -0.01 | -0.02 | -0.07 | -0.33 |
| IT-DM | -0.01 | -0.04 | -0.04 | -0.03 | -0.04 | -0.05 | -0.1 | -0.36 |
| IT-M | 0 | -0.04 | -0.04 | -0.02 | -0.04 | -0.04 | -0.1 | -0.36 |
| ITCPTC | 0.01 | -0.03 | -0.02 | -0.01 | -0.02 | -0.03 | -0.08 | -0.34 |
| Cl-ITIC | -0.04 | -0.07 | -0.07 | -0.06 | -0.07 | -0.08 | -0.13 | -0.39 |
| Br-ITIC | -0.04 | -0.07 | -0.07 | -0.06 | -0.07 | -0.07 | -0.12 | -0.39 |
| NFBDT | -0.03 | -0.06 | -0.06 | -0.05 | -0.06 | -0.06 | -0.1 | -0.37 |
| ITIC2 | 0.01 | -0.03 | -0.03 | -0.02 | -0.03 | -0.03 | -0.08 | -0.36 |
| ITVFFIC | -0.04 | -0.07 | -0.07 | -0.06 | -0.07 | -0.08 | -0.14 | -0.4 |
| INIC | 0 | -0.04 | -0.03 | -0.02 | -0.03 | -0.05 | -0.1 | -0.4 |
| INIC2 | 0.01 | -0.03 | -0.03 | -0.02 | -0.03 | -0.05 | -0.1 | -0.4 |
| INIC1 | -0.01 | -0.05 | -0.05 | -0.03 | -0.05 | -0.07 | -0.12 | -0.41 |
| INIC3 | -0.01 | -0.05 | -0.04 | -0.03 | -0.05 | -0.06 | -0.11 | -0.41 |
| IPIC | -0.11 | -0.14 | -0.14 | -0.13 | -0.14 | -0.15 | -0.2 | -0.44 |
| IPIC-4F | -0.12 | -0.15 | -0.15 | -0.14 | -0.15 | -0.16 | -0.2 | -0.45 |
| IPIC-4Cl | -0.13 | -0.15 | -0.16 | -0.15 | -0.16 | -0.17 | -0.22 | -0.46 |

^a $E_{\text{ver-theo}}$ and $E_{\text{max-exp}}$ are theoretical vertical and experimental maximum excitation energies, respectively.

Table S6 Charge transfer calculated with B3LYP ^a, APF, and PBE0^a

| Molecule | B3LYP | APF | PBE0 |
|----------|-------|-----|------|
|----------|-------|-----|------|

| | | | |
|----------|-------|-------|-------|
| NFBDT | 0.553 | 0.559 | 0.566 |
| ITOIC-2F | 0.637 | 0.642 | 0.648 |
| INIC2 | 0.647 | 0.651 | 0.656 |
| IEICO-4F | 0.6 | 0.613 | 0.626 |
| DC-IDT2T | 0.647 | 0.650 | 0.659 |
| IPIC | 0.598 | 0.605 | 0.609 |
| IPIC-4F | 0.6 | 0.607 | 0.611 |
| IT-DM | 0.593 | 0.598 | 0.605 |
| ITVFFIC | 0.605 | 0.611 | 0.622 |
| Flu-RH | 0.521 | 0.523 | 0.527 |

^a The values for B3LYP and PBE0 have been taken from our previous study.¹

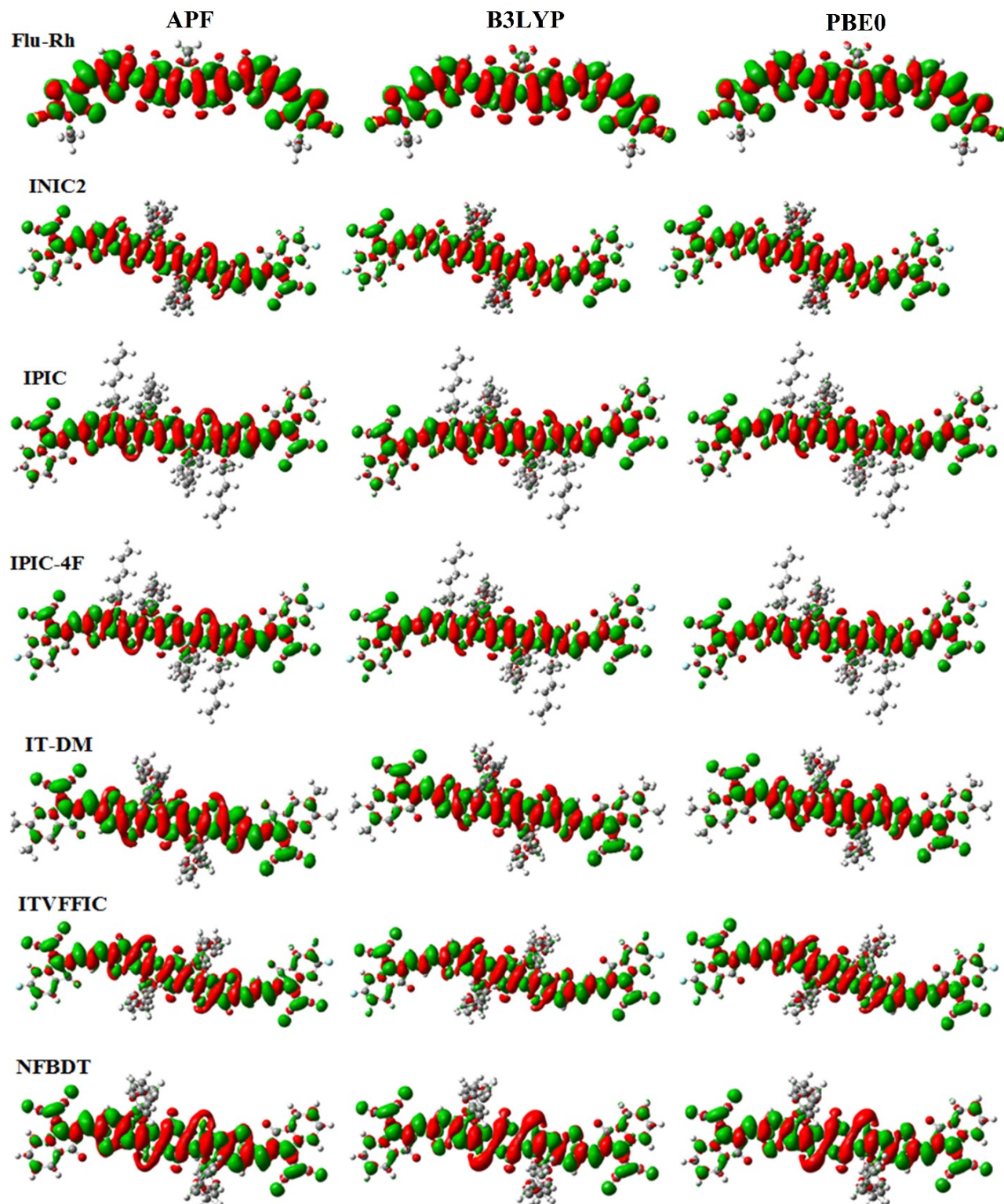


Fig. S1 Plots of the density difference between the ground and excited states computed for Flu-Rh, INIC2, IPIC, IPIC-4F, IT-DM, ITVFFIC, and NFBDT obtained using PCM-TD-APF, PCM-TD-B3LYP, and PCM-TD-PBE0 (contour threshold: 0.0002 a.u.)

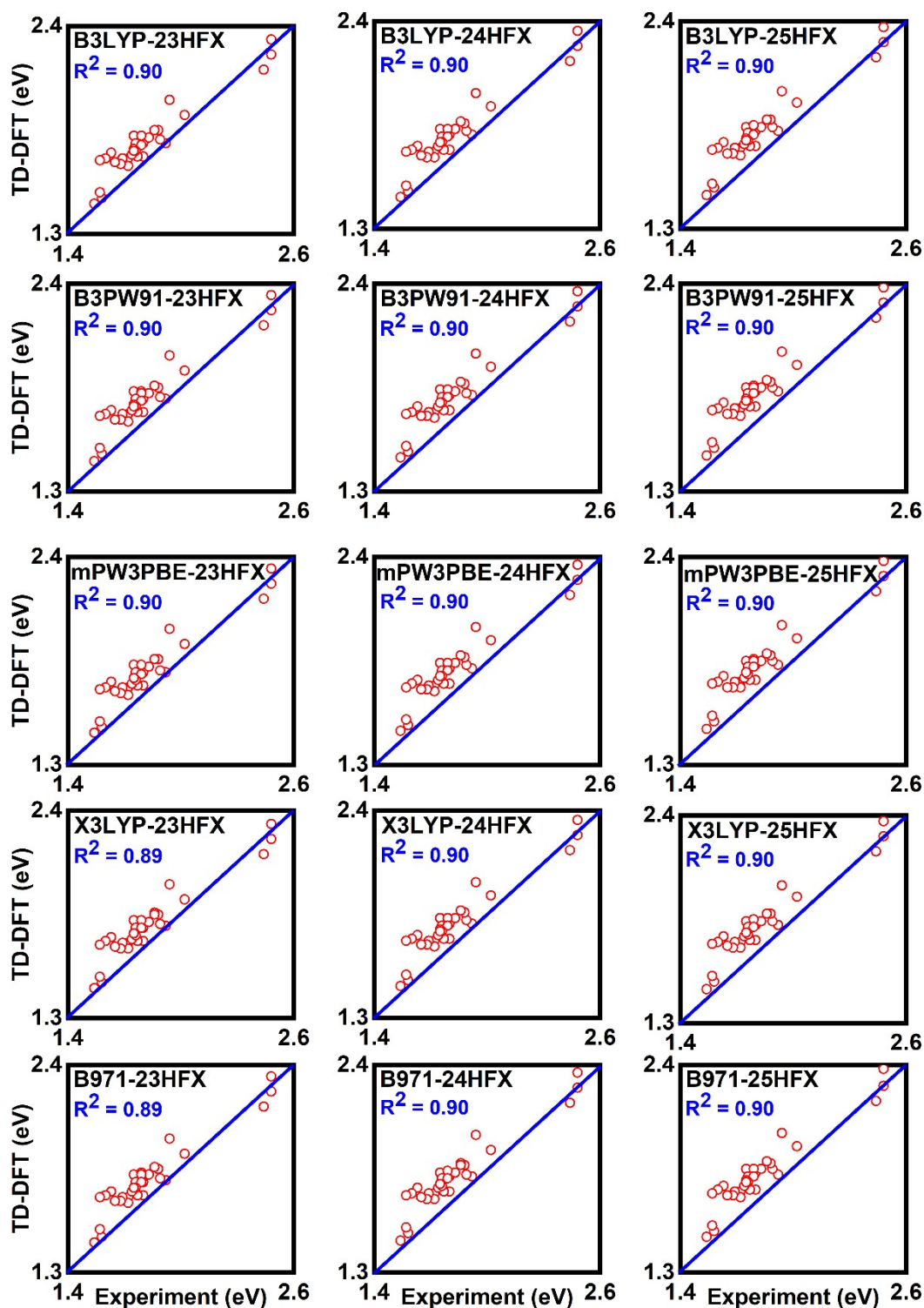


Fig. S2 Comparison between experimental maximum transition energies ($E_{\text{max-exp}}$) and theoretical vertical excitation energies ($E_{\text{ver-theo}}$) using B3LYP-23HFX, B3LYP-24HFX, B3LYP-25HFX, B3PW91-23HFX, B3PW91-24HFX, B3PW91-25HFX, mPW3PBE-23HFX, mPW3PBE-24HFX, mPW3PBE-25HFX, X3LYP-23HFX, X3LYP-24HFX, X3LYP-25HFX, B971-23HFX, B971-24HFX, and B971-25HFX. The solid line shows the theory-experiment perfect match. R^2 is the determination coefficient.

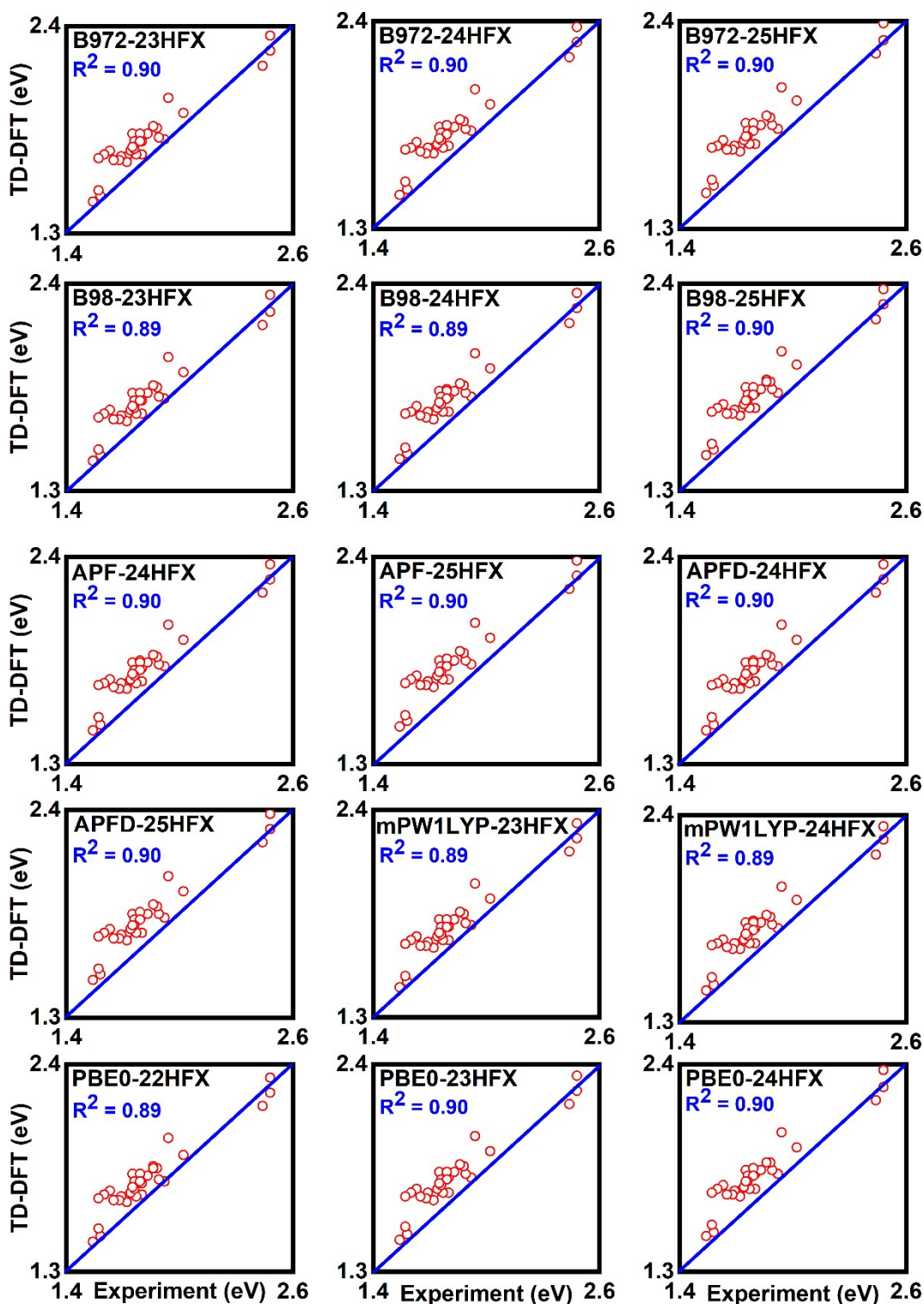


Fig. S3 Comparison between experimental maximum transition energies ($E_{\max\text{-exp}}$) and theoretical vertical excitation energies ($E_{\text{ver-theo}}$) using B972-23HFX, B972-24HFX, B972-25HFX, B98-23HFX, B98-24HFX, B98-25HFX, APF-24HFX, APF-25HFX, APFD-24HFX, APFD-25HFX, mPW1LYP-23HFX, mPW1LYP-24HFX, PBE0-22HFX, PBE0-23HFX, and PBE0-24HFX. The solid line shows the theory-experiment perfect match. R^2 is the determination coefficient.

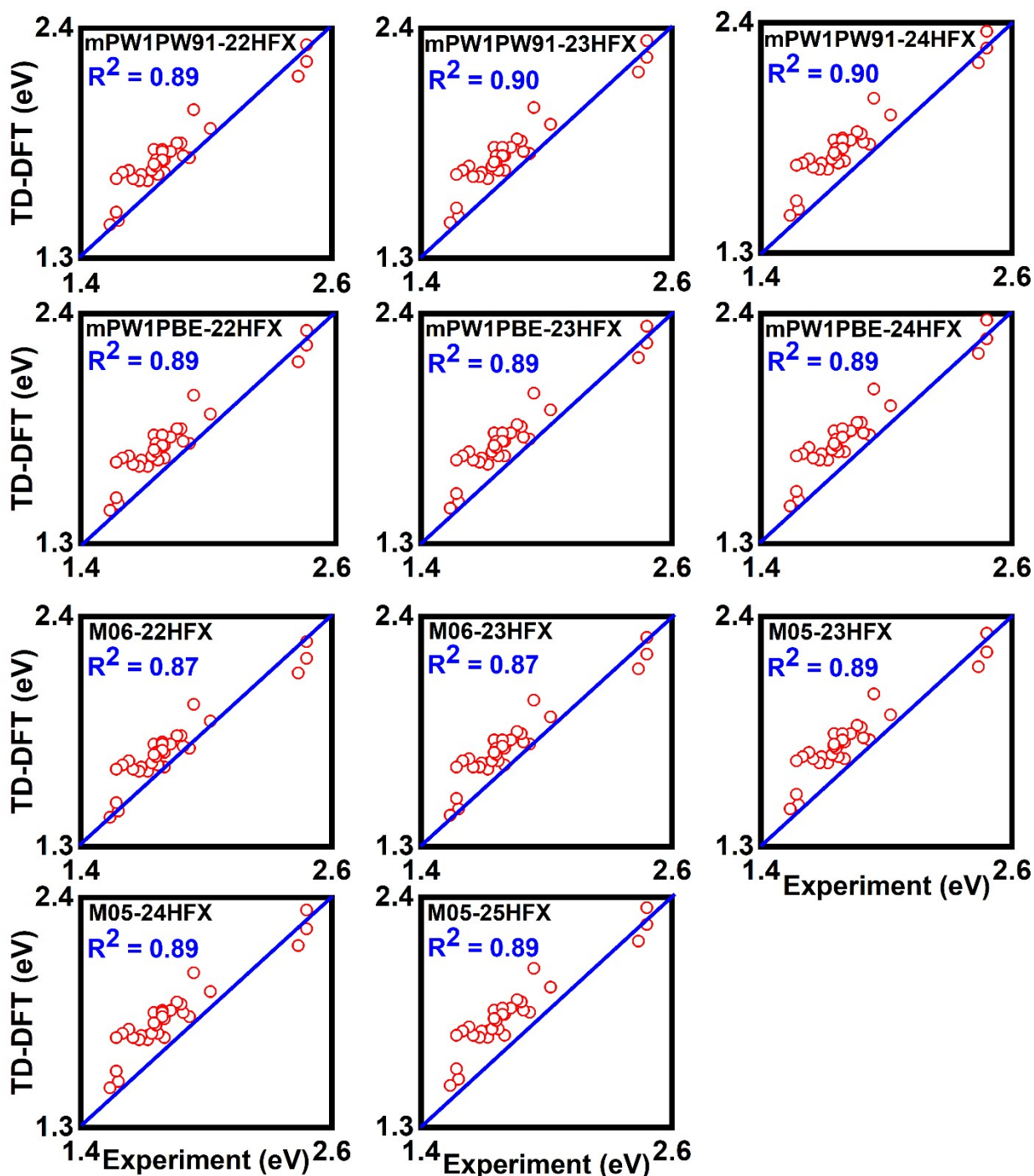


Fig. S4 Comparison between experimental maximum transition energies ($E_{\text{max-exp}}$) and theoretical vertical excitation energies ($E_{\text{ver-theo}}$) using mPW1PW91-22HFX, mPW1PW91-23HFX, mPW1PW91-24HFX, mPW1PBE-22HFX, mPW1PBE-23HFX, mPW1PBE-24HFX, M06-22HFX, M06-23HFX, M05-23HFX, M05-24HFX and M05-25HFX. The solid line shows the theory-experiment perfect match. R^2 is the determination coefficient.

Table S7 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-----------|---|------|-------------|------|-------------|------|-------------|------|-------------|------|-------------|------|---|------|
| | B3LYP | | B3LYP-21HFX | | B3LYP-22HFX | | B3LYP-23HFX | | B3LYP-24HFX | | B3LYP-25HFX | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 660 | 1.88 | 654 | 1.90 | 647 | 1.92 | 641 | 1.93 | 636 | 1.95 | 630 | 1.97 | 615 | 2.02 |
| Cz-RH | 547 | 2.27 | 542 | 2.29 | 537 | 2.31 | 532 | 2.33 | 528 | 2.35 | 524 | 2.37 | 500 | 2.48 |
| Flu-RH | 566 | 2.19 | 561 | 2.21 | 556 | 2.23 | 551 | 2.25 | 547 | 2.27 | 542 | 2.29 | 500 | 2.48 |
| FRd2 | 587 | 2.11 | 582 | 2.13 | 576 | 2.15 | 571 | 2.17 | 566 | 2.19 | 562 | 2.21 | 509 | 2.44 |
| ITDI | 715 | 1.73 | 708 | 1.75 | 701 | 1.77 | 695 | 1.78 | 688 | 1.80 | 682 | 1.82 | 647 | 1.92 |
| SiIDT-IC | 631 | 1.97 | 627 | 1.98 | 622 | 1.99 | 618 | 2.01 | 614 | 2.02 | 610 | 2.03 | 639 | 1.94 |
| IDIDT-C8 | 714 | 1.74 | 706 | 1.76 | 698 | 1.78 | 690 | 1.80 | 682 | 1.82 | 675 | 1.84 | 655 | 1.89 |
| IDT-BOC6 | 724 | 1.71 | 715 | 1.73 | 706 | 1.76 | 697 | 1.78 | 689 | 1.80 | 681 | 1.82 | 688 | 1.80 |
| ATT1 | 745 | 1.66 | 739 | 1.68 | 732 | 1.69 | 726 | 1.71 | 719 | 1.72 | 713 | 1.74 | 690 | 1.80 |
| DC-IDT2T | 749 | 1.66 | 742 | 1.67 | 734 | 1.69 | 727 | 1.71 | 720 | 1.72 | 714 | 1.74 | 700 | 1.77 |
| BZIC | 696 | 1.78 | 691 | 1.79 | 687 | 1.80 | 682 | 1.82 | 678 | 1.83 | 674 | 1.84 | 710 | 1.75 |
| ITOIC | 752 | 1.65 | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 724 | 1.71 | 717 | 1.73 | 722 | 1.72 |
| IDTOT2F | 766 | 1.62 | 759 | 1.63 | 752 | 1.65 | 745 | 1.66 | 738 | 1.68 | 732 | 1.69 | 723 | 1.72 |
| ITOIC-F | 751 | 1.65 | 744 | 1.67 | 737 | 1.68 | 731 | 1.70 | 724 | 1.71 | 718 | 1.73 | 732 | 1.69 |
| ITOIC-2F | 763 | 1.63 | 756 | 1.64 | 749 | 1.66 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 737 | 1.68 |
| IEICO | 858 | 1.45 | 850 | 1.46 | 841 | 1.47 | 833 | 1.49 | 826 | 1.50 | 818 | 1.52 | 785 | 1.58 |
| ATT2 | 839 | 1.48 | 831 | 1.49 | 824 | 1.50 | 817 | 1.52 | 810 | 1.53 | 803 | 1.54 | 791 | 1.57 |
| IEICO-4F | 875 | 1.42 | 867 | 1.43 | 859 | 1.44 | 852 | 1.46 | 844 | 1.47 | 837 | 1.48 | 805 | 1.54 |
| m-ITIC | 688 | 1.80 | 683 | 1.82 | 677 | 1.83 | 672 | 1.85 | 666 | 1.86 | 661 | 1.88 | 660 | 1.88 |
| IT-DM | 685 | 1.81 | 680 | 1.82 | 674 | 1.84 | 669 | 1.85 | 663 | 1.87 | 658 | 1.88 | 665 | 1.86 |
| IT-M | 686 | 1.81 | 680 | 1.82 | 675 | 1.84 | 669 | 1.85 | 664 | 1.87 | 659 | 1.88 | 668 | 1.86 |
| ITCPTC | 701 | 1.77 | 695 | 1.78 | 690 | 1.80 | 684 | 1.81 | 679 | 1.83 | 674 | 1.84 | 678 | 1.83 |
| Cl-ITIC | 699 | 1.77 | 693 | 1.79 | 687 | 1.80 | 682 | 1.82 | 676 | 1.83 | 671 | 1.85 | 691 | 1.79 |
| Br-ITIC | 700 | 1.77 | 694 | 1.79 | 688 | 1.80 | 683 | 1.82 | 677 | 1.83 | 672 | 1.85 | 692 | 1.79 |
| NFBBDT | 715 | 1.73 | 708 | 1.75 | 702 | 1.77 | 697 | 1.78 | 691 | 1.79 | 685 | 1.81 | 703 | 1.76 |
| ITIC2 | 739 | 1.68 | 732 | 1.69 | 725 | 1.71 | 719 | 1.72 | 713 | 1.74 | 707 | 1.75 | 714 | 1.74 |
| ITVFFIC | 758 | 1.64 | 752 | 1.65 | 746 | 1.66 | 739 | 1.68 | 734 | 1.69 | 728 | 1.70 | 750 | 1.65 |
| INIC | 720 | 1.72 | 713 | 1.74 | 706 | 1.76 | 699 | 1.77 | 693 | 1.79 | 687 | 1.80 | 692 | 1.79 |
| INIC2 | 734 | 1.69 | 727 | 1.71 | 720 | 1.72 | 713 | 1.74 | 706 | 1.76 | 700 | 1.77 | 704 | 1.76 |
| INIC1 | 730 | 1.70 | 723 | 1.72 | 716 | 1.73 | 710 | 1.75 | 703 | 1.76 | 697 | 1.78 | 710 | 1.75 |
| INIC3 | 730 | 1.70 | 724 | 1.71 | 717 | 1.73 | 711 | 1.74 | 705 | 1.76 | 699 | 1.77 | 710 | 1.75 |
| IPIC | 737 | 1.68 | 731 | 1.70 | 724 | 1.71 | 718 | 1.73 | 711 | 1.74 | 706 | 1.76 | 761 | 1.63 |
| IPIC-4F | 747 | 1.66 | 740 | 1.68 | 734 | 1.69 | 728 | 1.70 | 722 | 1.72 | 716 | 1.73 | 776 | 1.60 |
| IPIC-4Cl | 760 | 1.63 | 753 | 1.66 | 746 | 1.68 | 740 | 1.69 | 733 | 1.71 | 727 | 1.72 | 790 | 1.57 |

^aXC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S8 Experimental maximum absorption wavelengths (λ_{\max} in nm), experimental transition energies ($E_{\max\text{-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{\max} and $E_{\max\text{-exp}}$ | |
|-------------|---|------|--------------|------|--------------|------|--------------|------|--------------|------|--------------|------|--|------|
| | B3PW91 | | B3PW91-21HFX | | B3PW91-22HFX | | B3PW91-23HFX | | B3PW91-24HFX | | B3PW91-25HFX | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 658 | 1.88 | 651 | 1.90 | 645 | 1.92 | 639 | 1.94 | 633 | 1.96 | 628 | 1.97 | 615 | 2.02 |
| Cz-RH | 544 | 2.28 | 539 | 2.30 | 534 | 2.32 | 529 | 2.34 | 525 | 2.36 | 521 | 2.38 | 500 | 2.48 |
| Flu-RH | 563 | 2.20 | 558 | 2.22 | 553 | 2.24 | 548 | 2.26 | 544 | 2.28 | 539 | 2.30 | 500 | 2.48 |
| FRd2 | 584 | 2.12 | 578 | 2.15 | 573 | 2.16 | 568 | 2.18 | 563 | 2.20 | 558 | 2.22 | 509 | 2.44 |
| ITDI | 711 | 1.74 | 704 | 1.76 | 698 | 1.78 | 691 | 1.79 | 685 | 1.81 | 679 | 1.83 | 647 | 1.92 |
| SiIDT-IC-IC | 628 | 1.97 | 623 | 1.99 | 619 | 2.00 | 615 | 2.02 | 611 | 2.03 | 607 | 2.04 | 639 | 1.94 |
| IDIDT-C8 | 712 | 1.74 | 703 | 1.76 | 695 | 1.78 | 687 | 1.80 | 680 | 1.82 | 672 | 1.85 | 655 | 1.89 |
| IDT-BOC6 | 720 | 1.72 | 711 | 1.74 | 702 | 1.77 | 694 | 1.79 | 685 | 1.81 | 677 | 1.83 | 688 | 1.80 |
| ATT1 | 741 | 1.67 | 734 | 1.69 | 727 | 1.71 | 721 | 1.72 | 715 | 1.73 | 709 | 1.75 | 690 | 1.80 |
| DC-IDT2T | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 723 | 1.72 | 717 | 1.73 | 710 | 1.75 | 700 | 1.77 |
| BZIC | 692 | 1.79 | 688 | 1.80 | 683 | 1.82 | 679 | 1.83 | 674 | 1.84 | 670 | 1.85 | 710 | 1.75 |
| ITOIC | 748 | 1.66 | 741 | 1.67 | 734 | 1.69 | 727 | 1.71 | 720 | 1.72 | 713 | 1.74 | 722 | 1.72 |
| IDTOT2F | 762 | 1.63 | 755 | 1.64 | 748 | 1.66 | 741 | 1.67 | 734 | 1.69 | 728 | 1.70 | 723 | 1.72 |
| ITOIC-F | 747 | 1.66 | 740 | 1.68 | 733 | 1.69 | 727 | 1.71 | 720 | 1.72 | 714 | 1.74 | 732 | 1.69 |
| ITOIC-2F | 759 | 1.63 | 752 | 1.65 | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 725 | 1.71 | 737 | 1.68 |
| IEICO | 853 | 1.45 | 845 | 1.47 | 837 | 1.48 | 829 | 1.50 | 821 | 1.51 | 813 | 1.53 | 785 | 1.58 |
| ATT2 | 833 | 1.49 | 825 | 1.50 | 818 | 1.52 | 811 | 1.53 | 804 | 1.54 | 797 | 1.56 | 791 | 1.57 |
| IEICO-4F | 870 | 1.43 | 862 | 1.44 | 854 | 1.45 | 847 | 1.46 | 839 | 1.48 | 832 | 1.49 | 805 | 1.54 |
| m-ITIC | 686 | 1.81 | 680 | 1.82 | 674 | 1.84 | 669 | 1.85 | 664 | 1.87 | 658 | 1.88 | 660 | 1.88 |
| IT-DM | 683 | 1.82 | 677 | 1.83 | 671 | 1.85 | 666 | 1.86 | 660 | 1.88 | 655 | 1.89 | 665 | 1.86 |
| IT-M | 683 | 1.82 | 677 | 1.83 | 672 | 1.85 | 666 | 1.86 | 661 | 1.88 | 656 | 1.89 | 668 | 1.86 |
| ITCPTC | 698 | 1.78 | 692 | 1.79 | 686 | 1.81 | 681 | 1.82 | 676 | 1.83 | 671 | 1.85 | 678 | 1.83 |
| Cl-ITIC | 696 | 1.78 | 690 | 1.80 | 684 | 1.81 | 679 | 1.83 | 673 | 1.84 | 668 | 1.86 | 691 | 1.79 |
| Br-ITIC | 697 | 1.78 | 691 | 1.79 | 685 | 1.81 | 680 | 1.82 | 674 | 1.84 | 669 | 1.85 | 692 | 1.79 |
| NFBDT | 712 | 1.74 | 706 | 1.76 | 700 | 1.77 | 694 | 1.79 | 689 | 1.80 | 683 | 1.82 | 703 | 1.76 |
| ITIC2 | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 716 | 1.73 | 710 | 1.75 | 704 | 1.76 | 714 | 1.74 |
| ITVFFIC | 755 | 1.64 | 748 | 1.66 | 742 | 1.67 | 736 | 1.68 | 730 | 1.70 | 724 | 1.71 | 750 | 1.65 |
| INIC | 716 | 1.73 | 709 | 1.75 | 702 | 1.77 | 695 | 1.78 | 689 | 1.80 | 683 | 1.82 | 692 | 1.79 |
| INIC2 | 730 | 1.70 | 723 | 1.72 | 716 | 1.73 | 709 | 1.75 | 702 | 1.77 | 696 | 1.78 | 704 | 1.76 |
| INIC1 | 726 | 1.71 | 719 | 1.72 | 712 | 1.74 | 706 | 1.76 | 699 | 1.77 | 693 | 1.79 | 710 | 1.75 |
| INIC3 | 727 | 1.71 | 720 | 1.72 | 713 | 1.74 | 707 | 1.75 | 701 | 1.77 | 695 | 1.78 | 710 | 1.75 |
| IPIC | 734 | 1.69 | 728 | 1.70 | 721 | 1.72 | 715 | 1.73 | 708 | 1.75 | 702 | 1.77 | 761 | 1.63 |
| IPIC-4F | 744 | 1.67 | 737 | 1.68 | 731 | 1.70 | 725 | 1.71 | 719 | 1.72 | 713 | 1.74 | 776 | 1.60 |
| IPIC-4Cl | 751 | 1.65 | 744 | 1.67 | 737 | 1.68 | 731 | 1.70 | 724 | 1.71 | 718 | 1.73 | 790 | 1.57 |

^aXC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S9 Experimental maximum absorption wavelengths (λ_{\max} in nm), experimental transition energies ($E_{\max\text{-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{\max} and $E_{\max\text{-exp}}$ | |
|-----------|---|------|---------------|------|---------------|------|---------------|------|---------------|------|---------------|------|--|------|
| | mPW3PBE | | mPW3PBE-21HFX | | mPW3PBE-22HFX | | mPW3PBE-23HFX | | mPW3PBE-24HFX | | mPW3PBE-25HFX | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 658 | 1.88 | 651 | 1.90 | 645 | 1.92 | 639 | 1.94 | 633 | 1.96 | 628 | 1.97 | 615 | 2.02 |
| Cz-RH | 544 | 2.28 | 539 | 2.30 | 534 | 2.32 | 529 | 2.34 | 525 | 2.36 | 521 | 2.38 | 500 | 2.48 |
| Flu-RH | 563 | 2.20 | 558 | 2.22 | 553 | 2.24 | 548 | 2.26 | 544 | 2.28 | 539 | 2.30 | 500 | 2.48 |
| FRd2 | 584 | 2.12 | 578 | 2.15 | 573 | 2.16 | 568 | 2.18 | 563 | 2.20 | 558 | 2.22 | 509 | 2.44 |
| ITDI | 711 | 1.74 | 704 | 1.76 | 698 | 1.78 | 691 | 1.79 | 685 | 1.81 | 679 | 1.83 | 647 | 1.92 |
| SiIDT-IC | 628 | 1.97 | 623 | 1.99 | 619 | 2.00 | 615 | 2.02 | 611 | 2.03 | 607 | 2.04 | 639 | 1.94 |
| IDIDT-C8 | 711 | 1.74 | 703 | 1.76 | 695 | 1.78 | 687 | 1.80 | 679 | 1.83 | 672 | 1.85 | 655 | 1.89 |
| IDT-BOC6 | 720 | 1.72 | 711 | 1.74 | 702 | 1.77 | 693 | 1.79 | 685 | 1.81 | 677 | 1.83 | 688 | 1.80 |
| ATT1 | 741 | 1.67 | 734 | 1.69 | 728 | 1.70 | 721 | 1.72 | 715 | 1.73 | 709 | 1.75 | 690 | 1.80 |
| DC-IDT2T | 745 | 1.66 | 738 | 1.68 | 730 | 1.70 | 723 | 1.72 | 716 | 1.73 | 710 | 1.75 | 700 | 1.77 |
| BZIC | 692 | 1.79 | 687 | 1.80 | 683 | 1.82 | 678 | 1.83 | 674 | 1.84 | 670 | 1.85 | 710 | 1.75 |
| ITOIC | 748 | 1.66 | 741 | 1.67 | 733 | 1.69 | 726 | 1.71 | 720 | 1.72 | 713 | 1.74 | 722 | 1.72 |
| IDTOT2F | 762 | 1.63 | 755 | 1.64 | 747 | 1.66 | 741 | 1.67 | 734 | 1.69 | 727 | 1.71 | 723 | 1.72 |
| ITOIC-F | 747 | 1.66 | 740 | 1.68 | 733 | 1.69 | 726 | 1.71 | 720 | 1.72 | 714 | 1.74 | 732 | 1.69 |
| ITOIC-2F | 759 | 1.63 | 751 | 1.65 | 744 | 1.67 | 738 | 1.68 | 731 | 1.70 | 725 | 1.71 | 737 | 1.68 |
| IEICO | 853 | 1.45 | 845 | 1.47 | 836 | 1.48 | 828 | 1.50 | 821 | 1.51 | 813 | 1.53 | 785 | 1.58 |
| ATT2 | 833 | 1.49 | 825 | 1.50 | 817 | 1.52 | 810 | 1.53 | 803 | 1.54 | 797 | 1.56 | 791 | 1.57 |
| IEICO-4F | 870 | 1.43 | 862 | 1.44 | 854 | 1.45 | 846 | 1.47 | 839 | 1.48 | 832 | 1.49 | 805 | 1.54 |
| m-ITIC | 685 | 1.81 | 680 | 1.82 | 674 | 1.84 | 668 | 1.86 | 663 | 1.87 | 658 | 1.88 | 660 | 1.88 |
| IT-DM | 682 | 1.82 | 676 | 1.83 | 671 | 1.85 | 665 | 1.86 | 660 | 1.88 | 655 | 1.89 | 665 | 1.86 |
| IT-M | 683 | 1.82 | 677 | 1.83 | 671 | 1.85 | 666 | 1.86 | 661 | 1.88 | 656 | 1.89 | 668 | 1.86 |
| ITCPTC | 697 | 1.78 | 692 | 1.79 | 686 | 1.81 | 681 | 1.82 | 675 | 1.84 | 670 | 1.85 | 678 | 1.83 |
| Cl-ITIC | 696 | 1.78 | 690 | 1.80 | 684 | 1.81 | 678 | 1.83 | 673 | 1.84 | 668 | 1.86 | 691 | 1.79 |
| Br-ITIC | 697 | 1.78 | 691 | 1.79 | 685 | 1.81 | 679 | 1.83 | 674 | 1.84 | 669 | 1.85 | 692 | 1.79 |
| NFBDT | 712 | 1.74 | 706 | 1.76 | 700 | 1.77 | 694 | 1.79 | 688 | 1.80 | 683 | 1.82 | 703 | 1.76 |
| ITIC2 | 736 | 1.68 | 729 | 1.70 | 722 | 1.72 | 716 | 1.73 | 709 | 1.75 | 703 | 1.76 | 714 | 1.74 |
| ITVFFIC | 754 | 1.64 | 748 | 1.66 | 742 | 1.67 | 735 | 1.69 | 730 | 1.70 | 724 | 1.71 | 750 | 1.65 |
| INIC | 715 | 1.73 | 708 | 1.75 | 702 | 1.77 | 695 | 1.78 | 688 | 1.80 | 682 | 1.82 | 692 | 1.79 |
| INIC2 | 730 | 1.70 | 722 | 1.72 | 715 | 1.73 | 708 | 1.75 | 702 | 1.77 | 695 | 1.78 | 704 | 1.76 |
| INIC1 | 726 | 1.71 | 719 | 1.72 | 712 | 1.74 | 705 | 1.76 | 699 | 1.77 | 693 | 1.79 | 710 | 1.75 |
| INIC3 | 726 | 1.71 | 719 | 1.72 | 713 | 1.74 | 706 | 1.76 | 700 | 1.77 | 694 | 1.79 | 710 | 1.75 |
| IPIC | 734 | 1.69 | 727 | 1.71 | 721 | 1.72 | 714 | 1.74 | 708 | 1.75 | 702 | 1.77 | 761 | 1.63 |
| IPIC-4F | 743 | 1.67 | 737 | 1.68 | 730 | 1.70 | 724 | 1.71 | 718 | 1.73 | 712 | 1.74 | 776 | 1.60 |
| IPIC-4Cl | 751 | 1.65 | 744 | 1.67 | 737 | 1.68 | 730 | 1.70 | 724 | 1.71 | 717 | 1.73 | 790 | 1.57 |

^aXC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S10 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-----------|---|------|-------|------|-------------|------|-------------|------|-------------|------|-------------|------|---|------|
| | X3LYP-20HFX | | X3LYP | | X3LYP-22HFX | | X3LYP-23HFX | | X3LYP-24HFX | | X3LYP-25HFX | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 661 | 1.88 | 649 | 1.91 | 648 | 1.91 | 642 | 1.93 | 636 | 1.95 | 631 | 1.97 | 615 | 2.02 |
| Cz-RH | 547 | 2.27 | 538 | 2.30 | 537 | 2.31 | 533 | 2.33 | 528 | 2.35 | 524 | 2.37 | 500 | 2.48 |
| Flu-RH | 566 | 2.19 | 557 | 2.23 | 556 | 2.23 | 551 | 2.25 | 547 | 2.27 | 542 | 2.29 | 500 | 2.48 |
| FRd2 | 587 | 2.11 | 577 | 2.15 | 576 | 2.15 | 571 | 2.17 | 566 | 2.19 | 561 | 2.21 | 509 | 2.44 |
| ITDI | 714 | 1.74 | 702 | 1.77 | 701 | 1.77 | 694 | 1.79 | 688 | 1.80 | 682 | 1.82 | 647 | 1.92 |
| SiIDT-IC | 631 | 1.97 | 623 | 1.99 | 622 | 1.99 | 618 | 2.01 | 614 | 2.02 | 610 | 2.03 | 639 | 1.94 |
| IDIDT-C8 | 713 | 1.74 | 698 | 1.78 | 697 | 1.78 | 689 | 1.80 | 681 | 1.82 | 674 | 1.84 | 655 | 1.89 |
| IDT-BOC6 | 723 | 1.72 | 707 | 1.75 | 705 | 1.76 | 697 | 1.78 | 688 | 1.80 | 680 | 1.82 | 688 | 1.80 |
| ATT1 | 746 | 1.66 | 734 | 1.69 | 732 | 1.69 | 726 | 1.71 | 720 | 1.72 | 713 | 1.74 | 690 | 1.80 |
| DC-IDT2T | 749 | 1.66 | 735 | 1.69 | 734 | 1.69 | 727 | 1.71 | 720 | 1.72 | 713 | 1.74 | 700 | 1.77 |
| BZIC | 696 | 1.78 | 688 | 1.80 | 687 | 1.80 | 682 | 1.82 | 678 | 1.83 | 674 | 1.84 | 710 | 1.75 |
| ITOIC | 752 | 1.65 | 739 | 1.68 | 737 | 1.68 | 730 | 1.70 | 724 | 1.71 | 717 | 1.73 | 722 | 1.72 |
| IDTOT2F | 765 | 1.62 | 752 | 1.65 | 751 | 1.65 | 744 | 1.67 | 737 | 1.68 | 731 | 1.70 | 723 | 1.72 |
| ITOIC-F | 751 | 1.65 | 738 | 1.68 | 737 | 1.68 | 730 | 1.70 | 724 | 1.71 | 717 | 1.73 | 732 | 1.69 |
| ITOIC-2F | 762 | 1.63 | 749 | 1.66 | 748 | 1.66 | 741 | 1.67 | 735 | 1.69 | 728 | 1.70 | 737 | 1.68 |
| IEICO | 858 | 1.45 | 843 | 1.47 | 841 | 1.47 | 833 | 1.49 | 826 | 1.50 | 818 | 1.52 | 785 | 1.58 |
| ATT2 | 838 | 1.48 | 824 | 1.50 | 823 | 1.51 | 816 | 1.52 | 809 | 1.53 | 802 | 1.55 | 791 | 1.57 |
| IEICO-4F | 874 | 1.42 | 860 | 1.44 | 858 | 1.45 | 851 | 1.46 | 843 | 1.47 | 836 | 1.48 | 805 | 1.54 |
| m-ITIC | 688 | 1.80 | 678 | 1.83 | 677 | 1.83 | 671 | 1.85 | 666 | 1.86 | 661 | 1.88 | 660 | 1.88 |
| IT-DM | 685 | 1.81 | 675 | 1.84 | 674 | 1.84 | 668 | 1.86 | 663 | 1.87 | 658 | 1.88 | 665 | 1.86 |
| IT-M | 685 | 1.81 | 675 | 1.84 | 674 | 1.84 | 669 | 1.85 | 663 | 1.87 | 658 | 1.88 | 668 | 1.86 |
| ITCPTC | 700 | 1.77 | 690 | 1.80 | 689 | 1.80 | 684 | 1.81 | 679 | 1.83 | 673 | 1.84 | 678 | 1.83 |
| Cl-ITIC | 698 | 1.78 | 688 | 1.80 | 687 | 1.80 | 681 | 1.82 | 676 | 1.83 | 670 | 1.85 | 691 | 1.79 |
| Br-ITIC | 699 | 1.77 | 689 | 1.80 | 688 | 1.80 | 682 | 1.82 | 677 | 1.83 | 671 | 1.85 | 692 | 1.79 |
| NFBDT | 714 | 1.74 | 703 | 1.76 | 702 | 1.77 | 696 | 1.78 | 691 | 1.79 | 685 | 1.81 | 703 | 1.76 |
| ITIC2 | 739 | 1.68 | 726 | 1.71 | 725 | 1.71 | 719 | 1.72 | 712 | 1.74 | 706 | 1.76 | 714 | 1.74 |
| ITVFFIC | 757 | 1.64 | 745 | 1.66 | 744 | 1.67 | 738 | 1.68 | 732 | 1.69 | 726 | 1.71 | 750 | 1.65 |
| INIC | 719 | 1.72 | 706 | 1.76 | 705 | 1.76 | 698 | 1.78 | 692 | 1.79 | 686 | 1.81 | 692 | 1.79 |
| INIC2 | 733 | 1.69 | 720 | 1.72 | 719 | 1.72 | 712 | 1.74 | 705 | 1.76 | 699 | 1.77 | 704 | 1.76 |
| INIC1 | 729 | 1.70 | 717 | 1.73 | 715 | 1.73 | 709 | 1.75 | 702 | 1.77 | 696 | 1.78 | 710 | 1.75 |
| INIC3 | 729 | 1.70 | 717 | 1.73 | 716 | 1.73 | 710 | 1.75 | 703 | 1.76 | 697 | 1.78 | 710 | 1.75 |
| IPIC | 737 | 1.68 | 725 | 1.71 | 724 | 1.71 | 717 | 1.73 | 711 | 1.74 | 705 | 1.76 | 761 | 1.63 |
| IPIC-4F | 746 | 1.66 | 734 | 1.69 | 733 | 1.69 | 727 | 1.71 | 721 | 1.72 | 715 | 1.73 | 776 | 1.60 |
| IPIC-4Cl | 754 | 1.64 | 741 | 1.67 | 740 | 1.68 | 733 | 1.69 | 727 | 1.71 | 721 | 1.72 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S11 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-----------|---|------|------|------|------------|------|------------|------|------------|------|------------|------|---|------|
| | B971-20HFX | | B971 | | B971-22HFX | | B971-23HFX | | B971-24HFX | | B971-25HFX | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 661 | 1.88 | 654 | 1.90 | 647 | 1.92 | 641 | 1.93 | 635 | 1.95 | 630 | 1.97 | 615 | 2.02 |
| Cz-RH | 545 | 2.28 | 540 | 2.30 | 535 | 2.32 | 530 | 2.34 | 526 | 2.36 | 522 | 2.38 | 500 | 2.48 |
| Flu-RH | 564 | 2.20 | 559 | 2.22 | 554 | 2.24 | 549 | 2.26 | 545 | 2.28 | 541 | 2.29 | 500 | 2.48 |
| FRd2 | 585 | 2.12 | 580 | 2.14 | 574 | 2.16 | 569 | 2.18 | 564 | 2.20 | 560 | 2.21 | 509 | 2.44 |
| ITDI | 712 | 1.74 | 706 | 1.76 | 699 | 1.77 | 693 | 1.79 | 686 | 1.81 | 680 | 1.82 | 647 | 1.92 |
| SIIDT-IC | 629 | 1.97 | 624 | 1.99 | 620 | 2.00 | 616 | 2.01 | 612 | 2.03 | 608 | 2.04 | 639 | 1.94 |
| IDIDT-C8 | 712 | 1.74 | 703 | 1.76 | 695 | 1.78 | 687 | 1.80 | 680 | 1.82 | 672 | 1.85 | 655 | 1.89 |
| IDT-BOC6 | 721 | 1.72 | 712 | 1.74 | 703 | 1.76 | 695 | 1.78 | 686 | 1.81 | 678 | 1.83 | 688 | 1.80 |
| ATT1 | 744 | 1.67 | 737 | 1.68 | 730 | 1.70 | 724 | 1.71 | 717 | 1.73 | 711 | 1.74 | 690 | 1.80 |
| DC-IDT2T | 747 | 1.66 | 739 | 1.68 | 732 | 1.69 | 725 | 1.71 | 718 | 1.73 | 712 | 1.74 | 700 | 1.77 |
| BZIC | 694 | 1.79 | 689 | 1.80 | 684 | 1.81 | 680 | 1.82 | 676 | 1.83 | 671 | 1.85 | 710 | 1.75 |
| ITOIC | 750 | 1.65 | 742 | 1.67 | 735 | 1.69 | 728 | 1.70 | 721 | 1.72 | 715 | 1.73 | 722 | 1.72 |
| IDTOT2F | 763 | 1.63 | 755 | 1.64 | 748 | 1.66 | 741 | 1.67 | 735 | 1.69 | 728 | 1.70 | 723 | 1.72 |
| ITOIC-F | 748 | 1.66 | 741 | 1.67 | 734 | 1.69 | 728 | 1.70 | 721 | 1.72 | 715 | 1.73 | 732 | 1.69 |
| ITOIC-2F | 759 | 1.63 | 752 | 1.65 | 745 | 1.66 | 739 | 1.68 | 732 | 1.69 | 726 | 1.71 | 737 | 1.68 |
| IEICO | 856 | 1.45 | 847 | 1.46 | 839 | 1.48 | 831 | 1.49 | 823 | 1.51 | 816 | 1.52 | 785 | 1.58 |
| ATT2 | 835 | 1.49 | 828 | 1.50 | 820 | 1.51 | 813 | 1.53 | 806 | 1.54 | 799 | 1.55 | 791 | 1.57 |
| IEICO-4F | 871 | 1.42 | 863 | 1.44 | 856 | 1.45 | 848 | 1.46 | 841 | 1.47 | 834 | 1.49 | 805 | 1.54 |
| m-ITIC | 686 | 1.81 | 681 | 1.82 | 675 | 1.84 | 670 | 1.85 | 664 | 1.87 | 659 | 1.88 | 660 | 1.88 |
| IT-DM | 683 | 1.82 | 678 | 1.83 | 672 | 1.85 | 667 | 1.86 | 661 | 1.88 | 656 | 1.89 | 665 | 1.86 |
| IT-M | 684 | 1.81 | 678 | 1.83 | 672 | 1.85 | 667 | 1.86 | 662 | 1.87 | 657 | 1.89 | 668 | 1.86 |
| ITCPTC | 699 | 1.77 | 693 | 1.79 | 688 | 1.80 | 682 | 1.82 | 677 | 1.83 | 672 | 1.85 | 678 | 1.83 |
| Cl-ITIC | 696 | 1.78 | 691 | 1.79 | 685 | 1.81 | 679 | 1.83 | 674 | 1.84 | 669 | 1.85 | 691 | 1.79 |
| Br-ITIC | 698 | 1.78 | 692 | 1.79 | 686 | 1.81 | 680 | 1.82 | 675 | 1.84 | 670 | 1.85 | 692 | 1.79 |
| NFBBDT | 713 | 1.74 | 707 | 1.75 | 701 | 1.77 | 695 | 1.78 | 689 | 1.80 | 684 | 1.81 | 703 | 1.76 |
| ITIC2 | 737 | 1.68 | 730 | 1.70 | 723 | 1.72 | 717 | 1.73 | 710 | 1.75 | 704 | 1.76 | 714 | 1.74 |
| ITVFFIC | 755 | 1.64 | 748 | 1.66 | 742 | 1.67 | 736 | 1.68 | 730 | 1.70 | 724 | 1.71 | 750 | 1.65 |
| INIC | 717 | 1.73 | 710 | 1.75 | 703 | 1.76 | 696 | 1.78 | 690 | 1.80 | 684 | 1.81 | 692 | 1.79 |
| INIC2 | 731 | 1.70 | 724 | 1.71 | 717 | 1.73 | 710 | 1.75 | 703 | 1.76 | 697 | 1.78 | 704 | 1.76 |
| INIC1 | 727 | 1.71 | 720 | 1.72 | 713 | 1.74 | 707 | 1.75 | 700 | 1.77 | 694 | 1.79 | 710 | 1.75 |
| INIC3 | 727 | 1.71 | 720 | 1.72 | 714 | 1.74 | 707 | 1.75 | 701 | 1.77 | 695 | 1.78 | 710 | 1.75 |
| IPIC | 735 | 1.69 | 728 | 1.70 | 722 | 1.72 | 715 | 1.73 | 709 | 1.75 | 703 | 1.76 | 761 | 1.63 |
| IPIC-4F | 744 | 1.67 | 737 | 1.68 | 731 | 1.70 | 725 | 1.71 | 719 | 1.72 | 713 | 1.74 | 776 | 1.60 |
| IPIC-4Cl | 752 | 1.65 | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 725 | 1.71 | 719 | 1.72 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S12 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-----------|---|------|------|------|------------|------|------------|------|------------|------|------------|------|---|------|
| | B972-20HFX | | B972 | | B972-22HFX | | B972-23HFX | | B972-24HFX | | B972-25HFX | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 657 | 1.89 | 650 | 1.91 | 644 | 1.93 | 638 | 1.94 | 632 | 1.96 | 627 | 1.98 | 615 | 2.02 |
| Cz-RH | 542 | 2.29 | 537 | 2.31 | 532 | 2.33 | 528 | 2.35 | 523 | 2.37 | 519 | 2.39 | 500 | 2.48 |
| Flu-RH | 561 | 2.21 | 556 | 2.23 | 551 | 2.25 | 546 | 2.27 | 542 | 2.29 | 538 | 2.30 | 500 | 2.48 |
| FRd2 | 583 | 2.13 | 577 | 2.15 | 572 | 2.17 | 567 | 2.19 | 562 | 2.21 | 557 | 2.23 | 509 | 2.44 |
| ITDI | 709 | 1.75 | 702 | 1.77 | 695 | 1.78 | 689 | 1.80 | 683 | 1.82 | 677 | 1.83 | 647 | 1.92 |
| SiIDT-IC | 626 | 1.98 | 621 | 2.00 | 617 | 2.01 | 613 | 2.02 | 609 | 2.04 | 605 | 2.05 | 639 | 1.94 |
| IDIDT-C8 | 708 | 1.75 | 700 | 1.77 | 692 | 1.79 | 684 | 1.81 | 677 | 1.83 | 669 | 1.85 | 655 | 1.89 |
| IDT-BOC6 | 717 | 1.73 | 708 | 1.75 | 700 | 1.77 | 691 | 1.79 | 683 | 1.82 | 675 | 1.84 | 688 | 1.80 |
| ATT1 | 739 | 1.68 | 732 | 1.69 | 726 | 1.71 | 719 | 1.72 | 713 | 1.74 | 707 | 1.75 | 690 | 1.80 |
| DC-IDT2T | 743 | 1.67 | 736 | 1.68 | 728 | 1.70 | 721 | 1.72 | 715 | 1.73 | 708 | 1.75 | 700 | 1.77 |
| BZIC | 691 | 1.79 | 686 | 1.81 | 681 | 1.82 | 677 | 1.83 | 673 | 1.84 | 668 | 1.86 | 710 | 1.75 |
| ITOIC | 746 | 1.66 | 739 | 1.68 | 731 | 1.70 | 724 | 1.71 | 718 | 1.73 | 711 | 1.74 | 722 | 1.72 |
| IDTOT2F | 759 | 1.63 | 752 | 1.65 | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 725 | 1.71 | 723 | 1.72 |
| ITOIC-F | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 724 | 1.71 | 718 | 1.73 | 712 | 1.74 | 732 | 1.69 |
| ITOIC-2F | 756 | 1.64 | 749 | 1.66 | 742 | 1.67 | 735 | 1.69 | 729 | 1.70 | 723 | 1.72 | 737 | 1.68 |
| IEICO | 851 | 1.46 | 843 | 1.47 | 835 | 1.49 | 827 | 1.50 | 819 | 1.51 | 811 | 1.53 | 785 | 1.58 |
| ATT2 | 831 | 1.49 | 824 | 1.50 | 816 | 1.52 | 809 | 1.53 | 802 | 1.55 | 795 | 1.56 | 791 | 1.57 |
| IEICO-4F | 867 | 1.43 | 860 | 1.44 | 852 | 1.46 | 844 | 1.47 | 837 | 1.48 | 830 | 1.49 | 805 | 1.54 |
| m-ITIC | 684 | 1.81 | 678 | 1.83 | 672 | 1.85 | 667 | 1.86 | 662 | 1.87 | 657 | 1.89 | 660 | 1.88 |
| IT-DM | 681 | 1.82 | 675 | 1.84 | 670 | 1.85 | 664 | 1.87 | 659 | 1.88 | 654 | 1.90 | 665 | 1.86 |
| IT-M | 681 | 1.82 | 675 | 1.84 | 670 | 1.85 | 664 | 1.87 | 659 | 1.88 | 654 | 1.90 | 668 | 1.86 |
| ITCPTC | 696 | 1.78 | 690 | 1.80 | 685 | 1.81 | 679 | 1.83 | 674 | 1.84 | 669 | 1.85 | 678 | 1.83 |
| Cl-ITIC | 694 | 1.79 | 688 | 1.80 | 682 | 1.82 | 676 | 1.83 | 671 | 1.85 | 666 | 1.86 | 691 | 1.79 |
| Br-ITIC | 695 | 1.78 | 689 | 1.80 | 683 | 1.82 | 678 | 1.83 | 672 | 1.85 | 667 | 1.86 | 692 | 1.79 |
| NFBDT | 710 | 1.75 | 704 | 1.76 | 698 | 1.78 | 692 | 1.79 | 686 | 1.81 | 681 | 1.82 | 703 | 1.76 |
| ITIC2 | 734 | 1.69 | 727 | 1.71 | 720 | 1.72 | 714 | 1.74 | 707 | 1.75 | 701 | 1.77 | 714 | 1.74 |
| ITVFFIC | 752 | 1.65 | 746 | 1.66 | 739 | 1.68 | 733 | 1.69 | 727 | 1.71 | 722 | 1.72 | 750 | 1.65 |
| INIC | 714 | 1.74 | 707 | 1.75 | 700 | 1.77 | 693 | 1.79 | 687 | 1.80 | 681 | 1.82 | 692 | 1.79 |
| INIC2 | 728 | 1.70 | 720 | 1.72 | 713 | 1.74 | 707 | 1.75 | 700 | 1.77 | 694 | 1.79 | 704 | 1.76 |
| INIC1 | 724 | 1.71 | 717 | 1.73 | 710 | 1.75 | 704 | 1.76 | 697 | 1.78 | 691 | 1.79 | 710 | 1.75 |
| INIC3 | 724 | 1.71 | 717 | 1.73 | 711 | 1.74 | 704 | 1.76 | 698 | 1.78 | 692 | 1.79 | 710 | 1.75 |
| IPIC | 732 | 1.69 | 725 | 1.71 | 719 | 1.72 | 713 | 1.74 | 706 | 1.76 | 701 | 1.77 | 761 | 1.63 |
| IPIC-4F | 741 | 1.67 | 735 | 1.69 | 728 | 1.70 | 722 | 1.72 | 716 | 1.73 | 711 | 1.74 | 776 | 1.60 |
| IPIC-4Cl | 749 | 1.66 | 742 | 1.67 | 735 | 1.69 | 728 | 1.70 | 722 | 1.72 | 716 | 1.73 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S13 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-----------|---|------|-----------|------|-----|------|-----------|------|-----------|------|-----------|------|---|------|
| | B98-20HFX | | B98-21HFX | | B98 | | B98-23HFX | | B98-24HFX | | B98-25HFX | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 661 | 1.88 | 654 | 1.90 | 648 | 1.91 | 642 | 1.93 | 636 | 1.95 | 631 | 1.97 | 615 | 2.02 |
| Cz-RH | 546 | 2.27 | 541 | 2.29 | 536 | 2.31 | 531 | 2.34 | 527 | 2.35 | 523 | 2.37 | 500 | 2.48 |
| Flu-RH | 565 | 2.19 | 560 | 2.21 | 555 | 2.23 | 550 | 2.25 | 546 | 2.27 | 541 | 2.29 | 500 | 2.48 |
| FRd2 | 586 | 2.12 | 581 | 2.13 | 575 | 2.16 | 570 | 2.18 | 565 | 2.19 | 561 | 2.21 | 509 | 2.44 |
| ITDI | 714 | 1.74 | 707 | 1.75 | 700 | 1.77 | 694 | 1.79 | 687 | 1.80 | 681 | 1.82 | 647 | 1.92 |
| SiIDT-IC | 629 | 1.97 | 625 | 1.98 | 621 | 2.00 | 616 | 2.01 | 612 | 2.03 | 608 | 2.04 | 639 | 1.94 |
| IDIDT-C8 | 713 | 1.74 | 705 | 1.76 | 697 | 1.78 | 689 | 1.80 | 681 | 1.82 | 674 | 1.84 | 655 | 1.89 |
| IDT-BOC6 | 722 | 1.72 | 713 | 1.74 | 705 | 1.76 | 696 | 1.78 | 688 | 1.80 | 680 | 1.82 | 688 | 1.80 |
| ATT1 | 745 | 1.66 | 738 | 1.68 | 732 | 1.69 | 725 | 1.71 | 719 | 1.72 | 713 | 1.74 | 690 | 1.80 |
| DC-IDT2T | 748 | 1.66 | 741 | 1.67 | 734 | 1.69 | 726 | 1.71 | 720 | 1.72 | 713 | 1.74 | 700 | 1.77 |
| BZIC | 694 | 1.79 | 690 | 1.80 | 685 | 1.81 | 681 | 1.82 | 676 | 1.83 | 672 | 1.85 | 710 | 1.75 |
| ITOIC | 751 | 1.65 | 744 | 1.67 | 737 | 1.68 | 730 | 1.70 | 723 | 1.72 | 716 | 1.73 | 722 | 1.72 |
| IDTOT2F | 764 | 1.62 | 757 | 1.64 | 750 | 1.65 | 743 | 1.67 | 736 | 1.68 | 730 | 1.70 | 723 | 1.72 |
| ITOIC-F | 749 | 1.66 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 716 | 1.73 | 732 | 1.69 |
| ITOIC-2F | 761 | 1.63 | 754 | 1.64 | 747 | 1.66 | 740 | 1.68 | 734 | 1.69 | 727 | 1.71 | 737 | 1.68 |
| IEICO | 857 | 1.45 | 849 | 1.46 | 841 | 1.47 | 833 | 1.49 | 825 | 1.50 | 818 | 1.52 | 785 | 1.58 |
| ATT2 | 837 | 1.48 | 829 | 1.50 | 822 | 1.51 | 815 | 1.52 | 808 | 1.53 | 801 | 1.55 | 791 | 1.57 |
| IEICO-4F | 873 | 1.42 | 865 | 1.43 | 857 | 1.45 | 850 | 1.46 | 843 | 1.47 | 835 | 1.49 | 805 | 1.54 |
| m-ITIC | 687 | 1.80 | 682 | 1.82 | 676 | 1.83 | 671 | 1.85 | 666 | 1.86 | 660 | 1.88 | 660 | 1.88 |
| IT-DM | 684 | 1.81 | 679 | 1.83 | 673 | 1.84 | 668 | 1.86 | 662 | 1.87 | 657 | 1.89 | 665 | 1.86 |
| IT-M | 685 | 1.81 | 679 | 1.83 | 674 | 1.84 | 668 | 1.86 | 663 | 1.87 | 658 | 1.88 | 668 | 1.86 |
| ITCPTC | 700 | 1.77 | 694 | 1.79 | 689 | 1.80 | 683 | 1.82 | 678 | 1.83 | 673 | 1.84 | 678 | 1.83 |
| Cl-ITIC | 698 | 1.78 | 692 | 1.79 | 686 | 1.81 | 680 | 1.82 | 675 | 1.84 | 670 | 1.85 | 691 | 1.79 |
| Br-ITIC | 699 | 1.77 | 693 | 1.79 | 687 | 1.80 | 682 | 1.82 | 676 | 1.83 | 671 | 1.85 | 692 | 1.79 |
| NFBDT | 714 | 1.74 | 708 | 1.75 | 702 | 1.77 | 696 | 1.78 | 690 | 1.80 | 685 | 1.81 | 703 | 1.76 |
| ITIC2 | 738 | 1.68 | 731 | 1.70 | 725 | 1.71 | 718 | 1.73 | 712 | 1.74 | 706 | 1.76 | 714 | 1.74 |
| ITVFFIC | 756 | 1.64 | 749 | 1.66 | 743 | 1.67 | 737 | 1.68 | 731 | 1.70 | 726 | 1.71 | 750 | 1.65 |
| INIC | 718 | 1.73 | 711 | 1.74 | 705 | 1.76 | 698 | 1.78 | 691 | 1.79 | 685 | 1.81 | 692 | 1.79 |
| INIC2 | 732 | 1.69 | 725 | 1.71 | 718 | 1.73 | 711 | 1.74 | 705 | 1.76 | 698 | 1.78 | 704 | 1.76 |
| INIC1 | 728 | 1.70 | 721 | 1.72 | 715 | 1.73 | 708 | 1.75 | 702 | 1.77 | 695 | 1.78 | 710 | 1.75 |
| INIC3 | 728 | 1.70 | 721 | 1.72 | 715 | 1.73 | 709 | 1.75 | 702 | 1.77 | 696 | 1.78 | 710 | 1.75 |
| IPIC | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 717 | 1.73 | 710 | 1.75 | 704 | 1.76 | 761 | 1.63 |
| IPIC-4F | 745 | 1.66 | 738 | 1.68 | 732 | 1.69 | 726 | 1.71 | 720 | 1.72 | 714 | 1.74 | 776 | 1.60 |
| IPIC-4Cl | 753 | 1.65 | 746 | 1.66 | 739 | 1.68 | 733 | 1.69 | 726 | 1.71 | 720 | 1.72 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S14 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-----------|---|------|-----------|------|-----------|------|-----|------|-----------|------|-----------|------|---|------|
| | APF-20HFX | | APF-21HFX | | APF-22HFX | | APF | | APF-24HFX | | APF-25HFX | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 659 | 1.88 | 652 | 1.90 | 645 | 1.92 | 640 | 1.94 | 634 | 1.96 | 628 | 1.97 | 615 | 2.02 |
| Cz-RH | 543 | 2.28 | 538 | 2.30 | 534 | 2.32 | 529 | 2.34 | 525 | 2.36 | 520 | 2.38 | 500 | 2.48 |
| Flu-RH | 562 | 2.21 | 557 | 2.23 | 552 | 2.25 | 548 | 2.26 | 543 | 2.28 | 539 | 2.30 | 500 | 2.48 |
| FRd2 | 582 | 2.13 | 577 | 2.15 | 571 | 2.17 | 567 | 2.19 | 561 | 2.21 | 557 | 2.23 | 509 | 2.44 |
| ITDI | 709 | 1.75 | 703 | 1.76 | 696 | 1.78 | 690 | 1.80 | 683 | 1.82 | 677 | 1.83 | 647 | 1.92 |
| SiIDT-IC | 626 | 1.98 | 622 | 1.99 | 618 | 2.01 | 614 | 2.02 | 609 | 2.04 | 606 | 2.05 | 639 | 1.94 |
| IDIDT-C8 | 709 | 1.75 | 700 | 1.77 | 692 | 1.79 | 685 | 1.81 | 677 | 1.83 | 670 | 1.85 | 655 | 1.89 |
| IDT-BOC6 | 718 | 1.73 | 709 | 1.75 | 700 | 1.77 | 692 | 1.79 | 684 | 1.81 | 675 | 1.84 | 688 | 1.80 |
| ATT1 | 740 | 1.68 | 733 | 1.69 | 727 | 1.71 | 721 | 1.72 | 714 | 1.74 | 708 | 1.75 | 690 | 1.80 |
| DC-IDT2T | 744 | 1.67 | 736 | 1.68 | 729 | 1.70 | 722 | 1.72 | 715 | 1.73 | 708 | 1.75 | 700 | 1.77 |
| BZIC | 692 | 1.79 | 687 | 1.80 | 683 | 1.82 | 678 | 1.83 | 674 | 1.84 | 669 | 1.85 | 710 | 1.75 |
| ITOIC | 747 | 1.66 | 740 | 1.68 | 732 | 1.69 | 726 | 1.71 | 718 | 1.73 | 712 | 1.74 | 722 | 1.72 |
| IDTOT2F | 759 | 1.63 | 752 | 1.65 | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 725 | 1.71 | 723 | 1.72 |
| ITOIC-F | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 725 | 1.71 | 718 | 1.73 | 712 | 1.74 | 732 | 1.69 |
| ITOIC-2F | 756 | 1.64 | 749 | 1.66 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 722 | 1.72 | 737 | 1.68 |
| IEICO | 852 | 1.46 | 844 | 1.47 | 836 | 1.48 | 828 | 1.50 | 820 | 1.51 | 812 | 1.53 | 785 | 1.58 |
| ATT2 | 830 | 1.49 | 822 | 1.51 | 815 | 1.52 | 808 | 1.53 | 801 | 1.55 | 794 | 1.56 | 791 | 1.57 |
| IEICO-4F | 867 | 1.43 | 859 | 1.44 | 851 | 1.46 | 844 | 1.47 | 837 | 1.48 | 829 | 1.50 | 805 | 1.54 |
| m-ITIC | 684 | 1.81 | 678 | 1.83 | 673 | 1.84 | 667 | 1.86 | 662 | 1.87 | 657 | 1.89 | 660 | 1.88 |
| IT-DM | 681 | 1.82 | 675 | 1.84 | 669 | 1.85 | 664 | 1.87 | 659 | 1.88 | 654 | 1.90 | 665 | 1.86 |
| IT-M | 681 | 1.82 | 676 | 1.83 | 670 | 1.85 | 665 | 1.86 | 659 | 1.88 | 654 | 1.90 | 668 | 1.86 |
| ITCPTC | 696 | 1.78 | 690 | 1.80 | 685 | 1.81 | 680 | 1.82 | 674 | 1.84 | 669 | 1.85 | 678 | 1.83 |
| Cl-ITIC | 694 | 1.79 | 688 | 1.80 | 682 | 1.82 | 677 | 1.83 | 671 | 1.85 | 666 | 1.86 | 691 | 1.79 |
| Br-ITIC | 696 | 1.78 | 690 | 1.80 | 684 | 1.81 | 678 | 1.83 | 673 | 1.84 | 667 | 1.86 | 692 | 1.79 |
| NFBDT | 711 | 1.74 | 705 | 1.76 | 699 | 1.77 | 693 | 1.79 | 687 | 1.80 | 682 | 1.82 | 703 | 1.76 |
| ITIC2 | 735 | 1.69 | 728 | 1.70 | 721 | 1.72 | 715 | 1.73 | 708 | 1.75 | 702 | 1.77 | 714 | 1.74 |
| ITVFFIC | 751 | 1.65 | 745 | 1.66 | 739 | 1.68 | 733 | 1.69 | 727 | 1.71 | 721 | 1.72 | 750 | 1.65 |
| INIC | 714 | 1.74 | 707 | 1.75 | 700 | 1.77 | 694 | 1.79 | 687 | 1.80 | 681 | 1.82 | 692 | 1.79 |
| INIC2 | 727 | 1.71 | 720 | 1.72 | 713 | 1.74 | 707 | 1.75 | 700 | 1.77 | 693 | 1.79 | 704 | 1.76 |
| INIC1 | 724 | 1.71 | 717 | 1.73 | 710 | 1.75 | 704 | 1.76 | 697 | 1.78 | 691 | 1.79 | 710 | 1.75 |
| INIC3 | 723 | 1.72 | 716 | 1.73 | 710 | 1.75 | 704 | 1.76 | 697 | 1.78 | 691 | 1.79 | 710 | 1.75 |
| IPIC | 733 | 1.69 | 726 | 1.71 | 719 | 1.72 | 713 | 1.74 | 707 | 1.75 | 701 | 1.77 | 761 | 1.63 |
| IPIC-4F | 741 | 1.67 | 734 | 1.69 | 728 | 1.70 | 722 | 1.72 | 716 | 1.73 | 710 | 1.75 | 776 | 1.60 |
| IPIC-4Cl | 750 | 1.65 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 716 | 1.73 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S15 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-----------|---|------|------------|------|------------|------|------|------|------------|------|------------|------|---|------|
| | APFD-20HFX | | APFD-21HFX | | APFD-22HFX | | APFD | | APFD-24HFX | | APFD-25HFX | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 659 | 1.88 | 652 | 1.90 | 645 | 1.92 | 640 | 1.94 | 634 | 1.96 | 628 | 1.97 | 615 | 2.02 |
| Cz-RH | 543 | 2.28 | 538 | 2.30 | 534 | 2.32 | 529 | 2.34 | 525 | 2.36 | 520 | 2.38 | 500 | 2.48 |
| Flu-RH | 562 | 2.21 | 557 | 2.23 | 552 | 2.25 | 548 | 2.26 | 543 | 2.28 | 539 | 2.30 | 500 | 2.48 |
| FRd2 | 582 | 2.13 | 577 | 2.15 | 571 | 2.17 | 567 | 2.19 | 561 | 2.21 | 557 | 2.23 | 509 | 2.44 |
| ITDI | 709 | 1.75 | 703 | 1.76 | 696 | 1.78 | 690 | 1.80 | 683 | 1.82 | 677 | 1.83 | 647 | 1.92 |
| SiIDT-IC | 626 | 1.98 | 622 | 1.99 | 618 | 2.01 | 614 | 2.02 | 609 | 2.04 | 606 | 2.05 | 639 | 1.94 |
| IDIDT-C8 | 709 | 1.75 | 700 | 1.77 | 692 | 1.79 | 685 | 1.81 | 677 | 1.83 | 670 | 1.85 | 655 | 1.89 |
| IDT-BOC6 | 718 | 1.73 | 709 | 1.75 | 700 | 1.77 | 692 | 1.79 | 684 | 1.81 | 675 | 1.84 | 688 | 1.80 |
| ATT1 | 740 | 1.68 | 733 | 1.69 | 727 | 1.71 | 721 | 1.72 | 714 | 1.74 | 708 | 1.75 | 690 | 1.80 |
| DC-IDT2T | 744 | 1.67 | 736 | 1.68 | 729 | 1.70 | 722 | 1.72 | 715 | 1.73 | 708 | 1.75 | 700 | 1.77 |
| BZIC | 692 | 1.79 | 687 | 1.80 | 683 | 1.82 | 678 | 1.83 | 674 | 1.84 | 669 | 1.85 | 710 | 1.75 |
| ITOIC | 747 | 1.66 | 740 | 1.68 | 732 | 1.69 | 726 | 1.71 | 718 | 1.73 | 712 | 1.74 | 722 | 1.72 |
| IDTOT2F | 759 | 1.63 | 752 | 1.65 | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 725 | 1.71 | 723 | 1.72 |
| ITOIC-F | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 725 | 1.71 | 718 | 1.73 | 712 | 1.74 | 732 | 1.69 |
| ITOIC-2F | 756 | 1.64 | 749 | 1.66 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 722 | 1.72 | 737 | 1.68 |
| IEICO | 852 | 1.46 | 844 | 1.47 | 836 | 1.48 | 828 | 1.50 | 820 | 1.51 | 812 | 1.53 | 785 | 1.58 |
| ATT2 | 830 | 1.49 | 822 | 1.51 | 815 | 1.52 | 808 | 1.53 | 801 | 1.55 | 794 | 1.56 | 791 | 1.57 |
| IEICO-4F | 867 | 1.43 | 859 | 1.44 | 851 | 1.46 | 844 | 1.47 | 837 | 1.48 | 829 | 1.50 | 805 | 1.54 |
| m-ITIC | 684 | 1.81 | 678 | 1.83 | 673 | 1.84 | 667 | 1.86 | 662 | 1.87 | 657 | 1.89 | 660 | 1.88 |
| IT-DM | 681 | 1.82 | 675 | 1.84 | 669 | 1.85 | 664 | 1.87 | 659 | 1.88 | 654 | 1.90 | 665 | 1.86 |
| IT-M | 681 | 1.82 | 676 | 1.83 | 670 | 1.85 | 665 | 1.86 | 659 | 1.88 | 654 | 1.90 | 668 | 1.86 |
| ITCPTC | 696 | 1.78 | 690 | 1.80 | 685 | 1.81 | 680 | 1.82 | 674 | 1.84 | 669 | 1.85 | 678 | 1.83 |
| Cl-ITIC | 694 | 1.79 | 688 | 1.80 | 682 | 1.82 | 677 | 1.83 | 671 | 1.85 | 666 | 1.86 | 691 | 1.79 |
| Br-ITIC | 696 | 1.78 | 690 | 1.80 | 684 | 1.81 | 678 | 1.83 | 673 | 1.84 | 667 | 1.86 | 692 | 1.79 |
| NFBBDT | 711 | 1.74 | 705 | 1.76 | 699 | 1.77 | 693 | 1.79 | 687 | 1.80 | 682 | 1.82 | 703 | 1.76 |
| ITIC2 | 735 | 1.69 | 728 | 1.70 | 721 | 1.72 | 715 | 1.73 | 708 | 1.75 | 702 | 1.77 | 714 | 1.74 |
| ITVFFIC | 751 | 1.65 | 745 | 1.66 | 739 | 1.68 | 733 | 1.69 | 727 | 1.71 | 721 | 1.72 | 750 | 1.65 |
| INIC | 714 | 1.74 | 707 | 1.75 | 700 | 1.77 | 694 | 1.79 | 687 | 1.80 | 681 | 1.82 | 692 | 1.79 |
| INIC2 | 727 | 1.71 | 720 | 1.72 | 713 | 1.74 | 707 | 1.75 | 700 | 1.77 | 693 | 1.79 | 704 | 1.76 |
| INIC1 | 724 | 1.71 | 717 | 1.73 | 710 | 1.75 | 704 | 1.76 | 697 | 1.78 | 691 | 1.79 | 710 | 1.75 |
| INIC3 | 723 | 1.72 | 716 | 1.73 | 710 | 1.75 | 704 | 1.76 | 697 | 1.78 | 691 | 1.79 | 710 | 1.75 |
| IPIC | 733 | 1.69 | 726 | 1.71 | 719 | 1.72 | 713 | 1.74 | 707 | 1.75 | 701 | 1.77 | 761 | 1.63 |
| IPIC-4F | 741 | 1.67 | 734 | 1.69 | 728 | 1.70 | 722 | 1.72 | 716 | 1.73 | 710 | 1.75 | 776 | 1.60 |
| IPIC-4Cl | 750 | 1.65 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 716 | 1.73 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S16 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | | | |
|-----------|---|------|------------|------|------------|------|------------|------|------------|------|---|------|------------|------|
| | PBE0-20HFX | | PBE0-21HFX | | PBE0-22HFX | | PBE0-23HFX | | PBE0-24HFX | | PBE0 | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 659 | 1.88 | 652 | 1.90 | 646 | 1.92 | 640 | 1.94 | 634 | 1.96 | 628 | 2.02 | 615 | 2.02 |
| Cz-RH | 543 | 2.28 | 538 | 2.30 | 533 | 2.33 | 529 | 2.34 | 524 | 2.37 | 520 | 2.48 | 500 | 2.48 |
| Flu-RH | 562 | 2.21 | 557 | 2.23 | 552 | 2.25 | 548 | 2.26 | 543 | 2.28 | 538 | 2.48 | 500 | 2.48 |
| FRd2 | 581 | 2.13 | 576 | 2.15 | 570 | 2.18 | 565 | 2.19 | 560 | 2.21 | 556 | 2.44 | 509 | 2.44 |
| ITDI | 708 | 1.75 | 701 | 1.77 | 695 | 1.78 | 688 | 1.80 | 682 | 1.82 | 676 | 1.92 | 647 | 1.92 |
| SiIDT-IC | 626 | 1.98 | 621 | 2.00 | 617 | 2.01 | 613 | 2.02 | 609 | 2.04 | 605 | 1.94 | 639 | 1.94 |
| IDIDT-C8 | 707 | 1.75 | 699 | 1.77 | 691 | 1.79 | 683 | 1.82 | 675 | 1.84 | 668 | 1.89 | 655 | 1.89 |
| IDT-BOC6 | 716 | 1.73 | 707 | 1.75 | 699 | 1.77 | 690 | 1.80 | 682 | 1.82 | 674 | 1.8 | 688 | 1.80 |
| ATT1 | 740 | 1.68 | 733 | 1.69 | 726 | 1.71 | 720 | 1.72 | 714 | 1.74 | 708 | 1.8 | 690 | 1.80 |
| DC-IDT2T | 743 | 1.67 | 735 | 1.69 | 728 | 1.70 | 721 | 1.72 | 714 | 1.74 | 707 | 1.77 | 700 | 1.77 |
| BZIC | 691 | 1.79 | 687 | 1.80 | 682 | 1.82 | 678 | 1.83 | 673 | 1.84 | 669 | 1.75 | 710 | 1.75 |
| ITOIC | 746 | 1.66 | 739 | 1.68 | 731 | 1.70 | 724 | 1.71 | 718 | 1.73 | 711 | 1.72 | 722 | 1.72 |
| IDTOT2F | 757 | 1.64 | 750 | 1.65 | 743 | 1.67 | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 723 | 1.72 |
| ITOIC-F | 743 | 1.67 | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 717 | 1.73 | 710 | 1.69 | 732 | 1.69 |
| ITOIC-2F | 754 | 1.64 | 747 | 1.66 | 740 | 1.68 | 733 | 1.69 | 727 | 1.71 | 721 | 1.68 | 737 | 1.68 |
| IEICO | 851 | 1.46 | 843 | 1.47 | 835 | 1.49 | 827 | 1.50 | 819 | 1.51 | 811 | 1.58 | 785 | 1.58 |
| ATT2 | 828 | 1.50 | 820 | 1.51 | 813 | 1.53 | 806 | 1.54 | 799 | 1.55 | 792 | 1.57 | 791 | 1.57 |
| IEICO-4F | 865 | 1.43 | 857 | 1.45 | 849 | 1.46 | 842 | 1.47 | 835 | 1.49 | 827 | 1.54 | 805 | 1.54 |
| m-ITIC | 683 | 1.82 | 677 | 1.83 | 671 | 1.85 | 666 | 1.86 | 661 | 1.88 | 656 | 1.88 | 660 | 1.88 |
| IT-DM | 679 | 1.83 | 674 | 1.84 | 668 | 1.86 | 663 | 1.87 | 658 | 1.88 | 652 | 1.86 | 665 | 1.86 |
| IT-M | 680 | 1.82 | 674 | 1.84 | 669 | 1.85 | 663 | 1.87 | 658 | 1.88 | 653 | 1.86 | 668 | 1.86 |
| ITCPTC | 695 | 1.78 | 689 | 1.80 | 684 | 1.81 | 678 | 1.83 | 673 | 1.84 | 668 | 1.83 | 678 | 1.83 |
| Cl-ITIC | 693 | 1.79 | 687 | 1.80 | 681 | 1.82 | 676 | 1.83 | 670 | 1.85 | 665 | 1.79 | 691 | 1.79 |
| Br-ITIC | 694 | 1.79 | 688 | 1.80 | 683 | 1.82 | 677 | 1.83 | 672 | 1.85 | 666 | 1.79 | 692 | 1.79 |
| NFBDT | 710 | 1.75 | 704 | 1.76 | 698 | 1.78 | 692 | 1.79 | 686 | 1.81 | 681 | 1.76 | 703 | 1.76 |
| ITIC2 | 734 | 1.69 | 727 | 1.71 | 720 | 1.72 | 713 | 1.74 | 707 | 1.75 | 701 | 1.74 | 714 | 1.74 |
| ITVFFIC | 749 | 1.66 | 742 | 1.67 | 736 | 1.68 | 730 | 1.70 | 724 | 1.71 | 719 | 1.65 | 750 | 1.65 |
| INIC | 712 | 1.74 | 705 | 1.76 | 698 | 1.78 | 692 | 1.79 | 685 | 1.81 | 679 | 1.79 | 692 | 1.79 |
| INIC2 | 726 | 1.71 | 718 | 1.73 | 711 | 1.74 | 705 | 1.76 | 698 | 1.78 | 692 | 1.76 | 704 | 1.76 |
| INIC1 | 722 | 1.72 | 715 | 1.73 | 708 | 1.75 | 701 | 1.77 | 695 | 1.78 | 689 | 1.75 | 710 | 1.75 |
| INIC3 | 720 | 1.72 | 714 | 1.74 | 707 | 1.75 | 701 | 1.77 | 695 | 1.78 | 689 | 1.75 | 710 | 1.75 |
| IPIC | 732 | 1.69 | 725 | 1.71 | 718 | 1.73 | 712 | 1.74 | 706 | 1.76 | 700 | 1.63 | 761 | 1.63 |
| IPIC-4F | 739 | 1.68 | 732 | 1.69 | 726 | 1.71 | 720 | 1.72 | 714 | 1.74 | 708 | 1.6 | 776 | 1.60 |
| IPIC-4Cl | 748 | 1.66 | 741 | 1.67 | 734 | 1.69 | 728 | 1.70 | 722 | 1.72 | 721 | 1.57 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S17 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-----------|---|------|----------------|------|----------------|------|----------------|------|----------------|------|----------|------|---|------|
| | mPW1PW91-20HFX | | mPW1PW91-21HFX | | mPW1PW91-22HFX | | mPW1PW91-23HFX | | mPW1PW91-24HFX | | mPW1PW91 | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 660 | 1.88 | 652 | 1.90 | 646 | 1.92 | 640 | 1.94 | 634 | 1.96 | 629 | 1.97 | 615 | 2.02 |
| Cz-RH | 544 | 2.28 | 539 | 2.30 | 534 | 2.32 | 529 | 2.34 | 525 | 2.36 | 520 | 2.38 | 500 | 2.48 |
| Flu-RH | 562 | 2.21 | 557 | 2.23 | 553 | 2.24 | 548 | 2.26 | 543 | 2.28 | 539 | 2.30 | 500 | 2.48 |
| FRd2 | 582 | 2.13 | 576 | 2.15 | 571 | 2.17 | 566 | 2.19 | 561 | 2.21 | 556 | 2.23 | 509 | 2.44 |
| ITDI | 709 | 1.75 | 702 | 1.77 | 696 | 1.78 | 689 | 1.80 | 683 | 1.82 | 677 | 1.83 | 647 | 1.92 |
| SiIDT-IC | 626 | 1.98 | 622 | 1.99 | 618 | 2.01 | 613 | 2.02 | 609 | 2.04 | 605 | 2.05 | 639 | 1.94 |
| IDIDT-C8 | 708 | 1.75 | 700 | 1.77 | 692 | 1.79 | 684 | 1.81 | 676 | 1.83 | 669 | 1.85 | 655 | 1.89 |
| IDT-BOC6 | 717 | 1.73 | 709 | 1.75 | 700 | 1.77 | 691 | 1.79 | 683 | 1.82 | 675 | 1.84 | 688 | 1.80 |
| ATT1 | 741 | 1.67 | 734 | 1.69 | 727 | 1.71 | 721 | 1.72 | 714 | 1.74 | 708 | 1.75 | 690 | 1.80 |
| DC-IDT2T | 744 | 1.67 | 736 | 1.68 | 729 | 1.70 | 722 | 1.72 | 715 | 1.73 | 708 | 1.75 | 700 | 1.77 |
| BZIC | 692 | 1.79 | 687 | 1.80 | 683 | 1.82 | 678 | 1.83 | 674 | 1.84 | 670 | 1.85 | 710 | 1.75 |
| ITOIC | 747 | 1.66 | 740 | 1.68 | 732 | 1.69 | 725 | 1.71 | 719 | 1.72 | 712 | 1.74 | 722 | 1.72 |
| IDTOT2F | 758 | 1.64 | 751 | 1.65 | 744 | 1.67 | 737 | 1.68 | 731 | 1.70 | 724 | 1.71 | 723 | 1.72 |
| ITOIC-F | 744 | 1.67 | 737 | 1.68 | 731 | 1.70 | 724 | 1.71 | 718 | 1.73 | 711 | 1.74 | 732 | 1.69 |
| ITOIC-2F | 755 | 1.64 | 748 | 1.66 | 741 | 1.67 | 735 | 1.69 | 728 | 1.70 | 722 | 1.72 | 737 | 1.68 |
| IEICO | 853 | 1.45 | 844 | 1.47 | 836 | 1.48 | 828 | 1.50 | 820 | 1.51 | 813 | 1.53 | 785 | 1.58 |
| ATT2 | 829 | 1.50 | 822 | 1.51 | 814 | 1.52 | 807 | 1.54 | 800 | 1.55 | 794 | 1.56 | 791 | 1.57 |
| IEICO-4F | 867 | 1.43 | 859 | 1.44 | 851 | 1.46 | 843 | 1.47 | 836 | 1.48 | 829 | 1.50 | 805 | 1.54 |
| m-ITIC | 684 | 1.81 | 678 | 1.83 | 672 | 1.85 | 667 | 1.86 | 662 | 1.87 | 657 | 1.89 | 660 | 1.88 |
| IT-DM | 681 | 1.82 | 675 | 1.84 | 669 | 1.85 | 664 | 1.87 | 659 | 1.88 | 653 | 1.90 | 665 | 1.86 |
| IT-M | 681 | 1.82 | 675 | 1.84 | 670 | 1.85 | 664 | 1.87 | 659 | 1.88 | 654 | 1.90 | 668 | 1.86 |
| ITCPTC | 696 | 1.78 | 690 | 1.80 | 685 | 1.81 | 679 | 1.83 | 674 | 1.84 | 669 | 1.85 | 678 | 1.83 |
| Cl-ITIC | 694 | 1.79 | 688 | 1.80 | 682 | 1.82 | 677 | 1.83 | 671 | 1.85 | 666 | 1.86 | 691 | 1.79 |
| Br-ITIC | 695 | 1.78 | 689 | 1.80 | 684 | 1.81 | 678 | 1.83 | 673 | 1.84 | 667 | 1.86 | 692 | 1.79 |
| NFBBDT | 711 | 1.74 | 705 | 1.76 | 699 | 1.77 | 693 | 1.79 | 687 | 1.80 | 682 | 1.82 | 703 | 1.76 |
| ITIC2 | 735 | 1.69 | 728 | 1.70 | 721 | 1.72 | 714 | 1.74 | 708 | 1.75 | 702 | 1.77 | 714 | 1.74 |
| ITVFFIC | 750 | 1.65 | 744 | 1.67 | 738 | 1.68 | 732 | 1.69 | 726 | 1.71 | 720 | 1.72 | 750 | 1.65 |
| INIC | 713 | 1.74 | 706 | 1.76 | 700 | 1.77 | 693 | 1.79 | 687 | 1.80 | 680 | 1.82 | 692 | 1.79 |
| INIC2 | 727 | 1.71 | 720 | 1.72 | 713 | 1.74 | 706 | 1.76 | 699 | 1.77 | 693 | 1.79 | 704 | 1.76 |
| INIC1 | 723 | 1.72 | 716 | 1.73 | 709 | 1.75 | 703 | 1.76 | 696 | 1.78 | 690 | 1.80 | 710 | 1.75 |
| INIC3 | 722 | 1.72 | 715 | 1.73 | 709 | 1.75 | 703 | 1.76 | 696 | 1.78 | 691 | 1.79 | 710 | 1.75 |
| IPIC | 733 | 1.69 | 726 | 1.71 | 719 | 1.72 | 713 | 1.74 | 707 | 1.75 | 701 | 1.77 | 761 | 1.63 |
| IPIC-4F | 740 | 1.68 | 734 | 1.69 | 727 | 1.71 | 721 | 1.72 | 715 | 1.73 | 710 | 1.75 | 776 | 1.60 |
| IPIC-4Cl | 749 | 1.66 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 722 | 1.72 | 716 | 1.73 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange.

Table S18 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-----------|---|------|---------------|------|---------------|------|---------------|------|---------------|------|---------|------|---|------|
| | mPW1LYP-20HFX | | mPW1LYP-21HFX | | mPW1LYP-22HFX | | mPW1LYP-23HFX | | mPW1LYP-24HFX | | mPW1LYP | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 663 | 1.87 | 655 | 1.89 | 649 | 1.91 | 643 | 1.93 | 637 | 1.95 | 632 | 1.96 | 615 | 2.02 |
| Cz-RH | 547 | 2.27 | 542 | 2.29 | 538 | 2.30 | 533 | 2.33 | 529 | 2.34 | 524 | 2.37 | 500 | 2.48 |
| Flu-RH | 566 | 2.19 | 561 | 2.21 | 556 | 2.23 | 552 | 2.25 | 547 | 2.27 | 543 | 2.28 | 500 | 2.48 |
| FRd2 | 586 | 2.12 | 581 | 2.13 | 576 | 2.15 | 570 | 2.18 | 565 | 2.19 | 561 | 2.21 | 509 | 2.44 |
| ITDI | 713 | 1.74 | 706 | 1.76 | 700 | 1.77 | 693 | 1.79 | 687 | 1.80 | 681 | 1.82 | 647 | 1.92 |
| SiIDT-IC | 630 | 1.97 | 626 | 1.98 | 622 | 1.99 | 618 | 2.01 | 613 | 2.02 | 609 | 2.04 | 639 | 1.94 |
| IDIDT-C8 | 711 | 1.74 | 703 | 1.76 | 695 | 1.78 | 687 | 1.80 | 680 | 1.82 | 672 | 1.85 | 655 | 1.89 |
| IDT-BOC6 | 722 | 1.72 | 713 | 1.74 | 704 | 1.76 | 696 | 1.78 | 687 | 1.80 | 679 | 1.83 | 688 | 1.80 |
| ATT1 | 746 | 1.66 | 739 | 1.68 | 733 | 1.69 | 726 | 1.71 | 720 | 1.72 | 714 | 1.74 | 690 | 1.80 |
| DC-IDT2T | 748 | 1.66 | 741 | 1.67 | 734 | 1.69 | 726 | 1.71 | 720 | 1.72 | 713 | 1.74 | 700 | 1.77 |
| BZIC | 696 | 1.78 | 692 | 1.79 | 687 | 1.80 | 683 | 1.82 | 678 | 1.83 | 674 | 1.84 | 710 | 1.75 |
| ITOIC | 752 | 1.65 | 744 | 1.67 | 737 | 1.68 | 730 | 1.70 | 723 | 1.72 | 717 | 1.73 | 722 | 1.72 |
| IDTOT2F | 763 | 1.63 | 756 | 1.64 | 749 | 1.66 | 742 | 1.67 | 735 | 1.69 | 729 | 1.70 | 723 | 1.72 |
| ITOIC-F | 749 | 1.66 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 716 | 1.73 | 732 | 1.69 |
| ITOIC-2F | 760 | 1.63 | 753 | 1.65 | 746 | 1.66 | 740 | 1.68 | 733 | 1.69 | 727 | 1.71 | 737 | 1.68 |
| IEICO | 858 | 1.45 | 850 | 1.46 | 842 | 1.47 | 834 | 1.49 | 826 | 1.50 | 818 | 1.52 | 785 | 1.58 |
| ATT2 | 837 | 1.48 | 829 | 1.50 | 822 | 1.51 | 814 | 1.52 | 807 | 1.54 | 801 | 1.55 | 791 | 1.57 |
| IEICO-4F | 872 | 1.42 | 864 | 1.44 | 857 | 1.45 | 849 | 1.46 | 842 | 1.47 | 835 | 1.49 | 805 | 1.54 |
| m-ITIC | 687 | 1.80 | 681 | 1.82 | 676 | 1.83 | 671 | 1.85 | 665 | 1.86 | 660 | 1.88 | 660 | 1.88 |
| IT-DM | 684 | 1.81 | 678 | 1.83 | 673 | 1.84 | 667 | 1.86 | 662 | 1.87 | 657 | 1.89 | 665 | 1.86 |
| IT-M | 684 | 1.81 | 679 | 1.83 | 673 | 1.84 | 668 | 1.86 | 663 | 1.87 | 658 | 1.88 | 668 | 1.86 |
| ITCPTC | 700 | 1.77 | 694 | 1.79 | 689 | 1.80 | 683 | 1.82 | 678 | 1.83 | 673 | 1.84 | 678 | 1.83 |
| Cl-ITIC | 697 | 1.78 | 691 | 1.79 | 686 | 1.81 | 680 | 1.82 | 675 | 1.84 | 670 | 1.85 | 691 | 1.79 |
| Br-ITIC | 699 | 1.77 | 693 | 1.79 | 687 | 1.80 | 681 | 1.82 | 676 | 1.83 | 671 | 1.85 | 692 | 1.79 |
| NFBDT | 713 | 1.74 | 707 | 1.75 | 701 | 1.77 | 695 | 1.78 | 690 | 1.80 | 684 | 1.81 | 703 | 1.76 |
| ITIC2 | 738 | 1.68 | 731 | 1.70 | 724 | 1.71 | 718 | 1.73 | 711 | 1.74 | 705 | 1.76 | 714 | 1.74 |
| ITVFFIC | 754 | 1.64 | 748 | 1.66 | 742 | 1.67 | 736 | 1.68 | 730 | 1.70 | 724 | 1.71 | 750 | 1.65 |
| INIC | 718 | 1.73 | 711 | 1.74 | 704 | 1.76 | 698 | 1.78 | 691 | 1.79 | 685 | 1.81 | 692 | 1.79 |
| INIC2 | 732 | 1.69 | 724 | 1.71 | 717 | 1.73 | 711 | 1.74 | 704 | 1.76 | 698 | 1.78 | 704 | 1.76 |
| INIC1 | 728 | 1.70 | 721 | 1.72 | 714 | 1.74 | 707 | 1.75 | 701 | 1.77 | 695 | 1.78 | 710 | 1.75 |
| INIC3 | 727 | 1.71 | 720 | 1.72 | 714 | 1.74 | 707 | 1.75 | 701 | 1.77 | 695 | 1.78 | 710 | 1.75 |
| IPIC | 736 | 1.68 | 730 | 1.70 | 723 | 1.72 | 717 | 1.73 | 711 | 1.74 | 705 | 1.76 | 761 | 1.63 |
| IPIC-4F | 744 | 1.67 | 737 | 1.68 | 731 | 1.70 | 725 | 1.71 | 719 | 1.72 | 713 | 1.74 | 776 | 1.60 |
| IPIC-4Cl | 753 | 1.65 | 746 | 1.66 | 739 | 1.68 | 733 | 1.69 | 726 | 1.71 | 720 | 1.72 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S19 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-----------|---|------|---------------|------|---------------|------|---------------|------|---------------|------|---------|------|---|------|
| | mPW1PBE-20HFX | | mPW1PBE-21HFX | | mPW1PBE-22HFX | | mPW1PBE-23HFX | | mPW1PBE-24HFX | | mPW1PBE | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 659 | 1.88 | 652 | 1.90 | 646 | 1.92 | 640 | 1.94 | 634 | 1.96 | 629 | 1.97 | 615 | 2.02 |
| Cz-RH | 543 | 2.28 | 538 | 2.30 | 534 | 2.32 | 529 | 2.34 | 524 | 2.37 | 520 | 2.38 | 500 | 2.48 |
| Flu-RH | 562 | 2.21 | 557 | 2.23 | 552 | 2.25 | 548 | 2.26 | 543 | 2.28 | 539 | 2.30 | 500 | 2.48 |
| FRd2 | 582 | 2.13 | 576 | 2.15 | 571 | 2.17 | 566 | 2.19 | 561 | 2.21 | 556 | 2.23 | 509 | 2.44 |
| ITDI | 709 | 1.75 | 702 | 1.77 | 695 | 1.78 | 689 | 1.80 | 682 | 1.82 | 677 | 1.83 | 647 | 1.92 |
| SiIDT-IC | 626 | 1.98 | 622 | 1.99 | 617 | 2.01 | 613 | 2.02 | 609 | 2.04 | 605 | 2.05 | 639 | 1.94 |
| IDIDT-C8 | 708 | 1.75 | 699 | 1.77 | 691 | 1.79 | 684 | 1.81 | 676 | 1.83 | 669 | 1.85 | 655 | 1.89 |
| IDT-BOC6 | 717 | 1.73 | 708 | 1.75 | 700 | 1.77 | 691 | 1.79 | 683 | 1.82 | 675 | 1.84 | 688 | 1.80 |
| ATT1 | 740 | 1.68 | 733 | 1.69 | 727 | 1.71 | 720 | 1.72 | 714 | 1.74 | 708 | 1.75 | 690 | 1.80 |
| DC-IDT2T | 743 | 1.67 | 736 | 1.68 | 729 | 1.70 | 721 | 1.72 | 714 | 1.74 | 708 | 1.75 | 700 | 1.77 |
| BZIC | 691 | 1.79 | 687 | 1.80 | 682 | 1.82 | 678 | 1.83 | 673 | 1.84 | 669 | 1.85 | 710 | 1.75 |
| ITOIC | 747 | 1.66 | 739 | 1.68 | 732 | 1.69 | 725 | 1.71 | 718 | 1.73 | 712 | 1.74 | 722 | 1.72 |
| IDTOT2F | 758 | 1.64 | 751 | 1.65 | 744 | 1.67 | 737 | 1.68 | 730 | 1.70 | 724 | 1.71 | 723 | 1.72 |
| ITOIC-F | 744 | 1.67 | 737 | 1.68 | 730 | 1.70 | 724 | 1.71 | 717 | 1.73 | 711 | 1.74 | 732 | 1.69 |
| ITOIC-2F | 755 | 1.64 | 748 | 1.66 | 741 | 1.67 | 734 | 1.69 | 728 | 1.70 | 721 | 1.72 | 737 | 1.68 |
| IEICO | 852 | 1.46 | 844 | 1.47 | 835 | 1.49 | 827 | 1.50 | 820 | 1.51 | 812 | 1.53 | 785 | 1.58 |
| ATT2 | 829 | 1.50 | 821 | 1.51 | 814 | 1.52 | 807 | 1.54 | 800 | 1.55 | 793 | 1.56 | 791 | 1.57 |
| IEICO-4F | 866 | 1.43 | 858 | 1.45 | 850 | 1.46 | 843 | 1.47 | 836 | 1.48 | 828 | 1.50 | 805 | 1.54 |
| m-ITIC | 683 | 1.82 | 678 | 1.83 | 672 | 1.85 | 667 | 1.86 | 661 | 1.88 | 656 | 1.89 | 660 | 1.88 |
| IT-DM | 680 | 1.82 | 674 | 1.84 | 669 | 1.85 | 663 | 1.87 | 658 | 1.88 | 653 | 1.90 | 665 | 1.86 |
| IT-M | 681 | 1.82 | 675 | 1.84 | 669 | 1.85 | 664 | 1.87 | 659 | 1.88 | 654 | 1.90 | 668 | 1.86 |
| ITCPTC | 696 | 1.78 | 690 | 1.80 | 684 | 1.81 | 679 | 1.83 | 674 | 1.84 | 669 | 1.85 | 678 | 1.83 |
| Cl-ITIC | 693 | 1.79 | 688 | 1.80 | 682 | 1.82 | 676 | 1.83 | 671 | 1.85 | 666 | 1.86 | 691 | 1.79 |
| Br-ITIC | 695 | 1.78 | 689 | 1.80 | 683 | 1.82 | 678 | 1.83 | 672 | 1.85 | 667 | 1.86 | 692 | 1.79 |
| NFBDT | 711 | 1.74 | 704 | 1.76 | 698 | 1.78 | 693 | 1.79 | 687 | 1.80 | 681 | 1.82 | 703 | 1.76 |
| ITIC2 | 734 | 1.69 | 727 | 1.71 | 721 | 1.72 | 714 | 1.74 | 708 | 1.75 | 702 | 1.77 | 714 | 1.74 |
| ITVFFIC | 750 | 1.65 | 743 | 1.67 | 737 | 1.68 | 731 | 1.70 | 725 | 1.71 | 720 | 1.72 | 750 | 1.65 |
| INIC | 713 | 1.74 | 706 | 1.76 | 699 | 1.77 | 693 | 1.79 | 686 | 1.81 | 680 | 1.82 | 692 | 1.79 |
| INIC2 | 727 | 1.71 | 719 | 1.72 | 712 | 1.74 | 706 | 1.76 | 699 | 1.77 | 693 | 1.79 | 704 | 1.76 |
| INIC1 | 722 | 1.72 | 715 | 1.73 | 709 | 1.75 | 702 | 1.77 | 696 | 1.78 | 690 | 1.80 | 710 | 1.75 |
| INIC3 | 721 | 1.72 | 715 | 1.73 | 708 | 1.75 | 702 | 1.77 | 696 | 1.78 | 690 | 1.80 | 710 | 1.75 |
| IPIC | 732 | 1.69 | 725 | 1.71 | 719 | 1.72 | 713 | 1.74 | 706 | 1.76 | 700 | 1.77 | 761 | 1.63 |
| IPIC-4F | 740 | 1.68 | 733 | 1.69 | 727 | 1.71 | 721 | 1.72 | 715 | 1.73 | 709 | 1.75 | 776 | 1.60 |
| IPIC-4Cl | 749 | 1.66 | 742 | 1.67 | 735 | 1.69 | 729 | 1.70 | 722 | 1.72 | 716 | 1.73 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S20 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-------------|---|------|-----------|------|-----------|------|-----------|------|-----------|------|-----------|------|-----------|------|-----|------|---|------|
| | M06-20HFX | | M06-21HFX | | M06-22HFX | | M06-23HFX | | M06-24HFX | | M06-25HFX | | M06-26HFX | | M06 | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 666 | 1.86 | 660 | 1.88 | 653 | 1.90 | 647 | 1.92 | 642 | 1.93 | 637 | 1.95 | 632 | 1.96 | 627 | 1.98 | 615 | 2.02 |
| Cz-RH | 554 | 2.24 | 549 | 2.26 | 544 | 2.28 | 540 | 2.30 | 535 | 2.32 | 531 | 2.34 | 527 | 2.35 | 523 | 2.37 | 500 | 2.48 |
| Flu-RH | 574 | 2.16 | 569 | 2.18 | 564 | 2.20 | 559 | 2.22 | 555 | 2.23 | 550 | 2.25 | 546 | 2.27 | 542 | 2.29 | 500 | 2.48 |
| FRd2 | 594 | 2.09 | 589 | 2.11 | 583 | 2.13 | 578 | 2.15 | 573 | 2.16 | 569 | 2.18 | 564 | 2.20 | 560 | 2.21 | 509 | 2.44 |
| ITDI | 714 | 1.74 | 707 | 1.75 | 700 | 1.77 | 694 | 1.79 | 688 | 1.80 | 681 | 1.82 | 676 | 1.83 | 670 | 1.85 | 647 | 1.92 |
| SiIDT-IC-IC | 634 | 1.96 | 630 | 1.97 | 625 | 1.98 | 621 | 2.00 | 617 | 2.01 | 613 | 2.02 | 609 | 2.04 | 605 | 2.05 | 639 | 1.94 |
| IDIDT-C8 | 712 | 1.74 | 704 | 1.76 | 696 | 1.78 | 688 | 1.80 | 680 | 1.82 | 673 | 1.84 | 666 | 1.86 | 659 | 1.88 | 655 | 1.89 |
| IDT-BOC6 | 725 | 1.71 | 716 | 1.73 | 707 | 1.75 | 699 | 1.77 | 691 | 1.79 | 683 | 1.82 | 675 | 1.84 | 668 | 1.86 | 688 | 1.80 |
| ATT1 | 752 | 1.65 | 745 | 1.66 | 738 | 1.68 | 732 | 1.69 | 725 | 1.71 | 719 | 1.72 | 714 | 1.74 | 708 | 1.75 | 690 | 1.80 |
| DC-IDT2T | 748 | 1.66 | 741 | 1.67 | 733 | 1.69 | 726 | 1.71 | 719 | 1.72 | 713 | 1.74 | 706 | 1.76 | 700 | 1.77 | 700 | 1.77 |
| BZIC | 700 | 1.77 | 695 | 1.78 | 691 | 1.79 | 686 | 1.81 | 682 | 1.82 | 677 | 1.83 | 673 | 1.84 | 669 | 1.85 | 710 | 1.75 |
| ITOIC | 752 | 1.65 | 745 | 1.66 | 737 | 1.68 | 730 | 1.70 | 723 | 1.72 | 717 | 1.73 | 710 | 1.75 | 704 | 1.76 | 722 | 1.72 |
| IDTOT2F | 763 | 1.63 | 756 | 1.64 | 749 | 1.66 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 717 | 1.73 | 723 | 1.72 |
| ITOIC-F | 749 | 1.66 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 716 | 1.73 | 710 | 1.75 | 704 | 1.76 | 732 | 1.69 |
| ITOIC-2F | 760 | 1.63 | 753 | 1.65 | 746 | 1.66 | 739 | 1.68 | 733 | 1.69 | 726 | 1.71 | 720 | 1.72 | 714 | 1.74 | 737 | 1.68 |
| IEICO | 862 | 1.44 | 854 | 1.45 | 845 | 1.47 | 837 | 1.48 | 829 | 1.50 | 822 | 1.51 | 814 | 1.52 | 807 | 1.54 | 785 | 1.58 |
| ATT2 | 835 | 1.49 | 827 | 1.50 | 820 | 1.51 | 813 | 1.53 | 806 | 1.54 | 799 | 1.55 | 792 | 1.57 | 786 | 1.58 | 791 | 1.57 |
| IEICO-4F | 877 | 1.41 | 869 | 1.43 | 861 | 1.44 | 853 | 1.45 | 846 | 1.47 | 839 | 1.48 | 832 | 1.49 | 825 | 1.50 | 805 | 1.54 |
| m-ITIC | 691 | 1.79 | 685 | 1.81 | 679 | 1.83 | 674 | 1.84 | 668 | 1.86 | 663 | 1.87 | 658 | 1.88 | 653 | 1.90 | 660 | 1.88 |
| IT-DM | 688 | 1.80 | 682 | 1.82 | 676 | 1.83 | 670 | 1.85 | 665 | 1.86 | 660 | 1.88 | 655 | 1.89 | 650 | 1.91 | 665 | 1.86 |
| IT-M | 688 | 1.80 | 682 | 1.82 | 676 | 1.83 | 671 | 1.85 | 666 | 1.86 | 661 | 1.88 | 656 | 1.89 | 651 | 1.90 | 668 | 1.86 |
| ITCPTC | 703 | 1.76 | 697 | 1.78 | 691 | 1.79 | 686 | 1.81 | 681 | 1.82 | 676 | 1.83 | 670 | 1.85 | 666 | 1.86 | 678 | 1.83 |
| Cl-ITIC | 702 | 1.77 | 696 | 1.78 | 690 | 1.80 | 684 | 1.81 | 679 | 1.83 | 673 | 1.84 | 668 | 1.86 | 663 | 1.87 | 691 | 1.79 |
| Br-ITIC | 704 | 1.76 | 697 | 1.78 | 692 | 1.79 | 686 | 1.81 | 680 | 1.82 | 675 | 1.84 | 670 | 1.85 | 665 | 1.86 | 692 | 1.79 |
| NFBdT | 720 | 1.72 | 714 | 1.74 | 707 | 1.75 | 702 | 1.77 | 696 | 1.78 | 690 | 1.80 | 685 | 1.81 | 680 | 1.82 | 703 | 1.76 |
| ITIC2 | 745 | 1.66 | 738 | 1.68 | 731 | 1.70 | 725 | 1.71 | 718 | 1.73 | 712 | 1.74 | 706 | 1.76 | 700 | 1.77 | 714 | 1.74 |
| ITVFFIC | 757 | 1.64 | 750 | 1.65 | 744 | 1.67 | 738 | 1.68 | 732 | 1.69 | 726 | 1.71 | 721 | 1.72 | 715 | 1.73 | 750 | 1.65 |
| INIC | 719 | 1.72 | 712 | 1.74 | 705 | 1.76 | 698 | 1.78 | 692 | 1.79 | 685 | 1.81 | 679 | 1.83 | 674 | 1.84 | 692 | 1.79 |
| INIC2 | 733 | 1.69 | 725 | 1.71 | 718 | 1.73 | 711 | 1.74 | 705 | 1.76 | 698 | 1.78 | 692 | 1.79 | 686 | 1.81 | 704 | 1.76 |
| INIC1 | 728 | 1.70 | 721 | 1.72 | 714 | 1.74 | 708 | 1.75 | 701 | 1.77 | 695 | 1.78 | 689 | 1.80 | 683 | 1.82 | 710 | 1.75 |
| INIC3 | 727 | 1.71 | 720 | 1.72 | 714 | 1.74 | 708 | 1.75 | 701 | 1.77 | 695 | 1.78 | 690 | 1.80 | 684 | 1.81 | 710 | 1.75 |
| IPIC | 739 | 1.68 | 732 | 1.69 | 725 | 1.71 | 719 | 1.72 | 713 | 1.74 | 707 | 1.75 | 701 | 1.77 | 696 | 1.78 | 761 | 1.63 |
| IPIC-4F | 746 | 1.66 | 740 | 1.68 | 734 | 1.69 | 727 | 1.71 | 721 | 1.72 | 715 | 1.73 | 710 | 1.75 | 705 | 1.76 | 776 | 1.60 |
| IPIC-4Cl | 756 | 1.64 | 749 | 1.66 | 742 | 1.67 | 736 | 1.68 | 729 | 1.70 | 723 | 1.72 | 717 | 1.73 | 711 | 1.74 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S21 Experimental maximum absorption wavelengths (λ_{max} in nm), experimental transition energies ($E_{\text{max-exp}}$ in eV), theoretical vertical absorption wavelengths ($\lambda_{\text{ver-theo}}$ in nm), and theoretical vertical transition energies ($E_{\text{ver-theo}}$ in eV) of all FREAs computed in chloroform with PCM-TD-DFT-XC-HFX/6-31G(d,p)^a

| Molecule | $\lambda_{\text{ver-theo}}$ and $E_{\text{ver-theo}}$ | | | | | | | | | | | | | | | | λ_{max} and $E_{\text{max-exp}}$ | |
|-------------|---|------|-----------|------|-----------|------|-----------|------|-----------|------|-----------|------|-----------|------|-----|------|---|------|
| | M05-20HFX | | M05-21HFX | | M05-22HFX | | M05-23HFX | | M05-24HFX | | M05-25HFX | | M05-26HFX | | M05 | | Experiment | |
| | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| F(DPP)2B2 | 660 | 1.88 | 653 | 1.90 | 647 | 1.92 | 641 | 1.93 | 636 | 1.95 | 631 | 1.97 | 626 | 1.98 | 617 | 2.01 | 615 | 2.02 |
| Cz-RH | 550 | 2.25 | 545 | 2.28 | 540 | 2.30 | 535 | 2.32 | 531 | 2.34 | 527 | 2.35 | 522 | 2.38 | 515 | 2.41 | 500 | 2.48 |
| Flu-RH | 569 | 2.18 | 564 | 2.20 | 559 | 2.22 | 555 | 2.23 | 550 | 2.25 | 546 | 2.27 | 542 | 2.29 | 534 | 2.32 | 500 | 2.48 |
| FRd2 | 591 | 2.10 | 586 | 2.12 | 580 | 2.14 | 575 | 2.16 | 571 | 2.17 | 566 | 2.19 | 561 | 2.21 | 553 | 2.24 | 509 | 2.44 |
| ITDI | 705 | 1.76 | 698 | 1.78 | 691 | 1.79 | 684 | 1.81 | 678 | 1.83 | 672 | 1.85 | 666 | 1.86 | 655 | 1.89 | 647 | 1.92 |
| SiIDT-IC-IC | 624 | 1.99 | 620 | 2.00 | 615 | 2.02 | 611 | 2.03 | 607 | 2.04 | 603 | 2.06 | 599 | 2.07 | 591 | 2.10 | 639 | 1.94 |
| IDIDT-C8 | 704 | 1.76 | 696 | 1.78 | 688 | 1.80 | 680 | 1.82 | 672 | 1.85 | 665 | 1.86 | 658 | 1.88 | 644 | 1.93 | 655 | 1.89 |
| IDT-BOC6 | 715 | 1.73 | 706 | 1.76 | 698 | 1.78 | 689 | 1.80 | 681 | 1.82 | 673 | 1.84 | 665 | 1.86 | 650 | 1.91 | 688 | 1.80 |
| ATT1 | 743 | 1.67 | 737 | 1.68 | 730 | 1.70 | 723 | 1.72 | 717 | 1.73 | 711 | 1.74 | 705 | 1.76 | 694 | 1.79 | 690 | 1.80 |
| DC-IDT2T | 738 | 1.68 | 730 | 1.70 | 722 | 1.72 | 715 | 1.73 | 708 | 1.75 | 701 | 1.77 | 695 | 1.78 | 682 | 1.82 | 700 | 1.77 |
| BZIC | 689 | 1.80 | 684 | 1.81 | 679 | 1.83 | 674 | 1.84 | 670 | 1.85 | 665 | 1.86 | 661 | 1.88 | 652 | 1.90 | 710 | 1.75 |
| ITOIC | 742 | 1.67 | 734 | 1.69 | 727 | 1.71 | 719 | 1.72 | 712 | 1.74 | 706 | 1.76 | 699 | 1.77 | 687 | 1.80 | 722 | 1.72 |
| IDTOT2F | 751 | 1.65 | 744 | 1.67 | 737 | 1.68 | 730 | 1.70 | 723 | 1.72 | 717 | 1.73 | 710 | 1.75 | 698 | 1.78 | 723 | 1.72 |
| ITOIC-F | 738 | 1.68 | 731 | 1.70 | 724 | 1.71 | 717 | 1.73 | 711 | 1.74 | 704 | 1.76 | 698 | 1.78 | 687 | 1.80 | 732 | 1.69 |
| ITOIC-2F | 749 | 1.66 | 741 | 1.67 | 734 | 1.69 | 728 | 1.70 | 721 | 1.72 | 715 | 1.73 | 708 | 1.75 | 696 | 1.78 | 737 | 1.68 |
| IEICO | 850 | 1.46 | 842 | 1.47 | 833 | 1.49 | 825 | 1.50 | 817 | 1.52 | 809 | 1.53 | 801 | 1.55 | 787 | 1.58 | 785 | 1.58 |
| ATT2 | 821 | 1.51 | 813 | 1.53 | 806 | 1.54 | 798 | 1.55 | 791 | 1.57 | 785 | 1.58 | 778 | 1.59 | 766 | 1.62 | 791 | 1.57 |
| IEICO-4F | 863 | 1.44 | 855 | 1.45 | 847 | 1.46 | 839 | 1.48 | 832 | 1.49 | 825 | 1.50 | 818 | 1.52 | 804 | 1.54 | 805 | 1.54 |
| m-ITIC | 679 | 1.83 | 673 | 1.84 | 668 | 1.86 | 662 | 1.87 | 657 | 1.89 | 651 | 1.90 | 646 | 1.92 | 637 | 1.95 | 660 | 1.88 |
| IT-DM | 676 | 1.83 | 670 | 1.85 | 664 | 1.87 | 659 | 1.88 | 653 | 1.90 | 648 | 1.91 | 643 | 1.93 | 633 | 1.96 | 665 | 1.86 |
| IT-M | 677 | 1.83 | 671 | 1.85 | 665 | 1.86 | 659 | 1.88 | 654 | 1.90 | 649 | 1.91 | 644 | 1.93 | 634 | 1.96 | 668 | 1.86 |
| ITCPTC | 691 | 1.79 | 685 | 1.81 | 679 | 1.83 | 674 | 1.84 | 668 | 1.86 | 663 | 1.87 | 658 | 1.88 | 648 | 1.91 | 678 | 1.83 |
| Cl-ITIC | 691 | 1.79 | 685 | 1.81 | 679 | 1.83 | 674 | 1.84 | 668 | 1.86 | 662 | 1.87 | 657 | 1.89 | 647 | 1.92 | 691 | 1.79 |
| Br-ITIC | 693 | 1.79 | 687 | 1.80 | 681 | 1.82 | 675 | 1.84 | 670 | 1.85 | 664 | 1.87 | 659 | 1.88 | 648 | 1.91 | 692 | 1.79 |
| NFBBDT | 712 | 1.74 | 705 | 1.76 | 699 | 1.77 | 693 | 1.79 | 687 | 1.80 | 681 | 1.82 | 675 | 1.84 | 665 | 1.86 | 703 | 1.76 |
| ITIC2 | 736 | 1.68 | 728 | 1.70 | 721 | 1.72 | 714 | 1.74 | 708 | 1.75 | 701 | 1.77 | 695 | 1.78 | 683 | 1.82 | 714 | 1.74 |
| ITVFFIC | 742 | 1.67 | 735 | 1.69 | 729 | 1.70 | 723 | 1.72 | 717 | 1.73 | 711 | 1.74 | 705 | 1.76 | 694 | 1.79 | 750 | 1.65 |
| INIC | 707 | 1.75 | 699 | 1.77 | 692 | 1.79 | 685 | 1.81 | 678 | 1.83 | 673 | 1.84 | 666 | 1.86 | 655 | 1.89 | 692 | 1.79 |
| INIC2 | 720 | 1.72 | 713 | 1.74 | 706 | 1.76 | 699 | 1.77 | 692 | 1.79 | 685 | 1.81 | 679 | 1.83 | 667 | 1.86 | 704 | 1.76 |
| INIC1 | 716 | 1.73 | 709 | 1.75 | 702 | 1.77 | 695 | 1.78 | 688 | 1.80 | 682 | 1.82 | 676 | 1.83 | 664 | 1.87 | 710 | 1.75 |
| INIC3 | 714 | 1.74 | 707 | 1.75 | 700 | 1.77 | 694 | 1.79 | 688 | 1.80 | 682 | 1.82 | 676 | 1.83 | 665 | 1.86 | 710 | 1.75 |
| IPIC | 729 | 1.70 | 722 | 1.72 | 715 | 1.73 | 709 | 1.75 | 702 | 1.77 | 696 | 1.78 | 690 | 1.80 | 679 | 1.83 | 761 | 1.63 |
| IPIC-4F | 736 | 1.68 | 729 | 1.70 | 722 | 1.72 | 716 | 1.73 | 710 | 1.75 | 704 | 1.76 | 699 | 1.77 | 688 | 1.80 | 776 | 1.60 |
| IPIC-4Cl | 746 | 1.66 | 739 | 1.68 | 732 | 1.69 | 725 | 1.71 | 718 | 1.73 | 712 | 1.74 | 706 | 1.76 | 694 | 1.79 | 790 | 1.57 |

^a XC and HFX in PCM-TD-DFT-XC-HFX/6-31G(d,p) denote the exchange-correlation functional and percentage of Hartree-Fock exact-exchange, respectively.

Table S22 Statistical analysis of transition wavelengths and energies using actual theoretical data for excited states of all FREAs^a

| Functional Used | With various HFX (%) | without fit | | | | | | with linear fit | | | |
|-----------------|----------------------|-------------|-------|-----|------|-----|------|-----------------|------|-----|------|
| | | MSE | | MAE | | RMS | | MAE | | RMS | |
| | | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| B3LYP | B3LYP | -28 | 0.08 | 34 | 0.09 | 40 | 0.12 | 22 | 0.06 | 28 | 0.08 |
| | B3LYP-21HFX | -21 | 0.06 | 30 | 0.08 | 36 | 0.11 | 22 | 0.06 | 28 | 0.08 |
| | B3LYP-22HFX | -15 | 0.05 | 26 | 0.07 | 32 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | B3LYP-23HFX | -9 | 0.03 | 22 | 0.06 | 29 | 0.09 | 21 | 0.06 | 28 | 0.07 |
| | B3LYP-24HFX | -3 | 0.01 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | B3LYP-25HFX | 3 | 0.00 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| B3PW91 | B3PW91 | -24 | 0.07 | 32 | 0.09 | 37 | 0.11 | 22 | 0.06 | 28 | 0.08 |
| | B3PW91-21HFX | -18 | 0.05 | 27 | 0.07 | 33 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | B3PW91-22HFX | -11 | 0.04 | 24 | 0.07 | 30 | 0.09 | 21 | 0.06 | 28 | 0.08 |
| | B3PW91-23HFX | -5 | 0.02 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | B3PW91-24HFX | 1 | 0.01 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | B3PW91-25HFX | 7 | -0.01 | 22 | 0.06 | 28 | 0.08 | 20 | 0.06 | 27 | 0.07 |
| mPW3PBE | mPW3PBE | -24 | 0.07 | 32 | 0.09 | 37 | 0.11 | 22 | 0.06 | 28 | 0.08 |
| | mPW3PBE-21HFX | -18 | 0.05 | 27 | 0.07 | 33 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | mPW3PBE-22HFX | -11 | 0.04 | 24 | 0.07 | 30 | 0.09 | 21 | 0.06 | 28 | 0.08 |
| | mPW3PBE-23HFX | -5 | 0.02 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 28 | 0.07 |
| | mPW3PBE-24HFX | 1 | 0.00 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | mPW3PBE-25HFX | 7 | -0.01 | 23 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |

^a MSE: mean signed error; MAE: mean absolute error; RMS: root mean squared error; HFX: percentage of Hartree-Fock exact exchange.

Table S23 Statistical analysis of transition wavelengths and energies using actual theoretical data for excited states of all FREAs^a

| Functional Used | With various HFX (%) | without fit | | | | | | with linear fit | | | |
|-----------------|----------------------|-------------|-------|-----|------|-----|------|-----------------|------|-----|------|
| | | MSE | | MAE | | RMS | | MAE | | RMS | |
| | | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| X3LYP | X3LYP-20HFX | -27 | 0.08 | 34 | 0.09 | 40 | 0.12 | 22 | 0.06 | 29 | 0.08 |
| | X3LYP | -16 | 0.05 | 26 | 0.07 | 32 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | X3LYP-22HFX | -14 | 0.04 | 25 | 0.07 | 32 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | X3LYP-23HFX | -8 | 0.03 | 22 | 0.06 | 29 | 0.09 | 21 | 0.06 | 28 | 0.08 |
| | X3LYP-24HFX | -2 | 0.01 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | X3LYP-25HFX | 4 | 0.00 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| B971 | B971-20HFX | -26 | 0.07 | 33 | 0.09 | 38 | 0.11 | 22 | 0.06 | 29 | 0.08 |
| | B971 | -19 | 0.06 | 28 | 0.08 | 34 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | B971-22HFX | -12 | 0.04 | 24 | 0.07 | 31 | 0.09 | 22 | 0.06 | 28 | 0.08 |
| | B971-23HFX | -6 | 0.02 | 22 | 0.06 | 29 | 0.09 | 21 | 0.06 | 28 | 0.07 |
| | B971-24HFX | 0 | 0.01 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | B971-25HFX | 6 | -0.01 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| B972 | B972-20HFX | -22 | 0.06 | 30 | 0.08 | 36 | 0.11 | 22 | 0.06 | 28 | 0.08 |
| | B972 | -16 | 0.05 | 26 | 0.07 | 32 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | B972-22HFX | -9 | 0.03 | 23 | 0.06 | 29 | 0.09 | 21 | 0.06 | 28 | 0.08 |
| | B972-23HFX | -3 | 0.02 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | B972-24HFX | 3 | 0.00 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | B972-25HFX | 9 | -0.02 | 23 | 0.06 | 29 | 0.08 | 21 | 0.06 | 27 | 0.07 |

^a MSE: mean signed error; MAE: mean absolute error; RMS: root mean squared error; HFX: percentage of Hartree-Fock exact exchange.

Table S24 Statistical analysis of transition wavelengths and energies using actual theoretical data for excited states of all FREAs^a

| Functional Used | With various HFX (%) | without fit | | | | | | with linear fit | | | |
|-----------------|----------------------|-------------|------|-----|------|-----|------|-----------------|------|-----|------|
| | | MSE | | MAE | | RMS | | MAE | | RMS | |
| | | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| B98 | B98-20HFX | -27 | 0.07 | 34 | 0.09 | 39 | 0.11 | 22 | 0.06 | 29 | 0.08 |
| | B98-21HFX | -20 | 0.06 | 29 | 0.08 | 35 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | B98 | -14 | 0.04 | 25 | 0.07 | 31 | 0.09 | 22 | 0.06 | 28 | 0.08 |
| | B98-23HFX | -7 | 0.03 | 22 | 0.06 | 29 | 0.09 | 21 | 0.06 | 28 | 0.08 |
| | B98-24HFX | -1 | 0.01 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 28 | 0.07 |
| | B98-25HFX | 5 | 0.00 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |

^a MSE: mean signed error; MAE: mean absolute error; RMS: root mean squared error; HFX: percentage of Hartree-Fock exact exchange.

Table S25 Statistical analysis of transition wavelengths and energies using actual theoretical data for excited states of all FREAs^a

| Functional Used | With various HFX (%) | without fit | | | | | | with linear fit | | | |
|-----------------|----------------------|-------------|-------|-----|------|-----|------|-----------------|------|-----|------|
| | | MSE | | MAE | | RMS | | MAE | | RMS | |
| | | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| APF | APF-20HFX | -23 | 0.06 | 31 | 0.08 | 36 | 0.11 | 22 | 0.06 | 28 | 0.08 |
| | APF-21HFX | -16 | 0.05 | 26 | 0.07 | 32 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | APF-22HFX | -10 | 0.03 | 23 | 0.06 | 29 | 0.09 | 21 | 0.06 | 28 | 0.07 |
| | APF | -4 | 0.02 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 28 | 0.07 |
| | APF-24HFX | 3 | 0.00 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | APF-25HFX | 9 | -0.01 | 23 | 0.06 | 29 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| APFD | APFD-20HFX | -23 | 0.06 | 31 | 0.08 | 36 | 0.11 | 22 | 0.06 | 28 | 0.08 |
| | APFD-21HFX | -16 | 0.05 | 26 | 0.07 | 32 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | APFD-22HFX | -10 | 0.03 | 23 | 0.06 | 29 | 0.09 | 21 | 0.06 | 28 | 0.07 |
| | APFD | -4 | 0.02 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 28 | 0.07 |
| | APFD-24HFX | 3 | 0.00 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | APFD-25HFX | 9 | -0.01 | 23 | 0.06 | 29 | 0.08 | 21 | 0.06 | 27 | 0.07 |

^a MSE: mean signed error; MAE: mean absolute error; RMS: root mean squared error; HFX: percentage of Hartree-Fock exact exchange.

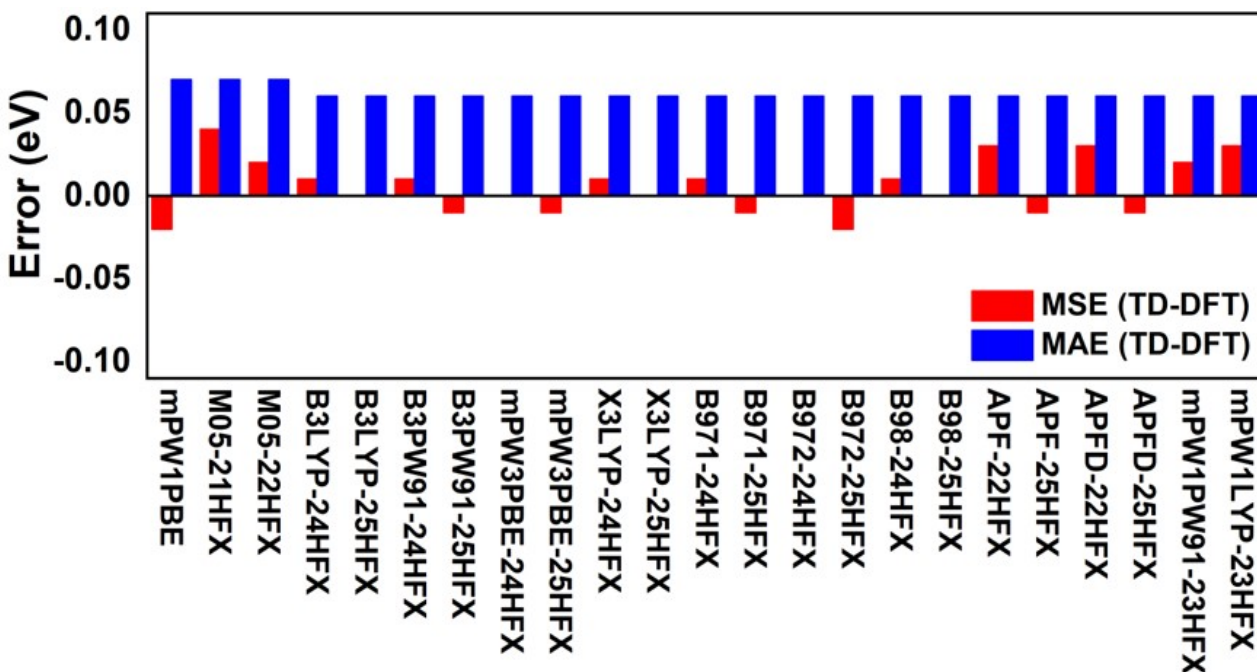


Fig. S5 MAEs and MSEs obtained from experimental data and that calculated with PCM-TD/6-31G(d,p) using new version of functionals with the best performing HFX ratio.

Table S26 Statistical analysis of transition wavelengths and energies using actual theoretical data for excited states of all FREAs^a

| Functional Used | With various HFX (%) | without fit | | | | | | with linear fit | | | |
|-----------------|----------------------|-------------|-------|-----|------|-----|------|-----------------|------|-----|------|
| | | MSE | | MAE | | RMS | | MAE | | RMS | |
| | | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| PBE0 | PBE0-20HFX | -21 | 0.06 | 30 | 0.08 | 36 | 0.11 | 22 | 0.06 | 28 | 0.08 |
| | PBE0-21HFX | -15 | 0.05 | 26 | 0.07 | 32 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | PBE0-22HFX | -8 | 0.03 | 23 | 0.06 | 29 | 0.09 | 22 | 0.06 | 28 | 0.08 |
| | PBE0-23HFX | -2 | 0.01 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 28 | 0.07 |
| | PBE0-24HFX | 4 | 0.00 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | PBE0 | 10 | -0.02 | 23 | 0.07 | 29 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| mPW1PW91 | mPW1PW91-20HFX | -22 | 0.06 | 30 | 0.08 | 36 | 0.11 | 22 | 0.06 | 29 | 0.08 |
| | mPW1PW91-21HFX | -16 | 0.05 | 26 | 0.07 | 32 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | mPW1PW91-22HFX | -9 | 0.03 | 23 | 0.06 | 30 | 0.09 | 22 | 0.06 | 28 | 0.08 |
| | mPW1PW91-23HFX | -3 | 0.02 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 28 | 0.07 |
| | mPW1PW91-24HFX | 3 | 0.00 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | mPW1PW91 | 9 | -0.02 | 23 | 0.06 | 29 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| mPW1LYP | mPW1LYP-20HFX | -27 | 0.07 | 33 | 0.09 | 39 | 0.12 | 23 | 0.06 | 29 | 0.08 |
| | mPW1LYP-21HFX | -20 | 0.06 | 29 | 0.08 | 35 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | mPW1LYP-22HFX | -14 | 0.04 | 25 | 0.07 | 31 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | mPW1LYP-23HFX | -7 | 0.03 | 22 | 0.06 | 29 | 0.09 | 21 | 0.06 | 28 | 0.08 |
| | mPW1LYP-24HFX | -1 | 0.01 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 28 | 0.07 |
| | mPW1LYP | 5 | 0.00 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| mPW1PBE | mPW1PBE-20HFX | -22 | 0.06 | 30 | 0.08 | 36 | 0.11 | 22 | 0.06 | 29 | 0.08 |
| | mPW1PBE-21HFX | -15 | 0.05 | 26 | 0.07 | 32 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | mPW1PBE-22HFX | -9 | 0.03 | 23 | 0.06 | 29 | 0.09 | 22 | 0.06 | 28 | 0.08 |
| | mPW1PBE-23HFX | -3 | 0.02 | 21 | 0.06 | 28 | 0.08 | 21 | 0.06 | 28 | 0.07 |
| | mPW1PBE-24HFX | 3 | 0.00 | 22 | 0.06 | 28 | 0.08 | 21 | 0.06 | 27 | 0.07 |
| | mPW1PBE | 9 | -0.02 | 23 | 0.07 | 29 | 0.08 | 21 | 0.06 | 27 | 0.07 |

^a MSE: mean signed error; MAE: mean absolute error; RMS: root mean squared error; HFX: percentage of Hartree-Fock exact exchange.

Table S27 Statistical analysis of transition wavelengths and energies using actual theoretical data for excited states of all FREAs^a

| Functional Used | With various HFX (%) | without fit | | | | | | with linear fit | | | |
|-----------------|----------------------|-------------|-------|-----|------|-----|------|-----------------|------|-----|------|
| | | MSE | | MAE | | RMS | | MAE | | RMS | |
| | | nm | eV | nm | eV | nm | eV | nm | eV | nm | eV |
| M05 | M05-20HFX | -19 | 0.06 | 29 | 0.08 | 36 | 0.11 | 24 | 0.07 | 30 | 0.08 |
| | M05-21HFX | -12 | 0.04 | 25 | 0.07 | 33 | 0.10 | 24 | 0.07 | 30 | 0.08 |
| | M05-22HFX | -6 | 0.02 | 23 | 0.07 | 31 | 0.10 | 23 | 0.07 | 30 | 0.08 |
| | M05-23HFX | 1 | 0.01 | 23 | 0.07 | 30 | 0.09 | 23 | 0.07 | 29 | 0.08 |
| | M05-24HFX | 7 | -0.01 | 25 | 0.07 | 31 | 0.09 | 23 | 0.07 | 29 | 0.08 |
| | M05-25HFX | 13 | -0.02 | 27 | 0.08 | 33 | 0.09 | 23 | 0.07 | 29 | 0.08 |
| | M05-26HFX | 18 | -0.04 | 30 | 0.08 | 35 | 0.10 | 23 | 0.06 | 29 | 0.08 |
| | M05 | 29 | -0.07 | 36 | 0.10 | 42 | 0.11 | 23 | 0.06 | 29 | 0.08 |
| M06 | M06-20HFX | -30 | 0.08 | 36 | 0.10 | 42 | 0.12 | 23 | 0.06 | 29 | 0.08 |
| | M06-21HFX | -23 | 0.07 | 31 | 0.08 | 37 | 0.11 | 23 | 0.06 | 29 | 0.08 |
| | M06-22HFX | -16 | 0.05 | 26 | 0.07 | 33 | 0.10 | 22 | 0.06 | 29 | 0.08 |
| | M06-23HFX | -10 | 0.03 | 23 | 0.07 | 30 | 0.10 | 22 | 0.06 | 28 | 0.08 |
| | M06-24HFX | -4 | 0.02 | 21 | 0.06 | 29 | 0.09 | 22 | 0.06 | 28 | 0.08 |
| | M06-25HFX | 2 | 0.00 | 22 | 0.06 | 29 | 0.09 | 22 | 0.06 | 28 | 0.08 |
| | M06-26HFX | 8 | -0.01 | 24 | 0.07 | 30 | 0.09 | 21 | 0.06 | 28 | 0.08 |
| | M06 | 13 | -0.03 | 26 | 0.07 | 31 | 0.09 | 21 | 0.06 | 28 | 0.07 |

^a MSE: mean signed error; MAE: mean absolute error; RMS: root mean squared error; HFX: percentage of Hartree-Fock exact exchange.

Cartesian Coordinates

Below are the cartesian coordinates for all the studied set of FREAs optimized in chloroform solvent using DFT-PBE0/6-31G(d,p) and PCM solvent model. All data is in Å. These cartesian coordinates have been taken from our previous study.¹

Cz-RH

```
0 1
C -1.10965700 -2.20947800 0.12249400
C -0.70982400 -3.56983600 0.08260400
C 0.71252000 -3.57044500 -0.11732300
C 1.10952100 -2.21043300 -0.18593600
N -0.00325700 -1.40518500 -0.05647400
C 1.67983900 -4.57176000 -0.24160800
C 3.00344100 -4.21529300 -0.42532000
C 3.39690600 -2.85774900 -0.49287600
C 2.43867900 -1.84428600 -0.36971700
C -2.43521800 -1.84226000 0.32923100
C -3.39062900 -2.85497100 0.47797300
C -2.99674300 -4.21287000 0.42311500
C -1.67443100 -4.57035100 0.23198000
C -0.00045600 0.03695400 -0.04118100
C 4.80662600 -2.53026000 -0.68733500
C -4.79647000 -2.52529000 0.69522300
S 5.45359400 -1.01113700 -0.16562700
C 7.04724900 -1.41694300 -0.75113500
C 7.03393200 -2.69269000 -1.30812700
C 5.78321500 -3.31805200 -1.27310900
C -5.76147600 -3.30386300 1.31165900
C -7.01103200 -2.67717100 1.36217600
C -7.03497700 -1.40988100 0.78645400
S -5.45335900 -1.01422800 0.16278700
C 8.24364100 -0.64306300 -0.70779500
C -8.23134400 -0.63525200 0.75676300
C 8.54283700 0.60108200 -0.24155000
C -8.53926000 0.60182300 0.27759000
C 7.65131300 1.56776800 0.39103800
N 8.35404900 2.73321100 0.72634900
C 9.67957100 2.77433200 0.41077000
S 10.16662800 1.27685100 -0.34974000
S -10.15932400 1.28199200 0.41124200
C -9.68811500 2.76521500 -0.38626000
N -8.37020600 2.71656100 -0.73128700
C -7.66114000 1.55639900 -0.39116200
O -6.47543900 1.42023500 -0.64630900
O 6.46011700 1.43695200 0.62223500
C -7.67607600 3.81641000 -1.39631500
C 7.64619100 3.84605800 1.35423500
C 7.06954300 4.80642400 0.32726300
C -7.07341400 4.79467100 -0.40169700
S -10.74307200 4.00752700 -0.65707600
S 10.73011400 4.01976500 0.68440300
H 1.40032500 -5.61956500 -0.18306200
H 3.76070300 -4.98936000 -0.48972200
H 2.72927500 -0.80046200 -0.43622000
H -2.72331900 -0.79861500 0.40715400
H -3.75205100 -4.98667100 0.50980300
H -1.39318300 -5.61856300 0.19181300
H -0.94891300 0.40877400 -0.43312200
H 0.14908800 0.43420200 0.96860800
H 0.79456500 0.40879400 -0.69018900
H 7.92435700 -3.13929400 -1.73789800
H 5.58695600 -4.29896100 -1.68917200
H -5.55714600 -4.27842400 1.73865600
H -7.89274500 -3.11640400 1.81679000
H 9.08106700 -1.18497900 -1.14657100
H -9.05966800 -1.16913400 1.22191800
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| | | | |
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| H | -6.90040900 | 3.35478200 | -2.01085600 |
| H | -8.40431900 | 4.30660800 | -2.04538300 |
| H | 6.85503700 | 3.39705500 | 1.95827800 |
| H | 8.35943700 | 4.34731300 | 2.01144500 |
| H | 6.54415300 | 5.61745000 | 0.83904700 |
| H | 7.86161400 | 5.24429100 | -0.28559500 |
| H | 6.35675800 | 4.29499400 | -0.32492600 |
| H | -6.55958800 | 5.59505200 | -0.94122300 |
| H | -7.84972700 | 5.24532500 | 0.22199600 |
| H | -6.34561600 | 4.29424500 | 0.24237900 |

Flu-RH

| | | | |
|-----|--------------|-------------|-------------|
| 0 1 | | | |
| C | -1.17353200 | -2.01317500 | -0.01464600 |
| C | -0.72823000 | -0.67892900 | -0.00992100 |
| C | 0.72822400 | -0.67892700 | 0.00952100 |
| C | 1.17352300 | -2.01317400 | 0.01461800 |
| C | -0.00000600 | -2.97990300 | 0.00012700 |
| C | 1.65003500 | 0.36735000 | 0.02307800 |
| C | 3.00448600 | 0.06957100 | 0.03968700 |
| C | 3.46843800 | -1.26007600 | 0.04296400 |
| C | 2.52349300 | -2.30523100 | 0.03062000 |
| C | -2.52350300 | -2.30523400 | -0.03056200 |
| C | -3.46844500 | -1.26008000 | -0.04320700 |
| C | -3.00449000 | 0.06956800 | -0.04030200 |
| C | -1.65003900 | 0.36734700 | -0.02376800 |
| C | -0.01557300 | -3.85819600 | 1.25962300 |
| C | 0.01555800 | -3.85856100 | -1.25911600 |
| C | 4.89706600 | -1.56039800 | 0.05890100 |
| C | -4.89707300 | -1.56040200 | -0.05906700 |
| S | 6.08134500 | -0.29322000 | 0.06192400 |
| C | 7.40064400 | -1.43396000 | 0.08268800 |
| C | 6.90045600 | -2.73273700 | 0.08571200 |
| C | 5.50477200 | -2.80630900 | 0.07242700 |
| C | -5.50477700 | -2.80631300 | -0.07261100 |
| C | -6.90046300 | -2.73274400 | -0.08580600 |
| C | -7.40065200 | -1.43396800 | -0.08269800 |
| S | -6.08135400 | -0.29322700 | -0.06195300 |
| C | 8.80364500 | -1.18268900 | 0.09723200 |
| C | -8.80365400 | -1.18269700 | -0.09715300 |
| C | 9.55707300 | -0.04809000 | 0.10163600 |
| C | -9.55708200 | -0.04809700 | -0.10148000 |
| C | 9.10322500 | 1.33915200 | 0.08903900 |
| N | 10.19995300 | 2.21168600 | 0.11156700 |
| C | 11.44220600 | 1.65104600 | 0.12519500 |
| S | 11.31837500 | -0.09341700 | 0.12488700 |
| S | -11.31838600 | -0.09342000 | -0.12463600 |
| C | -11.44221300 | 1.65104400 | -0.12486600 |
| N | -10.19995800 | 2.21168000 | -0.11139400 |
| C | -9.10323000 | 1.33914500 | -0.08889300 |
| O | 7.95173400 | 1.74204200 | 0.06484400 |
| S | 12.89219700 | 2.44250300 | 0.14634600 |
| C | 9.97330200 | 3.65461100 | 0.08739500 |
| C | 9.91799700 | 4.20027900 | -1.32974800 |
| S | -12.89219900 | 2.44250400 | -0.14625700 |
| O | -7.95173600 | 1.74203200 | -0.06480600 |
| C | -9.97330200 | 3.65460800 | -0.08737600 |
| C | -9.91786700 | 4.20040400 | 1.32971300 |
| H | 1.32356400 | 1.40313900 | 0.02150800 |
| H | 3.71785700 | 0.88891700 | 0.05081400 |
| H | 2.85454600 | -3.33942900 | 0.03300700 |
| H | -2.85456000 | -3.33943100 | -0.03262600 |
| H | -3.71786000 | 0.88891100 | -0.05168500 |
| H | -1.32356400 | 1.40313600 | -0.02249000 |
| H | -0.90053300 | -4.50249000 | 1.26687300 |
| H | 0.86897500 | -4.50240500 | 1.28878700 |
| H | -0.02683500 | -3.24713300 | 2.16636400 |
| H | 0.90052200 | -4.50285200 | -1.26618900 |
| H | -0.86898500 | -4.50278600 | -1.28808900 |
| H | 0.02681000 | -3.24775800 | -2.16603300 |
| H | 7.55322900 | -3.59924300 | 0.09806800 |
| H | 4.96073200 | -3.74267700 | 0.07346400 |
| H | -4.96073400 | -3.74268000 | -0.07374900 |
| H | -7.55323400 | -3.59925100 | -0.09817400 |
| H | 9.37091200 | -2.11284500 | 0.10880600 |
| H | -9.37092300 | -2.11285200 | -0.10872200 |
| H | 9.02739400 | 3.81878200 | 0.60769300 |
| H | 10.78217900 | 4.11376900 | 0.65909500 |

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| H | 9.74043700 | 5.27881700 | -1.29925000 |
| H | 10.86083000 | 4.02300700 | -1.85358500 |
| H | 9.10483200 | 3.73574400 | -1.89356600 |
| H | -9.02744000 | 3.81872800 | -0.60777300 |
| H | -10.78222800 | 4.11371800 | -0.65904600 |
| H | -9.74031100 | 5.27894000 | 1.29909900 |
| H | -10.86065000 | 4.02317900 | 1.85365300 |
| H | -9.10464800 | 3.73592200 | 1.89349800 |

FR-d2

| | | | |
|-----|--------------|-------------|-------------|
| 0 1 | | | |
| C | -0.72674600 | -2.52718200 | -0.30557000 |
| C | -1.39870900 | -1.30622400 | -0.48530600 |
| C | -0.42614600 | -0.19846700 | -0.85764300 |
| C | 0.89125300 | -0.95735800 | -0.86897000 |
| C | 0.69644500 | -2.31073400 | -0.54329800 |
| C | 2.16103100 | -0.47757500 | -1.13462600 |
| C | 3.26638800 | -1.34720100 | -1.08195000 |
| C | 3.05505600 | -2.69816400 | -0.75246200 |
| C | 1.78120900 | -3.18372400 | -0.48651800 |
| C | -1.43535800 | -3.67375100 | 0.04993000 |
| C | -2.81117300 | -3.58692100 | 0.21366400 |
| C | -3.49992600 | -2.37420300 | 0.02671500 |
| C | -2.77017000 | -1.22349300 | -0.32187100 |
| C | -0.74676800 | 0.38723700 | -2.24050100 |
| C | -0.42209900 | 0.91530000 | 0.19973300 |
| C | 4.61006000 | -0.83645800 | -1.40271900 |
| C | -7.88049500 | -2.35434900 | 0.40620300 |
| C | 4.80234200 | 0.13774700 | -2.36310400 |
| C | 6.06791100 | 0.67607800 | -2.68447100 |
| C | 7.23647900 | 0.26462000 | -2.07391700 |
| C | 7.10285300 | -0.76029100 | -1.08239000 |
| C | 5.80001600 | -1.29968300 | -0.74882800 |
| C | -7.11707800 | -1.21470200 | 0.81881100 |
| C | -5.67361800 | -1.20979000 | 0.69425600 |
| C | -4.96515500 | -2.34171300 | 0.16932100 |
| C | -5.75160500 | -3.41915500 | -0.19059300 |
| C | -7.15920900 | -3.42783600 | -0.07802200 |
| N | 8.09905300 | -1.32417900 | -0.39880000 |
| S | 7.42201900 | -2.41615100 | 0.59317800 |
| N | 5.85607200 | -2.23836400 | 0.20006400 |
| N | -7.60389200 | -0.10403600 | 1.37382800 |
| S | -6.33150200 | 0.85391500 | 1.68781500 |
| N | -5.11799700 | -0.08528500 | 1.15467400 |
| C | -9.32337500 | -2.42027700 | 0.49539000 |
| C | 10.59014200 | 1.44092200 | -2.16896100 |
| C | 10.25324300 | 1.78710900 | -3.46649700 |
| C | 8.91428800 | 1.41022100 | -3.65171600 |
| C | 8.50724300 | 0.83878500 | -2.46215600 |
| O | 9.51908600 | 0.86058300 | -1.56848700 |
| O | -10.03281200 | -1.27472300 | 0.42532700 |
| C | -11.34834500 | -1.59375700 | 0.52550000 |
| C | -11.47516600 | -2.96491500 | 0.66994400 |
| C | -10.17639700 | -3.49672200 | 0.64012000 |
| C | 11.85061400 | 1.61307000 | -1.53876700 |
| C | 12.29420800 | 1.42895500 | -0.26536000 |
| C | -12.38883100 | -0.62817000 | 0.50945100 |
| C | -12.41183100 | 0.70792400 | 0.25098100 |
| S | -13.89413000 | 1.64265800 | 0.44381600 |
| C | -13.12196700 | 3.13113200 | -0.05342200 |
| N | -11.82038800 | 2.90211800 | -0.36971700 |
| C | -11.33826800 | 1.58266700 | -0.24494800 |
| S | 13.99903200 | 1.63371400 | 0.13563200 |
| C | 13.73727800 | 1.24866000 | 1.82156100 |
| N | 12.42085000 | 0.99753300 | 2.04682300 |
| C | 11.53768900 | 1.10448000 | 0.95318200 |
| O | 10.33877000 | 0.96820000 | 1.08319400 |
| O | -10.20378500 | 1.28362400 | -0.55554700 |
| S | -13.92928900 | 4.57294100 | -0.11165900 |
| S | 14.96793900 | 1.21038500 | 2.92488200 |
| C | -10.91027000 | 3.95212400 | -0.81782200 |
| C | 11.88186300 | 0.69034500 | 3.36872500 |
| C | 11.48963000 | 1.94510600 | 4.13112200 |
| C | -10.16954300 | 4.59476500 | 0.34313200 |
| H | 2.31623400 | 0.57576100 | -1.35458300 |
| H | 3.90305600 | -3.37131700 | -0.71102100 |

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| H | 1.64215900 | -4.23271300 | -0.24053800 |
| H | -0.92678300 | -4.62025100 | 0.20980500 |
| H | -3.36453400 | -4.46901300 | 0.52151800 |
| H | -3.29001400 | -0.28219300 | -0.46428700 |
| H | -0.00204000 | 1.13941000 | -2.52042300 |
| H | -0.75374500 | -0.39248300 | -3.00736700 |
| H | -1.72836000 | 0.87184700 | -2.23312000 |
| H | -1.40105600 | 1.40295400 | 0.24579000 |
| H | -0.19052200 | 0.51628900 | 1.19115600 |
| H | 0.32392100 | 1.67725100 | -0.04818300 |
| H | 3.94256400 | 0.50732500 | -2.91286200 |
| H | 6.11349000 | 1.45847700 | -3.43583000 |
| H | -5.27594600 | -4.29360900 | -0.62310600 |
| H | -7.69359900 | -4.30635200 | -0.42633100 |
| H | 10.91386900 | 2.25125100 | -4.18552400 |
| H | 8.32200300 | 1.50575900 | -4.54989900 |
| H | -12.40590600 | -3.50238900 | 0.78683900 |
| H | -9.88654000 | -4.53187500 | 0.74607100 |
| H | 12.59666400 | 1.95548300 | -2.25378200 |
| H | -13.34538900 | -1.07950500 | 0.76661100 |
| H | -10.21409600 | 3.47231400 | -1.50882700 |
| H | -11.51001400 | 4.68467600 | -1.36130200 |
| H | 11.01413500 | 0.04979800 | 3.19847100 |
| H | 12.64848000 | 0.12455300 | 3.90192900 |
| H | 11.08760500 | 1.66853400 | 5.10974700 |
| H | 12.35566900 | 2.59342300 | 4.28728700 |
| H | 10.72032700 | 2.50208800 | 3.59007500 |
| H | -9.49579500 | 5.36875500 | -0.03485900 |
| H | -10.86904000 | 5.06070500 | 1.04215400 |
| H | -9.57183100 | 3.85309900 | 0.87978900 |

F(DPP)2B2

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|-----|--------------|-------------|-------------|
| 0 1 | | | |
| C | -1.11560800 | -1.79419100 | -0.15507400 |
| C | -0.52656100 | -0.61462100 | -0.64522300 |
| C | 0.92201600 | -0.77371800 | -0.61134100 |
| C | 1.21758900 | -2.04969100 | -0.09853300 |
| C | -0.05496500 | -2.80795000 | 0.24348500 |
| C | 1.95075300 | 0.09202800 | -0.98012600 |
| C | 3.26600800 | -0.32716200 | -0.83730000 |
| C | 3.57735800 | -1.59944700 | -0.32326700 |
| C | 2.52859800 | -2.46114700 | 0.05084000 |
| C | -2.48997300 | -1.91202800 | -0.07068500 |
| C | -3.30854400 | -0.84446600 | -0.48665200 |
| C | -2.70498400 | 0.32884600 | -0.97520400 |
| C | -1.32496400 | 0.45262400 | -1.05437100 |
| C | -0.12656700 | -3.12881600 | 1.74361800 |
| C | -0.17598400 | -4.09782900 | -0.58056300 |
| C | 4.96297200 | -2.03369500 | -0.17449900 |
| C | -4.75984900 | -0.97131500 | -0.40720000 |
| S | 6.25198200 | -0.88816900 | -0.03299800 |
| C | 7.45511900 | -2.14694200 | 0.09401400 |
| C | 6.84498100 | -3.39165100 | 0.02263500 |
| C | 5.45052600 | -3.32533200 | -0.12862900 |
| C | -5.51975200 | -2.12572200 | -0.38960700 |
| C | -6.90077900 | -1.89280800 | -0.30701500 |
| C | -7.22943900 | -0.54519800 | -0.25743200 |
| S | -5.78019400 | 0.42511200 | -0.30657100 |
| C | 8.84046900 | -1.79942000 | 0.23184400 |
| C | -8.56851500 | -0.04409400 | -0.17453000 |
| N | -8.93911300 | 1.28714700 | -0.11095100 |
| C | -10.35341600 | 1.43878100 | -0.03394000 |
| C | -10.85101700 | 0.08540500 | -0.06168800 |
| C | -9.74272900 | -0.79369300 | -0.14244000 |
| C | 9.45408900 | -0.56255300 | 0.06828100 |
| C | 10.84729500 | -0.70191200 | 0.28594400 |
| C | 11.11732300 | -2.07577300 | 0.61804500 |
| N | 9.84267000 | -2.70064400 | 0.56498200 |
| C | 9.18675700 | 0.80897700 | -0.28830800 |
| N | 10.47114000 | 1.42495000 | -0.27260400 |
| C | 11.46636500 | 0.52734400 | 0.07004600 |
| C | -12.02592800 | -0.65818800 | -0.07462700 |
| N | -11.65130900 | -1.99308500 | -0.14866600 |
| C | -10.23927400 | -2.14298100 | -0.19178500 |
| O | 12.14199000 | -2.68762200 | 0.91084000 |

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| O | 8.16093100 | 1.42434200 | -0.54929100 |
| C | 12.86535800 | 0.81770000 | 0.17597000 |
| C | 13.82990800 | -0.10636700 | 0.55154700 |
| C | 15.12920400 | 0.42471500 | 0.57486900 |
| C | 15.19112400 | 1.75814000 | 0.22137500 |
| S | 13.61211100 | 2.35887900 | -0.15731100 |
| O | -10.89814700 | 2.53233900 | 0.04639900 |
| O | -9.69218400 | -3.24213500 | -0.24691500 |
| C | -8.09282800 | 2.45619800 | -0.09575800 |
| C | -12.48675000 | -3.16885400 | -0.10226000 |
| C | 9.71857100 | -4.09025800 | 0.93395300 |
| C | 10.59228800 | 2.83312900 | -0.56509600 |
| C | -13.38611400 | -0.20201300 | -0.02800900 |
| S | -13.73027600 | 1.47010600 | 0.33986000 |
| C | -15.43624300 | 1.22502200 | 0.19955600 |
| C | -15.71772900 | -0.08753700 | -0.12068700 |
| C | -14.57136000 | -0.88955400 | -0.24821500 |
| C | 16.36818500 | 2.62117100 | 0.14416100 |
| C | -16.37933100 | 2.32323000 | 0.40598600 |
| C | 16.26582600 | 4.01452900 | 0.27442100 |
| C | 17.39663400 | 4.81855600 | 0.20210600 |
| C | 18.65238600 | 4.24826200 | 0.00628400 |
| C | 18.76710400 | 2.86533900 | -0.12295100 |
| C | 17.63819700 | 2.05861400 | -0.06031800 |
| C | -16.0005400 | 3.66020300 | 0.21235400 |
| C | -16.91049800 | 4.69092100 | 0.41116500 |
| C | -18.21803900 | 4.40832800 | 0.79966300 |
| C | -18.60679400 | 3.08417500 | 0.99431500 |
| C | -17.69746200 | 2.05138900 | 0.80522400 |
| H | 1.73693900 | 1.07804400 | -1.38242700 |
| H | 4.06979800 | 0.33470300 | -1.14780800 |
| H | 2.75657500 | -3.43466900 | 0.47654900 |
| H | -2.94299000 | -2.81190600 | 0.33616500 |
| H | -3.33066300 | 1.14831000 | -1.31820700 |
| H | -0.88360300 | 1.36750700 | -1.43883800 |
| H | -1.07690700 | -3.61437900 | 1.98724700 |
| H | 0.68199200 | -3.80944600 | 2.02879300 |
| H | -0.03976800 | -2.21996400 | 2.34542900 |
| H | -1.12570800 | -4.60013700 | -0.37026000 |
| H | -0.12800400 | -3.88702700 | -1.65252200 |
| H | 0.63368700 | -4.79021200 | -0.32865300 |
| H | 7.38336800 | -4.32804100 | 0.04303400 |
| H | 4.82169000 | -4.20132300 | -0.23660600 |
| H | -5.08588300 | -3.11594900 | -0.46493500 |
| H | -7.66372800 | -2.66675500 | -0.29383600 |
| H | 13.57105900 | -1.13142700 | 0.80320200 |
| H | 16.00182000 | -0.14488700 | 0.87249200 |
| H | -8.76347600 | 3.31441300 | -0.02641700 |
| H | -7.42486200 | 2.45859800 | 0.77018100 |
| H | -7.50616800 | 2.53950400 | -1.01493600 |
| H | -13.17700900 | -3.12717600 | 0.74376000 |
| H | -13.04756200 | -3.30626000 | -1.03184600 |
| H | -11.81274200 | -4.01773800 | 0.02142200 |
| H | 10.68470600 | -4.38488600 | 1.34625100 |
| H | 8.94299100 | -4.22702600 | 1.69127200 |
| H | 9.50609100 | -4.72428000 | 0.06756200 |
| H | 11.20210600 | 3.00821500 | -1.45591700 |
| H | 9.57902900 | 3.19072700 | -0.75623900 |
| H | 11.00918200 | 3.38482400 | 0.28212500 |
| H | -16.72326300 | -0.45392500 | -0.29166300 |
| H | -14.62055600 | -1.93227800 | -0.52570900 |
| H | 15.29582300 | 4.47010700 | 0.45525200 |
| H | 17.29689400 | 5.89459900 | 0.30881100 |
| H | 19.53587400 | 4.87716800 | -0.04701200 |
| H | 19.74073400 | 2.41211900 | -0.28420700 |
| H | 17.73597800 | 0.98534000 | -0.19161500 |
| H | -14.99037300 | 3.89297600 | -0.11542500 |
| H | -16.59846600 | 5.71896500 | 0.25313800 |
| H | -18.92914000 | 5.21459800 | 0.95218100 |
| H | -19.62149700 | 2.85443200 | 1.30589400 |
| H | -18.00208500 | 1.02552000 | 0.98885500 |

ITDI

| | | | |
|-----|------------|-------------|-------------|
| O 1 | | | |
| C | 1.06458400 | -2.12073000 | -0.18799300 |
| C | 1.81095000 | -0.96015400 | 0.12297100 |
| C | 3.20104300 | -1.33576400 | 0.04759000 |

| | | | |
|---|--------------|-------------|-------------|
| C | 3.33504300 | -2.66796100 | -0.29432700 |
| C | 1.97702100 | -3.30869500 | -0.48375400 |
| C | -0.31393500 | -2.07455100 | -0.20574900 |
| C | -0.97966100 | -0.86935800 | 0.09897100 |
| C | -0.21936100 | 0.27304800 | 0.40742100 |
| C | 1.16786600 | 0.24042900 | 0.41879400 |
| S | 4.71343900 | -0.56299400 | 0.28048200 |
| C | 5.56042900 | -2.05045100 | -0.09631700 |
| C | 4.67332700 | -3.08094400 | -0.37892600 |
| C | 1.78784000 | -3.81525700 | -1.92108200 |
| C | 1.74962600 | -4.44932700 | 0.51925300 |
| C | 6.99368800 | -2.12234300 | -0.09154900 |
| C | 7.77640200 | -3.27303400 | -0.14825400 |
| C | 9.14287300 | -3.00058600 | -0.15142600 |
| C | 9.45397100 | -1.64344300 | -0.06174200 |
| S | 7.98478700 | -0.70490700 | -0.02750600 |
| C | -2.43687700 | -0.82684200 | 0.09614700 |
| S | -3.29768000 | 0.66511700 | -0.11407900 |
| C | -4.84363800 | -0.12281200 | 0.01904400 |
| C | -4.67292800 | -1.48242100 | 0.20397800 |
| C | -3.32389200 | -1.87580300 | 0.24601600 |
| C | -8.45851600 | 1.34481300 | -0.14250300 |
| C | -7.54068800 | 2.39641800 | -0.25311800 |
| C | -6.20841200 | 2.00270200 | -0.21007000 |
| C | -6.06564800 | 0.62507000 | -0.06495800 |
| S | -7.60175400 | -0.17377700 | 0.01434100 |
| C | 10.76907200 | -1.12921000 | -0.15442500 |
| C | -9.84803700 | 1.60632400 | -0.16410900 |
| C | 11.30869700 | 0.12832400 | -0.06534500 |
| C | -10.96931500 | 0.81358200 | -0.07130600 |
| C | 12.61189100 | 0.36638600 | -0.75152400 |
| C | 12.72484600 | 1.83470800 | -0.90209100 |
| C | 11.64024700 | 2.45355400 | -0.25640300 |
| C | 10.83966200 | 1.40983700 | 0.41847900 |
| C | -12.35642400 | 1.26125900 | -0.10451100 |
| C | -13.21184100 | 0.06152700 | 0.04142000 |
| C | -12.38905100 | -1.06904800 | 0.15409500 |
| C | -10.97517800 | -0.65288800 | 0.08777400 |
| C | 9.99871400 | 1.62076200 | 1.49275800 |
| C | -12.83583400 | 2.54923000 | -0.24375300 |
| O | 13.38999600 | -0.47841300 | -1.15602300 |
| O | -10.00683500 | -1.39584700 | 0.15407100 |
| C | 13.69334500 | 2.56119100 | -1.57459000 |
| C | 13.55997800 | 3.94783700 | -1.61666500 |
| C | 12.47664400 | 4.57179500 | -0.99349600 |
| C | 11.51070900 | 3.84033200 | -0.30166900 |
| C | -14.59735000 | -0.10034800 | 0.08284600 |
| C | -15.11203900 | -1.38789700 | 0.23556200 |
| C | -14.27869000 | -2.50314800 | 0.34569000 |
| C | -12.89485000 | -2.34897400 | 0.30503400 |
| C | 9.59447700 | 0.56546400 | 2.35824100 |
| N | 9.29844600 | -0.26612800 | 3.11607800 |
| C | 9.60129600 | 2.91736600 | 1.92603400 |
| N | 9.24584600 | 3.96183600 | 2.29550600 |
| C | -14.22195400 | 2.87609700 | -0.26459400 |
| N | -15.33862700 | 3.20262900 | -0.28878200 |
| C | -12.01420000 | 3.70403100 | -0.38354200 |
| N | -11.38783400 | 4.67821900 | -0.50053200 |
| H | -0.89022500 | -2.95520500 | -0.47467700 |
| H | -0.72616900 | 1.19885200 | 0.66478700 |
| H | 1.73356300 | 1.13374800 | 0.66474000 |
| H | 5.00298900 | -4.07799100 | -0.64774200 |
| H | 0.77843600 | -4.21631300 | -2.05573700 |
| H | 1.93965200 | -3.01099400 | -2.64593000 |
| H | 2.50045500 | -4.61688000 | -2.13905100 |
| H | 2.45802900 | -5.26344800 | 0.33655500 |
| H | 1.87986200 | -4.10209200 | 1.54773900 |
| H | 0.73778900 | -4.85343100 | 0.41619900 |
| H | 7.35639600 | -4.27074000 | -0.17717100 |
| H | 9.91428500 | -3.76098300 | -0.20597900 |
| H | -5.50246000 | -2.17135600 | 0.32104200 |
| H | -3.00551100 | -2.89761200 | 0.41498900 |
| H | -7.86689600 | 3.42555700 | -0.35941800 |
| H | -5.37062200 | 2.68736800 | -0.27675900 |
| H | 11.49853600 | -1.87249300 | -0.48250700 |
| H | -10.02618500 | 2.67142400 | -0.27628800 |
| H | 14.52433700 | 2.05177500 | -2.05232600 |
| H | 14.29761600 | 4.54916000 | -2.13881200 |
| H | 12.38117200 | 5.65190800 | -1.04639100 |
| H | 10.68112300 | 4.35384700 | 0.16850400 |

| | | | |
|---|--------------|-------------|------------|
| H | -15.27935800 | 0.73564100 | 0.00141700 |
| H | -16.18885600 | -1.52148400 | 0.26908100 |
| H | -14.71417100 | -3.49050400 | 0.46335300 |
| H | -12.22008500 | -3.19517000 | 0.38832600 |

SiDT-IC

| | | | |
|-----|--------------|-------------|-------------|
| 0 1 | | | |
| C | -0.47726400 | 1.33102100 | -0.00018700 |
| C | -1.36881400 | 0.22524300 | -0.00012100 |
| C | -0.89006900 | -1.09257200 | -0.00002600 |
| C | 0.47705900 | -1.33076000 | 0.00000800 |
| C | 1.36861100 | -0.22498200 | -0.00005400 |
| C | 0.88986600 | 1.09283200 | -0.00015400 |
| Si | 1.46006600 | -2.95395300 | 0.00014600 |
| C | 3.07409700 | -1.98785600 | 0.00010000 |
| C | 2.76845500 | -0.62311300 | -0.00000100 |
| Si | -1.46027200 | 2.95421300 | -0.00030000 |
| C | -3.07430400 | 1.98811700 | -0.00023100 |
| C | -2.76865700 | 0.62337400 | -0.00014900 |
| C | -1.19524900 | 3.97094600 | -1.55374700 |
| C | 1.19500700 | -3.97067100 | 1.55359700 |
| C | 1.19507100 | -3.97092600 | -1.55315000 |
| C | -1.19524100 | 3.97116800 | 1.55300100 |
| C | 4.45482900 | -2.18386200 | 0.00013500 |
| C | 5.21362900 | -1.00321100 | 0.00006800 |
| S | 4.15195300 | 0.39535200 | -0.00004200 |
| C | -4.45503600 | 2.18412500 | -0.00022700 |
| C | -5.21382300 | 1.00346500 | -0.00014800 |
| S | -4.15214900 | -0.39509600 | -0.00008300 |
| C | 6.62777500 | -1.06784800 | 0.00008100 |
| C | -6.62796700 | 1.06801400 | -0.00008200 |
| C | 7.62876500 | -0.12449700 | 0.00003700 |
| C | -7.62879500 | 0.12450600 | 0.00000100 |
| C | -9.06497500 | 0.38134100 | 0.00010000 |
| C | -9.74903400 | -0.93151300 | -0.00003000 |
| C | -8.78025700 | -1.94599600 | -0.00011700 |
| C | -7.43562600 | -1.33904800 | -0.00008100 |
| C | 9.06491200 | -0.38157500 | 0.00005200 |
| C | 9.74920400 | 0.93114200 | 0.00006800 |
| C | 8.78062800 | 1.94580600 | 0.00003300 |
| C | 7.43588500 | 1.33910100 | 0.00000300 |
| C | 11.10012400 | 1.28192300 | 0.00010700 |
| C | 11.43524200 | 2.63588500 | 0.00010800 |
| C | 10.45806400 | 3.63386100 | 0.00006900 |
| C | 9.10804100 | 3.29106000 | 0.00003200 |
| C | -11.09988300 | -1.28258500 | -0.00006800 |
| C | -11.43472300 | -2.63661600 | -0.00018400 |
| C | -10.45734600 | -3.63439600 | -0.00025900 |
| C | -9.10739700 | -3.29131700 | -0.00022700 |
| O | -6.37631700 | -1.94811200 | -0.00012800 |
| C | -9.71509000 | 1.59975000 | 0.00033600 |
| O | 6.37670800 | 1.94839100 | -0.00003600 |
| C | 9.71495500 | -1.60002100 | 0.00003300 |
| C | -11.13296300 | 1.73616300 | 0.00042900 |
| N | -12.28356300 | 1.90979800 | 0.00051300 |
| C | -9.05919000 | 2.86401200 | 0.00054800 |
| N | -8.57280200 | 3.92156300 | 0.00072900 |
| C | 11.13283100 | -1.73640000 | 0.00004800 |
| N | 12.28347000 | -1.90977700 | 0.00006600 |
| C | 9.05907700 | -2.86429400 | -0.00001600 |
| N | 8.57288700 | -3.92193600 | -0.00007000 |
| H | -1.59359400 | -1.92272500 | 0.00002400 |
| H | 1.59339000 | 1.92298600 | -0.00020200 |
| H | -1.89043300 | 4.81614700 | -1.58286200 |
| H | -0.17720900 | 4.37268000 | -1.58271500 |
| H | -1.35122500 | 3.36764200 | -2.45236300 |
| H | 1.89017200 | -4.81588700 | 1.58272500 |
| H | 0.17695800 | -4.37238300 | 1.58255600 |
| H | 1.35098600 | -3.36736600 | 2.45221100 |
| H | 1.35104200 | -3.36775700 | -2.45185600 |
| H | 1.89027200 | -4.81611700 | -1.58213000 |
| H | 0.17703900 | -4.37268500 | -1.58206400 |
| H | -0.17719100 | 4.37287900 | 1.58192100 |
| H | -1.89040300 | 4.81639200 | 1.58198400 |
| H | -1.35124300 | 3.36800000 | 2.45170400 |
| H | 4.94197000 | -3.15428300 | 0.00020500 |

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|---|--------------|-------------|-------------|
| H | -4.94218100 | 3.15454500 | -0.00026700 |
| H | 6.95175600 | -2.10412400 | 0.00014100 |
| H | -6.95208000 | 2.10425500 | -0.00010600 |
| H | 11.88908800 | 0.54156200 | 0.00013800 |
| H | 12.48396500 | 2.91644500 | 0.00013900 |
| H | 10.75560300 | 4.67781300 | 0.00007000 |
| H | 8.32463200 | 4.04238900 | 0.00000200 |
| H | -11.88900700 | -0.54240500 | -0.00001600 |
| H | -12.48338900 | -2.91738900 | -0.00021800 |
| H | -10.75467300 | -4.67840800 | -0.00034600 |
| H | -8.32383500 | -4.04248700 | -0.00028800 |

IDIDT-C8

| | | | |
|-----|--------------|-------------|-------------|
| 0 1 | | | |
| C | -4.18491500 | -1.71369200 | -0.02138900 |
| C | -2.83441500 | -1.45841900 | 0.08234400 |
| C | -2.38077300 | -0.19284500 | 0.51190400 |
| C | -3.28832300 | 0.81534600 | 0.83751900 |
| C | -4.64535300 | 0.54887700 | 0.73260300 |
| C | -5.11775200 | -0.70645100 | 0.30599600 |
| C | -1.66816300 | -2.39817600 | -0.21453900 |
| C | -0.48079400 | -1.49101300 | 0.08649000 |
| C | -0.94284000 | -0.25230000 | 0.50653200 |
| C | 0.93697100 | -1.53580800 | 0.07946800 |
| C | 1.48065100 | -0.33181900 | 0.50278000 |
| S | 0.30754700 | 0.86883400 | 0.90480000 |
| C | 2.06162600 | -2.50418300 | -0.26782200 |
| C | 3.28767200 | -1.65719200 | 0.06543100 |
| C | 2.91942900 | -0.36876900 | 0.50900800 |
| C | 4.61790200 | -2.00403000 | -0.03543400 |
| C | 5.61483000 | -1.06789100 | 0.31289700 |
| C | 5.22818100 | 0.21140800 | 0.75281200 |
| C | 3.89211100 | 0.57050800 | 0.85177600 |
| C | -1.72800200 | -3.60996000 | 0.72885200 |
| C | -1.71128200 | -2.86155800 | -1.67726000 |
| C | 2.07389200 | -2.86527600 | -1.76190100 |
| C | 2.04320800 | -3.77784300 | 0.58812900 |
| C | -6.54384400 | -0.97800900 | 0.20187400 |
| C | 7.01852700 | -1.43797900 | 0.21811600 |
| S | -7.69676600 | 0.30608100 | 0.07335800 |
| C | -9.03480400 | -0.81828700 | 0.01663700 |
| C | -8.54952100 | -2.12928300 | 0.08456900 |
| C | -7.16477700 | -2.22259800 | 0.18650700 |
| C | 7.56578300 | -2.71437200 | 0.20641800 |
| C | 8.95720600 | -2.71531200 | 0.08641900 |
| C | 9.51929300 | -1.44161200 | 0.03356500 |
| S | 8.25942600 | -0.23977600 | 0.08663400 |
| C | -10.42559600 | -0.57711900 | -0.08576600 |
| C | 10.89729600 | -1.19967900 | -0.19504300 |
| C | -11.19403300 | 0.56144400 | -0.16062600 |
| C | -12.64799600 | 0.62395500 | -0.25759300 |
| C | -13.02792800 | 2.05449200 | -0.29083200 |
| C | -11.86293400 | 2.83319000 | -0.22746700 |
| C | -10.68581800 | 1.94709600 | -0.14775300 |
| C | 11.67218000 | -0.07124700 | -0.24043700 |
| C | 12.93851000 | -0.13984400 | -1.02789400 |
| C | 13.31762000 | 1.26405400 | -1.30278500 |
| C | 12.42772900 | 2.12563400 | -0.63789100 |
| C | 11.49982500 | 1.30760700 | 0.17112900 |
| O | 13.50538500 | -1.14599200 | -1.41320000 |
| O | -9.52075900 | 2.30998200 | -0.08391500 |
| C | 10.80862600 | 1.74960800 | 1.28024500 |
| C | -13.54660100 | -0.42340000 | -0.31508600 |
| C | -14.26723100 | 2.69161600 | -0.36864500 |
| C | -14.29812200 | 4.08608000 | -0.38100000 |
| C | -13.12840500 | 4.84667600 | -0.31838900 |
| C | -11.88815100 | 4.21742900 | -0.24029800 |
| C | 14.34961400 | 1.73970700 | -2.09472800 |
| C | 14.48161500 | 3.11945700 | -2.23865800 |
| C | 13.59180900 | 3.98441900 | -1.59696200 |
| C | 12.56294200 | 3.50484000 | -0.78599100 |
| C | 10.27373800 | 0.85404900 | 2.24891000 |
| N | 9.87884000 | 0.14948400 | 3.08614200 |
| C | 10.71083000 | 3.12418700 | 1.63856800 |
| N | 10.59858200 | 4.23936500 | 1.95060000 |

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|---|--------------|-------------|-------------|
| C | -14.95687400 | -0.24757400 | -0.41074700 |
| N | -16.11500500 | -0.16580300 | -0.48925200 |
| C | -13.18284100 | -1.80012300 | -0.29016400 |
| N | -12.93928500 | -2.93830200 | -0.27378400 |
| H | -4.53574900 | -2.67847000 | -0.37631500 |
| H | -2.94759000 | 1.78937800 | 1.17499700 |
| H | -5.35644400 | 1.32258800 | 1.00779600 |
| H | 4.90447100 | -2.98589800 | -0.40182100 |
| H | 5.98927300 | 0.92837000 | 1.04767200 |
| H | 3.61761500 | 1.56092200 | 1.20152100 |
| H | -0.89589700 | -4.29215500 | 0.53931900 |
| H | -1.68913900 | -3.29725700 | 1.77573700 |
| H | -2.65720400 | -4.16588700 | 0.56936100 |
| H | -0.89295500 | -3.55474300 | -1.88843600 |
| H | -2.64919800 | -3.38788700 | -1.87995800 |
| H | -1.63653000 | -2.01451600 | -2.36434900 |
| H | 1.19730000 | -3.46162000 | -2.02634700 |
| H | 2.08199300 | -1.96656000 | -2.38445900 |
| H | 2.96356000 | -3.45676700 | -1.99950900 |
| H | 1.17825600 | -4.39925400 | 0.34270300 |
| H | 2.94171100 | -4.37289100 | 0.39757800 |
| H | 2.00867500 | -3.53829400 | 1.65422600 |
| H | -9.21788800 | -2.98395400 | 0.07084000 |
| H | -6.62884300 | -3.15936500 | 0.27907100 |
| H | 6.96901500 | -3.61287500 | 0.30376800 |
| H | 9.56564300 | -3.61248200 | 0.05093700 |
| H | -10.96663300 | -1.51822800 | -0.10464400 |
| H | 11.44163100 | -2.08977200 | -0.51723400 |
| H | -15.19733500 | 2.14113800 | -0.41843300 |
| H | -15.25844200 | 4.58880200 | -0.44093800 |
| H | -13.19024500 | 5.93036900 | -0.33039400 |
| H | -10.96104200 | 4.77974000 | -0.18982300 |
| H | 15.02579200 | 1.04626200 | -2.58481800 |
| H | 15.27609000 | 3.52799200 | -2.85527300 |
| H | 13.70100600 | 5.05627900 | -1.73004700 |
| H | 11.88767300 | 4.20158000 | -0.30481000 |

IDT-BOC6

| | | | |
|-----|-------------|-------------|-------------|
| 0 1 | | | |
| C | 1.31905400 | 0.40432100 | -0.01575300 |
| C | 0.99366000 | -0.97305400 | -0.00191800 |
| C | -0.32739900 | -1.38512800 | -0.00803700 |
| C | -1.31851200 | -0.39878600 | -0.02117500 |
| C | -0.99291500 | 0.97842400 | -0.03583900 |
| C | 0.32802300 | 1.39070000 | -0.02826400 |
| C | -2.76023100 | -0.48373800 | -0.00810300 |
| C | -3.32835000 | 0.77192500 | 0.00080800 |
| C | -2.25752700 | 1.85113100 | -0.03456100 |
| C | 2.76077000 | 0.48956700 | -0.01580100 |
| C | 3.32919800 | -0.76580000 | -0.02068000 |
| C | 2.25884500 | -1.84543500 | -0.00514200 |
| S | -3.93107900 | -1.73326700 | -0.04745800 |
| C | -5.23806400 | -0.55555100 | -0.01485100 |
| C | -4.73059000 | 0.73721200 | -0.00683000 |
| S | 3.93140400 | 1.73957100 | -0.04479400 |
| C | 5.23853800 | 0.56192900 | -0.02832300 |
| C | 4.73143500 | -0.73095400 | -0.02313800 |
| C | -1.50639700 | 4.74295200 | 2.36194300 |
| C | -1.59670800 | 3.97364000 | 1.20763300 |
| C | -2.24158400 | 2.73219700 | 1.21924500 |
| C | -2.78642600 | 2.28919500 | 2.42577600 |
| C | -2.69529800 | 3.06392000 | 3.57875300 |
| C | -2.05742700 | 4.30597800 | 3.57024700 |
| C | -1.97585000 | 3.08816500 | -3.66388700 |
| C | -1.72655200 | 2.38392800 | -2.48782900 |
| C | -2.43763600 | 2.66575300 | -1.32142500 |
| C | -3.41200500 | 3.66993300 | -1.37376100 |
| C | -3.65813400 | 4.36805100 | -2.54881800 |
| C | -2.94139800 | 4.09363400 | -3.71865300 |
| C | 2.82883400 | -2.26457900 | -2.46137900 |
| C | 2.74626500 | -3.02596600 | -3.62399400 |
| C | 2.08530200 | -4.25557800 | -3.64135100 |
| C | 1.50226600 | -4.69479000 | -2.44884800 |
| C | 1.58417300 | -3.93936200 | -1.28503000 |
| C | 2.25169300 | -2.70976100 | -1.27093600 |
| C | 3.39109900 | -3.69696500 | 1.30863100 |

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| C | 3.62997000 | -4.41237900 | 2.47517700 |
| C | 2.92030900 | -4.14153900 | 3.64996100 |
| C | 1.96996200 | -3.12060200 | 3.60996600 |
| C | 1.72786700 | -2.39955800 | 2.44283300 |
| C | 2.43119600 | -2.67862300 | 1.27076100 |
| C | 2.02592900 | -5.09241300 | -4.88806000 |
| C | 3.15799600 | -4.94067200 | 4.90016200 |
| C | -1.98822500 | 5.15706200 | 4.80680900 |
| C | -3.19113500 | 4.87197000 | -4.97948500 |
| C | 6.64582400 | 0.92503400 | 0.01955700 |
| C | -6.64487500 | -0.91869000 | 0.04293400 |
| C | 7.12104000 | 2.22780100 | -0.28906200 |
| C | 8.47386300 | 2.49932100 | -0.25000200 |
| C | 9.43467200 | 1.50932700 | 0.05132200 |
| C | 8.95644400 | 0.22287500 | 0.40822800 |
| C | 7.59237700 | -0.04090300 | 0.38994200 |
| C | -7.12162000 | -2.22284200 | -0.25742000 |
| C | -8.47344500 | -2.49660600 | -0.20208500 |
| C | -9.43271700 | -1.50748900 | 0.10705700 |
| C | -8.95283200 | -0.21834500 | 0.45182100 |
| C | -7.58947600 | 0.04740100 | 0.41823900 |
| O | 6.17671500 | 3.14284900 | -0.60425800 |
| O | 9.87905300 | -0.66696000 | 0.81052300 |
| O | -9.87246800 | 0.67201000 | 0.86002700 |
| O | -6.17930000 | -3.13730300 | -0.57958200 |
| C | 6.58411800 | 4.46288700 | -0.90902700 |
| C | 9.45629500 | -1.96087200 | 1.20666000 |
| C | -6.58815500 | -4.45690800 | -0.88432500 |
| C | -9.44835800 | 1.97026500 | 1.23966600 |
| C | 10.80425800 | 1.92796600 | 0.09076200 |
| C | -10.80051600 | -1.92944800 | 0.16821500 |
| C | 12.03059200 | 1.31884800 | 0.08053200 |
| C | -12.02861100 | -1.32379800 | 0.17623500 |
| C | 13.18435600 | 2.15315500 | 0.54760500 |
| C | 14.31094200 | 1.22076300 | 0.75498200 |
| C | 13.92924900 | -0.06353600 | 0.33460200 |
| C | 12.56286300 | 0.00558900 | -0.22966500 |
| C | -13.17175600 | -2.15952200 | 0.66633900 |
| C | -14.29708600 | -1.22938000 | 0.89012700 |
| C | -13.92643600 | 0.05429800 | 0.45815700 |
| C | -12.57013400 | -0.01336100 | -0.13009800 |
| C | 15.56186100 | 1.48482200 | 1.28851500 |
| C | 16.45421600 | 0.42324200 | 1.42031600 |
| C | 16.08069000 | -0.86252000 | 1.02190800 |
| C | 14.82538300 | -1.12291600 | 0.47151000 |
| C | -15.53742000 | -1.49454800 | 1.44730600 |
| C | -16.42991800 | -0.43467800 | 1.59147200 |
| C | -16.06695000 | 0.85054900 | 1.18171600 |
| C | -14.82254100 | 1.11198600 | 0.60757300 |
| O | 13.17762000 | 3.35305600 | 0.75507400 |
| C | 12.01444800 | -0.92757900 | -1.08169600 |
| O | -13.15799800 | -3.35857200 | 0.87844700 |
| C | -12.03991600 | 0.91723200 | -0.99624200 |
| C | 10.83687400 | -0.67975400 | -1.84016200 |
| N | 9.90488200 | -0.49473900 | -2.51147000 |
| C | 12.63136800 | -2.17719400 | -1.37431700 |
| N | 13.09533300 | -3.21386800 | -1.62781300 |
| C | -10.87409000 | 0.66945900 | -1.77269100 |
| N | -9.95247100 | 0.48368800 | -2.45793900 |
| C | -12.66674300 | 2.16285900 | -1.28486600 |
| N | -13.13935800 | 3.19625000 | -1.53576800 |
| H | -0.58836500 | -2.43941000 | -0.00446800 |
| H | 0.58856600 | 2.44515300 | -0.03063600 |
| H | -5.36019100 | 1.61840900 | -0.03159000 |
| H | 5.36096300 | -1.61232300 | -0.04363900 |
| H | -0.99881700 | 5.70404600 | 2.32247900 |
| H | -1.16908500 | 4.34916900 | 0.28223500 |
| H | -3.28621700 | 1.32585500 | 2.46850800 |
| H | -3.12986300 | 2.69299000 | 4.50415200 |
| H | -1.40532700 | 2.84623400 | -4.55751500 |
| H | -0.97033500 | 1.60531800 | -2.48587300 |
| H | -3.97937200 | 3.91426600 | -0.47972700 |
| H | -4.42236600 | 5.14184200 | -2.55886800 |
| H | 3.34898900 | -1.31158000 | -2.48491500 |
| H | 3.20747200 | -2.65423100 | -4.53595400 |
| H | 0.97644400 | -5.64665700 | -2.42968300 |
| H | 1.13190400 | -4.31716000 | -0.37224100 |
| H | 3.95165900 | -3.93896000 | 0.40973700 |
| H | 4.38134000 | -5.19883100 | 2.47355900 |
| H | 1.40524500 | -2.88107900 | 4.50798500 |

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| H | 0.98312700 | -1.60989600 | 2.45139000 |
| H | 2.14155500 | -4.47951100 | -5.78601700 |
| H | 2.82659200 | -5.84156300 | -4.89791700 |
| H | 1.07733200 | -5.63215000 | -4.96195100 |
| H | 4.21709000 | -5.18670100 | 5.02159700 |
| H | 2.82934700 | -4.39713600 | 5.78997700 |
| H | 2.60751600 | -5.88857900 | 4.87267400 |
| H | -2.08959700 | 4.55377800 | 5.71298000 |
| H | -1.04176000 | 5.70265800 | 4.86339200 |
| H | -2.79229900 | 5.90254100 | 4.81771500 |
| H | -4.25891400 | 5.05924300 | -5.12749900 |
| H | -2.69370500 | 5.84852000 | -4.94545700 |
| H | -2.81307800 | 4.34134100 | -5.85725400 |
| H | 8.83326800 | 3.49436300 | -0.48578300 |
| H | 7.24036500 | -1.01579500 | 0.69813500 |
| H | -8.83353800 | -3.49327700 | -0.42985000 |
| H | -7.23620000 | 1.02455400 | 0.71771100 |
| H | 5.67016200 | 5.01523700 | -1.12592400 |
| H | 7.09756300 | 4.92775400 | -0.05947300 |
| H | 7.23820700 | 4.48218600 | -1.78824100 |
| H | 10.36539700 | -2.50240800 | 1.46682700 |
| H | 8.79827400 | -1.91115700 | 2.08102000 |
| H | 8.94549400 | -2.47919000 | 0.38787000 |
| H | -5.67577100 | -5.00730200 | -1.11243300 |
| H | -7.09228500 | -4.92522600 | -0.03105200 |
| H | -7.25115700 | -4.47391300 | -1.75681000 |
| H | -10.35574500 | 2.51235000 | 1.50464100 |
| H | -8.78107300 | 1.93011300 | 2.10751600 |
| H | -8.94740000 | 2.48201800 | 0.41075900 |
| H | 10.91596800 | 3.00693400 | 0.22321200 |
| H | -10.90725200 | -3.00826700 | 0.30592400 |
| H | 15.82297800 | 2.49363000 | 1.59273700 |
| H | 17.44216600 | 0.59070500 | 1.83775900 |
| H | 16.78225200 | -1.68238400 | 1.14188100 |
| H | 14.56947000 | -2.13300300 | 0.17699500 |
| H | -15.79038900 | -2.50283900 | 1.76001100 |
| H | -17.40968400 | -0.60304600 | 2.02743800 |
| H | -16.76826700 | 1.66912200 | 1.31152600 |
| H | -14.57448200 | 2.12156100 | 0.30469500 |

ATT-1

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|----|-------------|-------------|-------------|
| 01 | | | |
| C | 1.29595600 | -0.46342200 | 0.27274300 |
| C | 1.03799300 | 0.92916700 | 0.28216500 |
| C | -0.26075800 | 1.40393500 | 0.26982100 |
| C | -1.29591100 | 0.46343500 | 0.27270000 |
| C | -1.03794900 | -0.92915700 | 0.28177300 |
| C | 0.26080400 | -1.40392200 | 0.26946400 |
| C | -2.72890700 | 0.61337400 | 0.25067100 |
| C | -3.36054200 | -0.61440800 | 0.23090100 |
| C | -2.34102900 | -1.74172400 | 0.27164400 |
| C | 2.72895500 | -0.61335800 | 0.25086400 |
| C | 3.36059300 | 0.61442800 | 0.23151800 |
| C | 2.34108000 | 1.74173500 | 0.27244300 |
| C | -2.35985300 | -2.62405500 | -0.98127300 |
| C | -2.56755700 | -2.54404800 | 1.55982100 |
| C | 2.36008700 | 2.62441400 | -0.98022700 |
| C | 2.56740900 | 2.54370000 | 1.56088100 |
| C | 1.78945800 | 3.90058500 | -0.95665500 |
| C | 1.72552900 | 4.67518500 | -2.10996400 |
| C | 2.23042500 | 4.20821500 | -3.32646600 |
| C | 2.79435900 | 2.93022900 | -3.34591900 |
| C | 2.85817700 | 2.15020600 | -2.19560400 |
| C | 1.83777600 | 2.30808800 | 2.72598000 |
| C | 2.12578100 | 3.00009600 | 3.90067500 |
| C | 3.14930200 | 3.94655800 | 3.95437100 |
| C | 3.88429800 | 4.17381000 | 2.78549400 |
| C | 3.60046700 | 3.48765500 | 1.61204700 |
| C | -1.78926500 | -3.90024200 | -0.95795500 |
| C | -1.72516500 | -4.67452900 | -2.11147200 |
| C | -2.22984100 | -4.20721400 | -3.32792400 |
| C | -2.79373800 | -2.92920000 | -3.34712200 |
| C | -2.85772600 | -2.14949500 | -2.19660900 |
| C | -1.83807800 | -2.30885700 | 2.72507000 |
| C | -2.12633000 | -3.00120200 | 3.89953900 |
| C | -3.14994700 | -3.94754400 | 3.95281700 |
| C | -3.88475800 | -4.17444500 | 2.78372300 |

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| C | -3.60069600 | -3.48797800 | 1.61054700 |
| C | -2.19391600 | -5.05995900 | -4.56449300 |
| C | -3.44188200 | -4.71552200 | 5.21073700 |
| C | 3.44059600 | 4.71441800 | 5.21251100 |
| S | 3.83875200 | -1.91906500 | 0.24832100 |
| C | 5.19530800 | -0.80384500 | 0.22995200 |
| C | 4.75822900 | 0.51575900 | 0.22413700 |
| S | -3.83870600 | 1.91907700 | 0.24837300 |
| C | -5.19526200 | 0.80386600 | 0.22953800 |
| C | -4.75817400 | -0.51573700 | 0.22339100 |
| C | 2.19466400 | 5.06134200 | -4.56277600 |
| C | -6.54775400 | 1.27167300 | 0.20023700 |
| C | 6.54780200 | -1.27165100 | 0.20058600 |
| C | -7.06130900 | 2.55188700 | 0.45376700 |
| C | -8.47359500 | 2.58992700 | 0.32463400 |
| C | -9.07864900 | 1.37838600 | -0.01941200 |
| S | -7.82146200 | 0.16881500 | -0.20066900 |
| C | 7.06137500 | -2.55184800 | 0.45414200 |
| C | 8.47365000 | -2.58989400 | 0.32490200 |
| C | 9.07867500 | -1.37837000 | -0.01925300 |
| S | 7.82147000 | -0.16881300 | -0.20048900 |
| C | -6.52218800 | 3.81947200 | 0.83506800 |
| C | -7.49642200 | 4.76076300 | 0.97133900 |
| S | -9.11619400 | 4.16639700 | 0.65387300 |
| C | 6.52227800 | -3.81940800 | 0.83555700 |
| C | 7.49652000 | -4.76069400 | 0.97179900 |
| S | 9.11626900 | -4.16635000 | 0.65417500 |
| C | -10.47689500 | 1.23495700 | -0.18343200 |
| C | 10.47690900 | -1.23495200 | -0.18340000 |
| C | -11.28206400 | 0.17820100 | -0.50407700 |
| C | 11.28205500 | -0.17822200 | -0.50418700 |
| C | -10.89895600 | -1.19211000 | -0.78490200 |
| N | -12.03537000 | -1.97942900 | -1.05557000 |
| C | -13.22332100 | -1.32806200 | -1.03012200 |
| S | -13.02828700 | 0.35822000 | -0.62624800 |
| C | 10.89892800 | 1.19206800 | -0.78508900 |
| N | 12.03531900 | 1.97935700 | -1.05594000 |
| C | 13.22327000 | 1.32798800 | -1.03053700 |
| S | 13.02826700 | -0.35825700 | -0.62649300 |
| O | 9.77229800 | 1.66078300 | -0.79667200 |
| O | -9.77232500 | -1.66082300 | -0.79655200 |
| C | -14.49778600 | -1.82897800 | -1.27269500 |
| C | 14.49771500 | 1.82888400 | -1.27325100 |
| C | -11.83228400 | -3.39489200 | -1.37783000 |
| C | -11.72144000 | -3.63888900 | -2.87340500 |
| C | 11.83221100 | 3.39478500 | -1.37834000 |
| C | 11.72121900 | 3.63861700 | -2.87393200 |
| C | -7.36430800 | 6.17474800 | 1.34670100 |
| O | -8.30894900 | 6.93274200 | 1.43994600 |
| O | -6.09335600 | 6.51650600 | 1.56913300 |
| C | -5.88628400 | 7.88244100 | 1.94206100 |
| C | 7.36443300 | -6.17465900 | 1.34724600 |
| O | 8.30907900 | -6.93265200 | 1.44045500 |
| O | 6.09349800 | -6.51640100 | 1.56980200 |
| C | 5.88645300 | -7.88231500 | 1.94282100 |
| C | -14.81685100 | -3.16273100 | -1.62834700 |
| N | -15.13958500 | -4.24122000 | -1.92769300 |
| C | -15.59597200 | -0.93477000 | -1.17059600 |
| N | -16.48772800 | -0.19096100 | -1.08356700 |
| C | 14.81675500 | 3.16261700 | -1.62900200 |
| N | 15.13944700 | 4.24107900 | -1.92849000 |
| C | 15.59590900 | 0.93468400 | -1.17117200 |
| N | 16.48767500 | 0.19088900 | -1.08413000 |
| H | -0.46955000 | 2.46939800 | 0.25269200 |
| H | 0.46959800 | -2.46938000 | 0.25205300 |
| H | 1.40022700 | 4.30022000 | -0.02448100 |
| H | 1.27635900 | 5.66438900 | -2.06193800 |
| H | 3.19185400 | 2.53556400 | -4.27799200 |
| H | 3.29906200 | 1.15901500 | -2.24913600 |
| H | 1.03503400 | 1.57743900 | 2.72500000 |
| H | 1.53901100 | 2.79658400 | 4.79331500 |
| H | 4.69255800 | 4.90129700 | 2.79469800 |
| H | 4.18385200 | 3.69574000 | 0.71919500 |
| H | -1.40020500 | -4.30014400 | -0.02582400 |
| H | -1.27603600 | -5.66376100 | -2.06364600 |
| H | -3.19106200 | -2.53426300 | -4.27915300 |
| H | -3.29857200 | -1.15827600 | -2.24994000 |
| H | -1.03524700 | -1.57830500 | 2.72442900 |
| H | -1.53964600 | -2.79803900 | 4.79231400 |
| H | -4.69303400 | -4.90192100 | 2.79256600 |

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| H | -4.18391500 | -3.69578900 | 0.71752300 |
| H | -1.35475300 | -5.76067800 | -4.54228600 |
| H | -3.11129000 | -5.65303200 | -4.65943400 |
| H | -2.10739900 | -4.44972100 | -5.46784000 |
| H | -3.00190100 | -5.71892000 | 5.17025600 |
| H | -3.03170800 | -4.21220800 | 6.09010100 |
| H | -4.51834800 | -4.84199300 | 5.35983600 |
| H | 3.03584800 | 4.20757300 | 6.09237600 |
| H | 4.51672400 | 4.84690300 | 5.35861400 |
| H | 2.99461000 | 5.71528100 | 5.17475600 |
| H | 5.44008800 | 1.35897000 | 0.23361400 |
| H | -5.44002400 | -1.35896000 | 0.23253800 |
| H | 3.11102400 | 5.65622900 | -4.65615000 |
| H | 2.11060100 | 4.45128200 | -5.46646800 |
| H | 1.35413700 | 5.76046500 | -4.54151500 |
| H | -5.47771600 | 4.04174100 | 1.01105900 |
| H | 5.47781800 | -4.04164900 | 1.01165600 |
| H | -11.00371200 | 2.17384200 | -0.01419800 |
| H | 11.00373800 | -2.17382800 | -0.01415100 |
| H | -10.90237300 | -3.66750500 | -0.87545800 |
| H | -12.64062100 | -3.97052300 | -0.92711200 |
| H | -11.54730500 | -4.70330600 | -3.05183500 |
| H | -12.63557800 | -3.35460500 | -3.40016900 |
| H | -10.88211200 | -3.07846300 | -3.29300500 |
| H | 10.90235000 | 3.66745600 | -0.87590900 |
| H | 12.64059400 | 3.97046400 | -0.92776200 |
| H | 11.54708000 | 4.70301700 | -3.05246300 |
| H | 12.63529800 | 3.35426300 | -3.40076000 |
| H | 10.88184000 | 3.07815700 | -3.29338500 |
| H | -4.81216300 | 7.98785300 | 2.08434100 |
| H | -6.23513400 | 8.55101100 | 1.15212600 |
| H | -6.41918800 | 8.11036800 | 2.86767700 |
| H | 4.81235400 | -7.98769200 | 2.08529200 |
| H | 6.23514400 | -8.55092600 | 1.15285000 |
| H | 6.41951300 | -8.11022300 | 2.86835200 |

DC-IDT2T

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|-----|-------------|-------------|-------------|
| 0 1 | | | |
| C | 1.28809700 | 0.48474300 | 0.00952000 |
| C | 1.05284800 | -0.91126900 | 0.04064300 |
| C | 0.23798700 | 1.40750600 | -0.02671300 |
| C | -1.05283500 | 0.91128700 | -0.04030600 |
| C | -1.28808300 | -0.48472500 | -0.00919700 |
| C | -0.23797200 | -1.40748900 | 0.02703600 |
| C | -2.36947600 | 1.70177900 | -0.06445200 |
| C | -3.37047400 | 0.55830300 | -0.02570100 |
| C | -2.71890200 | -0.65899700 | -0.01294900 |
| C | -4.76754000 | 0.43530100 | -0.03772700 |
| C | -5.17881800 | -0.89006100 | -0.02759400 |
| S | -3.80522400 | -1.98439400 | -0.01250800 |
| C | 2.36948900 | -1.70176000 | 0.06486500 |
| C | 3.37048800 | -0.55828400 | 0.02613400 |
| C | 2.71891700 | 0.65901500 | 0.01331100 |
| C | 4.76755300 | -0.43528600 | 0.03830100 |
| C | 5.17883500 | 0.89007300 | 0.02818800 |
| S | 3.80524300 | 1.98441300 | 0.01292600 |
| C | 2.42253600 | -2.59978700 | -1.17594600 |
| C | 2.58674800 | -2.48414300 | 1.36664200 |
| C | -2.42246200 | 2.59977000 | 1.17638800 |
| C | -2.58680000 | 2.48419900 | -1.36619500 |
| C | 1.85768600 | -3.87862800 | -1.14856900 |
| C | 1.82310100 | -4.66840800 | -2.29247500 |
| C | 2.35325400 | -4.21494400 | -3.50348100 |
| C | 2.91247100 | -2.93522300 | -3.52678300 |
| C | 2.94671500 | -2.13975100 | -2.38559300 |
| C | 3.62413600 | -3.42111100 | 1.44349200 |
| C | 3.89784000 | -4.08849800 | 2.63031800 |
| C | 3.14806000 | -3.84832500 | 3.78679500 |
| C | 2.12096100 | -2.90730800 | 3.70772800 |
| C | 1.84304800 | -2.23427500 | 2.52003800 |
| C | -1.85767100 | 3.87863400 | 1.14900500 |
| C | -1.82302600 | 4.66838000 | 2.29293800 |
| C | -2.35305800 | 4.21485300 | 3.50396900 |
| C | -2.91221800 | 2.93510500 | 3.52727600 |
| C | -2.94652300 | 2.13967000 | 2.38606500 |
| C | -3.62422400 | 3.42114300 | -1.44297100 |
| C | -3.89799000 | 4.08856500 | -2.62975400 |

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|---|--------------|-------------|-------------|
| C | -3.14824200 | 3.84845700 | -3.78627500 |
| C | -2.12111100 | 2.90748000 | -3.70727900 |
| C | -1.84313200 | 2.23440500 | -2.51962000 |
| C | 2.34834600 | -5.08458900 | -4.72878300 |
| C | 3.42652600 | -4.59726700 | 5.05921000 |
| C | -2.34808600 | 5.08444800 | 4.72930800 |
| C | -3.42683200 | 4.59741900 | -5.05864900 |
| C | 6.51530700 | 1.40788500 | 0.02785600 |
| C | -6.51528700 | -1.40787700 | -0.02712700 |
| S | -7.88252700 | -0.34218900 | 0.01901600 |
| C | -9.00041200 | -1.68971900 | -0.00716300 |
| C | -8.28731600 | -2.89480000 | -0.04855800 |
| C | -6.90657700 | -2.74535000 | -0.05969700 |
| S | 7.88252200 | 0.34221700 | -0.01946400 |
| C | 9.00043200 | 1.68970600 | 0.00770100 |
| C | 8.28736100 | 2.89476300 | 0.05019900 |
| C | 6.90662100 | 2.74532300 | 0.06146400 |
| C | -10.41322600 | -1.69931300 | 0.01255200 |
| C | 10.41324500 | 1.69928800 | -0.01220900 |
| C | -11.37374000 | -0.71322200 | 0.05112200 |
| C | 11.37373300 | 0.71320600 | -0.05161500 |
| C | -12.81773800 | -0.90638800 | 0.06871300 |
| C | -13.44325600 | 0.43568800 | 0.09187000 |
| C | -12.43039300 | 1.40626400 | 0.09645900 |
| C | -11.11469700 | 0.73840800 | 0.07381600 |
| C | 12.81773300 | 0.90635500 | -0.06921500 |
| C | 13.44322200 | -0.43571600 | -0.09337400 |
| C | 12.43033800 | -1.40626800 | -0.09856500 |
| C | 11.11465900 | -0.73840200 | -0.07535300 |
| C | -14.77689500 | 0.84571100 | 0.10876100 |
| C | -15.05187700 | 2.21330100 | 0.12989900 |
| C | -14.03161300 | 3.16677600 | 0.13494900 |
| C | -12.69795000 | 2.76450500 | 0.11805900 |
| C | 14.77685100 | -0.84575700 | -0.11062500 |
| C | 15.05180300 | -2.21333800 | -0.13270400 |
| C | 14.03151800 | -3.16678800 | -0.13834000 |
| C | 12.69786500 | -2.76450000 | -0.12110200 |
| O | -10.02792800 | 1.29818100 | 0.07310400 |
| O | 10.02787900 | -1.29815500 | -0.07498500 |
| C | 13.52172700 | 2.09535000 | -0.06986300 |
| C | -13.52170700 | -2.09539700 | 0.07014400 |
| C | 14.94382800 | 2.16921300 | -0.08869900 |
| N | 16.10104600 | 2.29146100 | -0.10345400 |
| C | 12.92163400 | 3.38670600 | -0.05552300 |
| N | 12.48111600 | 4.46422200 | -0.04499900 |
| C | -14.94380900 | -2.16927800 | 0.08883300 |
| N | -16.10102600 | -2.29154200 | 0.10351800 |
| C | -12.92158400 | -3.38675000 | 0.05681900 |
| N | -12.48103800 | -4.46426300 | 0.04713900 |
| H | 0.42989100 | 2.47620800 | -0.04201800 |
| H | -0.42987800 | -2.47619000 | 0.04235800 |
| H | -5.46412000 | 1.26624000 | -0.05784200 |
| H | 5.46412900 | -1.26622500 | 0.05858600 |
| H | 1.44975800 | -4.26778500 | -0.21995800 |
| H | 1.37722200 | -5.65897300 | -2.24160100 |
| H | 3.33021300 | -2.55136500 | -4.45453900 |
| H | 3.38569500 | -1.14786900 | -2.44170200 |
| H | 4.21966900 | -3.63813900 | 0.56084800 |
| H | 4.71016800 | -4.81089800 | 2.65974500 |
| H | 1.52365900 | -2.69279500 | 4.59076300 |
| H | 1.03814100 | -1.50637800 | 2.49931000 |
| H | -1.44983700 | 4.26784000 | 0.22037300 |
| H | -1.37719500 | 5.65896600 | 2.24205700 |
| H | -3.32986800 | 2.55120000 | 4.45505400 |
| H | -3.38545300 | 1.14776700 | 2.44217500 |
| H | -4.21972600 | 3.63812000 | -0.56029300 |
| H | -4.71033800 | 4.81094500 | -2.65912500 |
| H | -1.52382600 | 2.69302700 | -4.59034000 |
| H | -1.03819500 | 1.50653900 | -2.49895000 |
| H | 1.50134000 | -5.77624000 | -4.72415100 |
| H | 2.29732700 | -4.48642600 | -5.64282200 |
| H | 3.26171100 | -5.68865000 | -4.78561100 |
| H | 4.49925400 | -4.75839200 | 5.20063000 |
| H | 3.04353000 | -4.05987700 | 5.93077600 |
| H | 2.95009900 | -5.58473600 | 5.04671500 |
| H | -1.50133500 | 5.77640800 | 4.72444300 |
| H | -3.26165900 | 5.68816500 | 4.78645200 |
| H | -2.29656300 | 4.48626200 | 5.64330500 |
| H | -4.49965600 | 4.75750900 | -5.20054800 |
| H | -2.95141300 | 5.58536700 | -5.04569200 |

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| H | -3.04289400 | 4.06060700 | -5.93015400 |
| H | -8.79503100 | -3.85324500 | -0.07065200 |
| H | -6.20746900 | -3.57312300 | -0.09397100 |
| H | 8.79509400 | 3.85318200 | 0.07304000 |
| H | 6.20752800 | 3.57307200 | 0.09664700 |
| H | -10.77996900 | -2.72094900 | -0.00836600 |
| H | 10.78001100 | 2.72090000 | 0.00941700 |
| H | -15.59796000 | 0.14107900 | 0.10530400 |
| H | -16.08711900 | 2.53993400 | 0.14262300 |
| H | -14.28228200 | 4.22283200 | 0.15181300 |
| H | -11.88227100 | 3.48073000 | 0.12116200 |
| H | 15.59793300 | -0.14114500 | -0.10674000 |
| H | 16.08703700 | -2.53998500 | -0.14570600 |
| H | 14.28216300 | -4.22283800 | -0.15592800 |
| H | 11.88217000 | -3.48070400 | -0.12464000 |

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|---|--------------|-------------|-------------|
| C | 1.22606400 | 1.27659200 | -0.25496400 |
| C | 0.85743700 | -0.09873200 | -0.20173100 |
| C | -0.52077100 | -0.46456000 | -0.22948200 |
| C | -1.52322300 | 0.54130900 | -0.09777700 |
| C | -1.14032000 | 1.90975200 | -0.07575100 |
| C | 0.21473200 | 2.27396600 | -0.20502600 |
| N | -1.13608700 | -1.69835300 | -0.37124500 |
| C | -2.49357000 | -1.49539100 | -0.28842600 |
| C | -2.75404900 | -0.13036900 | -0.10806100 |
| C | 2.62882400 | 1.30493800 | -0.27486200 |
| C | 3.08213200 | -0.01965000 | -0.18992700 |
| N | 2.00563400 | -0.87479800 | -0.13712400 |
| N | -1.87393300 | 3.02714700 | 0.00681800 |
| N | -0.96437300 | 3.98378000 | -0.06675800 |
| N | 0.29706400 | 3.61072500 | -0.19892500 |
| C | -1.34070700 | 5.37966200 | -0.07679200 |
| C | -0.57884000 | -2.92833400 | -0.90370900 |
| C | 2.14184800 | -2.22438900 | 0.38575400 |
| C | -3.64127700 | -2.28294400 | -0.39994100 |
| C | -4.79861900 | -1.51618100 | -0.25626400 |
| S | -4.43720200 | 0.19622800 | -0.03282100 |
| S | 3.93107800 | 2.41529000 | -0.30533200 |
| C | 5.09801300 | 1.08948300 | -0.17569900 |
| C | 4.46958600 | -0.15484200 | -0.12906400 |
| C | -6.10096100 | -2.04893300 | -0.42409300 |
| C | 6.46743400 | 1.43280000 | -0.25613500 |
| C | -7.36106400 | -1.53525100 | -0.26456600 |
| C | 7.63502200 | 0.71982300 | -0.12527700 |
| C | -8.46530300 | -2.16405600 | -1.04678000 |
| C | -9.56621800 | -1.17501800 | -1.05362900 |
| C | -9.21641900 | -0.08226400 | -0.24112600 |
| C | -7.91528200 | -0.37166800 | 0.39797700 |
| C | -10.76754700 | -1.22718300 | -1.74086900 |
| C | -11.63563100 | -0.14331000 | -1.62455800 |
| C | -11.29045800 | 0.95543200 | -0.83385200 |
| C | -10.08759200 | 0.99963500 | -0.12839800 |
| C | 8.85185400 | 1.33042500 | -0.74095400 |
| C | 9.85249900 | 0.24715300 | -0.83161700 |
| C | 9.33583100 | -0.91066200 | -0.22694800 |
| C | 8.01379400 | -0.59027900 | 0.35906600 |
| C | 11.10340600 | 0.27781100 | -1.42451100 |
| C | 11.85438000 | -0.89606000 | -1.42783400 |
| C | 11.34444400 | -2.05910700 | -0.84663300 |
| C | 10.09010600 | -2.08308300 | -0.23567500 |
| C | -7.46024400 | 0.19306100 | 1.57155600 |
| C | 7.39562000 | -1.32807500 | 1.35089900 |
| O | -8.43820400 | -3.24263400 | -1.61143300 |
| O | 8.97034800 | 2.47700200 | -1.13321600 |
| C | -6.42891700 | -0.40401800 | 2.35089300 |
| N | -5.63457700 | -0.90420500 | 3.03791400 |
| C | -8.08409600 | 1.31604900 | 2.18532900 |
| N | -8.56368800 | 2.24072600 | 2.70354300 |
| C | 6.32223300 | -0.82447800 | 2.13411800 |
| N | 5.45921800 | -0.43848700 | 2.81272200 |
| C | 7.85702200 | -2.60670600 | 1.77610300 |
| N | 8.18854400 | -3.66060200 | 2.14126500 |
| H | -2.25024800 | 5.49237800 | 0.51096800 |
| H | -0.52851500 | 5.95632900 | 0.36300300 |
| H | -1.51883900 | 5.71521900 | -1.10159900 |

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| H | -0.34461000 | -3.64907700 | -0.11622100 |
| H | -1.30843800 | -3.37563400 | -1.58162500 |
| H | 0.31837400 | -2.70877900 | -1.48147700 |
| H | 2.99677100 | -2.24799500 | 1.06459400 |
| H | 1.25610600 | -2.48781600 | 0.96233200 |
| H | 2.29883400 | -2.95933200 | -0.40755000 |
| H | -3.67355100 | -3.35324100 | -0.56634700 |
| H | 5.00977000 | -1.09194300 | -0.10752500 |
| H | -6.10936800 | -3.03680900 | -0.88896400 |
| H | 6.66565700 | 2.45584600 | -0.58472600 |
| H | -11.01071400 | -2.09187700 | -2.35031600 |
| H | -12.58391100 | -0.14726000 | -2.15282100 |
| H | -11.97258000 | 1.79711000 | -0.76425300 |
| H | -9.84788200 | 1.86770500 | 0.47322900 |
| H | 11.47266200 | 1.19519600 | -1.87201200 |
| H | 12.83775500 | -0.91177000 | -1.88714400 |
| H | 11.93594100 | -2.96918200 | -0.86812800 |
| H | 9.72596400 | -3.00393900 | 0.20215400 |

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| C | -1.01900500 | -0.94599700 | 0.03285000 |
| C | -1.30505600 | 0.44072100 | 0.05837200 |
| C | -0.28747400 | 1.39998400 | 0.08705200 |
| C | 1.02046100 | 0.95046200 | 0.09744100 |
| C | 1.30645300 | -0.43618300 | 0.06873700 |
| C | 0.28893200 | -1.39547100 | 0.04182400 |
| C | -2.30655800 | -1.78315100 | 0.01924900 |
| C | 2.30815400 | 1.78742500 | 0.11336600 |
| C | -2.74181300 | 0.56631600 | 0.05863800 |
| C | -3.34671100 | -0.67513600 | 0.05452400 |
| C | -4.74550700 | -0.60209400 | 0.04504000 |
| C | -5.20610500 | 0.70889400 | 0.04900800 |
| S | -3.87158300 | 1.85601700 | 0.04852500 |
| C | 2.74311400 | -0.56181000 | 0.06272900 |
| C | 3.34820700 | 0.67949800 | 0.07013700 |
| C | 4.74706000 | 0.60615000 | 0.06813300 |
| C | 5.20725400 | -0.70491200 | 0.05322300 |
| S | 3.87245200 | -1.85168600 | 0.04689800 |
| C | -2.32352800 | -2.67361700 | 1.26647900 |
| C | -2.50147200 | -2.58228700 | -1.27567300 |
| C | 2.32398100 | 2.68440500 | -1.12922500 |
| C | -1.71827500 | -3.93398100 | 1.24585000 |
| C | -1.65509900 | -4.71467200 | 2.39485600 |
| C | -2.19523900 | -4.27014600 | 3.60470500 |
| C | -2.79387600 | -3.00823100 | 3.62171700 |
| C | -2.85729400 | -2.22224100 | 2.47526600 |
| C | -3.50867100 | -3.55247000 | -1.34260600 |
| C | -3.76537600 | -4.23612000 | -2.52390400 |
| C | -3.02749700 | -3.98024200 | -3.68473200 |
| C | -2.03005800 | -3.00719600 | -3.61541400 |
| C | -1.76967000 | -2.31745500 | -2.43324600 |
| C | 1.72418600 | 3.94715500 | -1.10011900 |
| C | 1.65921200 | 4.73332000 | -2.24533000 |
| C | 2.19206900 | 4.29199000 | -3.45952500 |
| C | 2.78528600 | 3.02762700 | -3.48491600 |
| C | 2.85038100 | 2.23612600 | -2.34244100 |
| C | -2.16026800 | -5.13150000 | 4.83541000 |
| C | -3.28746300 | -4.74553500 | -4.95136700 |
| C | 2.15476400 | 5.15879100 | -4.68630800 |
| C | 3.29615400 | 4.72228900 | 5.09911000 |
| C | 3.51539600 | 3.54571100 | 1.48486500 |
| C | 3.77358600 | 4.22286000 | 2.66951700 |
| C | 3.03403400 | 3.96401000 | 3.82869000 |
| C | 2.03324900 | 2.99488300 | 3.75397700 |
| C | 1.77126400 | 2.31171200 | 2.56824800 |
| C | 2.50488000 | 2.57927300 | 1.41248400 |
| C | -9.07447000 | 1.26805100 | 0.05572100 |
| C | -8.44032000 | 2.52585600 | 0.06962700 |
| C | -7.03654400 | 2.45277300 | 0.07909100 |
| C | -6.56906800 | 1.14243400 | 0.04874800 |
| S | -7.87253600 | -0.00630500 | 0.04447300 |
| C | -10.47665900 | 1.19533500 | -0.01271000 |
| C | -11.37140000 | 0.14542100 | -0.03770400 |
| C | -11.02569100 | -1.27804500 | 0.11044100 |
| C | -12.29932300 | -2.02400500 | 0.15018600 |
| C | -13.36705100 | -1.12422100 | 0.01386600 |

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| C | -12.81797800 | 0.24323900 | -0.14113700 |
| O | -9.90766800 | -1.76624200 | 0.20140700 |
| C | -13.58126000 | 1.37070800 | -0.38153200 |
| C | -12.48678700 | -3.38674100 | 0.30366200 |
| C | -13.79448500 | -3.86772600 | 0.32621700 |
| C | -14.86830600 | -2.98498200 | 0.19658600 |
| C | -14.67373800 | -1.61212100 | 0.03802500 |
| C | 9.07485800 | -1.26823800 | 0.00518600 |
| C | 8.43963400 | -2.52506200 | 0.04252700 |
| C | 7.03623900 | -2.45000700 | 0.07103300 |
| C | 6.56983600 | -1.13942900 | 0.03593000 |
| S | 7.87427900 | 0.00753400 | -0.00108200 |
| O | 6.19894400 | -3.51873600 | 0.10923800 |
| C | 10.47559700 | -1.19808900 | -0.08973900 |
| C | 11.37084200 | -0.14969000 | -0.14385300 |
| C | 11.03023700 | 1.27573800 | -0.00270300 |
| C | 12.30575000 | 2.01962400 | 0.00668200 |
| C | 13.36914500 | 1.11663200 | -0.14191600 |
| C | 12.81479500 | -0.25087500 | -0.27566200 |
| O | 9.91488600 | 1.76684800 | 0.10389600 |
| C | 13.57082500 | -1.38122400 | -0.52528500 |
| C | 12.49861300 | 3.38331300 | 0.14434700 |
| C | 13.80738800 | 3.86186600 | 0.13784000 |
| C | 14.87698900 | 2.97587400 | -0.00394900 |
| C | 14.67694000 | 1.60204600 | -0.14655800 |
| O | -9.15632400 | 3.66348600 | 0.11423700 |
| O | -6.19976100 | 3.52239900 | 0.09531400 |
| O | 9.15522500 | -3.66266300 | 0.09043500 |
| C | -8.92280600 | 4.59447900 | -0.95274800 |
| C | -6.24418200 | 4.28564400 | 1.30788500 |
| C | 6.25074500 | -4.26213800 | 1.33404700 |
| C | 8.90299200 | -4.60911200 | -0.95839800 |
| C | -13.04567400 | 2.67129500 | -0.60444100 |
| N | -12.66496700 | 3.75349600 | -0.80277300 |
| C | -15.00264500 | 1.35535400 | -0.46198600 |
| N | -16.16334800 | 1.40111400 | -0.53586800 |
| C | 14.99025600 | -1.36915200 | -0.63514000 |
| N | 16.14908300 | -1.41752300 | -0.73293600 |
| C | 13.02803300 | -2.68158400 | -0.73151200 |
| N | 12.64126300 | -3.76374700 | -0.91796600 |
| H | -0.51739500 | 2.46129100 | 0.09852200 |
| H | 0.51900200 | -2.45672300 | 0.02877900 |
| H | -5.41128200 | -1.45821800 | 0.03393500 |
| H | 5.41323600 | 1.46195200 | 0.07941700 |
| H | -1.30134400 | -4.31632000 | 0.31839500 |
| H | -1.17873400 | -5.69122100 | 2.34887000 |
| H | -3.22023700 | -2.63144200 | 4.54848500 |
| H | -3.32754300 | -1.24450300 | 2.52564200 |
| H | -4.09391900 | -3.78215700 | -0.45627300 |
| H | -4.55483300 | -4.98375800 | -2.54558200 |
| H | -1.44270000 | -2.77999900 | -4.50196000 |
| H | -0.98816500 | -1.56432200 | -2.42015700 |
| H | 1.31262700 | 4.32688700 | -0.16920800 |
| H | 1.18677800 | 5.71145000 | -2.19295300 |
| H | 3.20556900 | 2.65301900 | -4.41531900 |
| H | 3.31563100 | 1.25637700 | -2.39972200 |
| H | -3.05604100 | -5.76057800 | 4.90036700 |
| H | -1.29422500 | -5.79920600 | 4.83125300 |
| H | -2.12202400 | -4.52638500 | 5.74551100 |
| H | -4.35627600 | -4.93086100 | -5.09315600 |
| H | -2.91479900 | -4.20706000 | -5.82671900 |
| H | -2.79006900 | -5.72246700 | -4.93019000 |
| H | 3.05158200 | 5.78636700 | -4.75154400 |
| H | 2.11220000 | 4.55765600 | -5.59883200 |
| H | 1.29001100 | 5.82810100 | -4.67635100 |
| H | 4.36619600 | 4.89612700 | 5.24626600 |
| H | 2.80913500 | 5.70444500 | 5.07906200 |
| H | 2.91416600 | 4.18469800 | 5.97097600 |
| H | 4.10199700 | 3.77762000 | 0.60004500 |
| H | 4.56557000 | 4.96768700 | 2.69521400 |
| H | 1.44441300 | 2.76560200 | 4.63904100 |
| H | 0.98691100 | 1.56161800 | 2.55079900 |
| H | -10.89591900 | 2.19769500 | -0.03977000 |
| H | -11.63076300 | -4.04679100 | 0.40343500 |
| H | -15.53408400 | -0.96275700 | -0.05742700 |
| H | 10.89330200 | -2.20122200 | -0.11311000 |
| H | 11.64584300 | 4.04594300 | 0.25438700 |
| H | 15.53415600 | 0.95009800 | -0.25214700 |
| H | -9.56492600 | 5.44921300 | -0.74458200 |
| H | -7.87555500 | 4.90400800 | -0.98518600 |

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|---|--------------|-------------|-------------|
| H | -9.20778900 | 4.14485100 | -1.90825300 |
| H | -7.24607600 | 4.69030800 | 1.47800300 |
| H | -5.94672100 | 3.66736300 | 2.16058500 |
| H | -5.53283900 | 5.10133700 | 1.17848700 |
| H | 7.25347900 | -4.66520500 | 1.50327700 |
| H | 5.96002300 | -3.62945900 | 2.17835100 |
| H | 5.53757600 | -5.07893600 | 1.22298600 |
| H | 9.54716600 | -5.46169100 | -0.74786200 |
| H | 7.85498000 | -4.91732700 | -0.96922700 |
| H | 9.17328100 | -4.17453600 | -1.92509300 |
| H | 13.99966900 | 4.92490800 | 0.24448300 |
| H | 15.89208000 | 3.36078900 | -0.00374700 |
| H | -15.88244700 | -3.37174300 | 0.21915800 |
| H | -13.98263300 | -4.93010600 | 0.44601200 |

IDTOT2F

| | | | |
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| 0 1 | | | |
| C | 0.34590700 | -1.34791500 | -0.20664600 |
| C | 1.33369100 | -0.33509300 | -0.20143700 |
| C | 0.99818300 | 1.02219400 | -0.19412400 |
| C | -0.34594200 | 1.34800800 | -0.20669500 |
| C | -1.33372400 | 0.33518500 | -0.20138900 |
| C | -0.99821700 | -1.02210100 | -0.19402700 |
| C | -0.97437600 | 2.74981800 | -0.19768100 |
| C | -2.45066700 | 2.37854800 | -0.16259600 |
| C | -2.60777200 | 1.00966600 | -0.19100300 |
| C | 0.97433900 | -2.74972700 | -0.19761200 |
| C | 2.45062700 | -2.37845500 | -0.16266700 |
| C | 2.60774100 | -1.00957600 | -0.19112200 |
| C | 0.69608800 | -3.53384900 | -1.48844400 |
| C | 0.49255400 | -3.47149800 | 1.06634500 |
| C | -0.49248600 | 3.47166400 | 1.06619700 |
| C | -0.69623000 | 3.53388200 | -1.48856700 |
| C | 1.00795300 | -4.89735200 | -1.55788600 |
| C | 0.82310300 | -5.61311100 | -2.73301600 |
| C | 0.32435800 | -4.99963100 | -3.88753600 |
| C | 0.02640200 | -3.63905700 | -3.81779700 |
| C | 0.20762500 | -2.91657100 | -2.64024600 |
| C | 1.10673800 | -3.23666800 | 2.29958900 |
| C | 0.61586100 | -3.81585200 | 3.46513300 |
| C | -0.50998900 | -4.64358700 | 3.44514500 |
| C | -1.13183900 | -4.86014400 | 2.21323800 |
| C | -0.64222300 | -4.28633400 | 1.04382500 |
| C | 0.64223600 | 4.28659800 | 1.04350100 |
| C | 1.13196400 | 4.86046800 | 2.21281900 |
| C | 0.51028600 | 4.64389000 | 3.44483000 |
| C | -0.61549000 | 3.81609000 | 3.46498800 |
| C | -1.10648700 | 3.23682900 | 2.29951200 |
| C | -1.00829200 | 4.89735900 | -1.55805800 |
| C | -0.82352000 | 5.61310600 | -2.73318300 |
| C | -0.32467200 | 4.99964800 | -3.88769600 |
| C | -0.02644100 | 3.63916000 | -3.81788200 |
| C | -0.20759900 | 2.91666200 | -2.64030300 |
| C | 0.10219400 | -5.78755600 | -5.14739900 |
| C | -1.02021400 | -5.29406500 | 4.69961100 |
| C | 1.02071700 | 5.29446300 | 4.69916300 |
| C | -0.10309000 | 5.78754700 | -5.14768000 |
| C | -3.68571900 | 3.06155500 | -0.16536000 |
| C | -4.77787300 | 2.18849400 | -0.20654100 |
| S | -4.25020600 | 0.51988300 | -0.22840600 |
| C | 3.68566600 | -3.06148200 | -0.16546900 |
| C | 4.77782800 | -2.18843800 | -0.20671300 |
| S | 4.25017900 | -0.51981400 | -0.22859600 |
| C | -6.16595600 | 2.53449700 | -0.27089300 |
| S | -7.40663100 | 1.36648600 | 0.04435900 |
| C | -8.67376800 | 2.52013600 | -0.28324000 |
| C | -8.11109000 | 3.75284600 | -0.62149700 |
| C | -6.71958100 | 3.77305700 | -0.59920500 |
| C | 6.16590500 | -2.53446300 | -0.27112500 |
| S | 7.40661400 | -1.36650100 | 0.04416900 |
| C | 8.67371500 | -2.52016400 | -0.28353800 |
| C | 8.11099800 | -3.75283600 | -0.62186100 |
| C | 6.71948800 | -3.77301500 | -0.59953000 |
| C | -10.05639100 | 2.24457900 | -0.36459800 |

| | | | |
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| C | -10.82904600 | 1.14322600 | -0.08671600 |
| C | 10.05634300 | -2.24463100 | -0.36490900 |
| C | 10.82903200 | -1.14332700 | -0.08693600 |
| C | -12.12419400 | 1.01582500 | -0.81029600 |
| C | -12.51374300 | -0.40765400 | -0.68719500 |
| C | -11.59519100 | -1.07171300 | 0.14077400 |
| C | -10.62974300 | -0.07952400 | 0.65918300 |
| C | 12.12416900 | -1.01588900 | -0.81053200 |
| C | 12.51377600 | 0.40755800 | -0.68727300 |
| C | 11.59526900 | 1.07155500 | 0.14079500 |
| C | 10.62979500 | 0.07934300 | 0.65911400 |
| C | -13.58557800 | -1.05418000 | -1.28170900 |
| C | -13.71628400 | -2.41050100 | -1.04095100 |
| C | -12.79962000 | -3.08638600 | -0.22768700 |
| C | -11.73754000 | -2.43750400 | 0.38156800 |
| C | 13.58562000 | 1.05411100 | -1.28174100 |
| C | 13.71638500 | 2.41039900 | -1.04083000 |
| C | 12.79976700 | 3.08622500 | -0.22746600 |
| C | 11.73767600 | 2.43731400 | 0.38174200 |
| O | 3.81458100 | -4.41157400 | -0.15690100 |
| O | -3.81467600 | 4.41164400 | -0.15679200 |
| C | -4.08724900 | 4.98099700 | 1.12934200 |
| C | 4.08737500 | -4.98092900 | 1.12918400 |
| O | -12.71369000 | 1.88517700 | -1.42550900 |
| C | -9.87768200 | -0.22989000 | 1.80764900 |
| O | 12.71361000 | -1.88519000 | -1.42586900 |
| C | 9.87776600 | 0.22959900 | 1.80761500 |
| F | 14.71191400 | 3.10841000 | -1.57923500 |
| F | 12.97241400 | 4.39260600 | -0.04704400 |
| F | -14.71180000 | -3.10848800 | -1.57941200 |
| F | -12.97221400 | -4.39279400 | -0.04741100 |
| C | -9.31064200 | 0.88110800 | 2.49271500 |
| N | -8.88906700 | 1.77606300 | 3.10492300 |
| C | -9.74602500 | -1.47191700 | 2.48987400 |
| N | -9.61023400 | -2.47943000 | 3.05594500 |
| C | 9.31069700 | -0.88145600 | 2.49256200 |
| N | 8.88910400 | -1.77648400 | 3.10465100 |
| C | 9.74616800 | 1.47154700 | 2.48999600 |
| N | 9.61040800 | 2.47899000 | 3.05619800 |
| H | 1.76306700 | 1.79313200 | -0.17602100 |
| H | -1.76309800 | -1.79304000 | -0.17584900 |
| H | 1.40551900 | -5.40118600 | -0.68335600 |
| H | 1.07369200 | -6.67119200 | -2.75549900 |
| H | -0.35716000 | -3.12943000 | -4.69845700 |
| H | -0.03650500 | -1.85922500 | -2.62835000 |
| H | 1.97447500 | -2.58457000 | 2.35448300 |
| H | 1.11598100 | -3.61556900 | 4.40970400 |
| H | -2.01662300 | -5.49052700 | 2.16462800 |
| H | -1.14749200 | -4.48228100 | 0.10284000 |
| H | 1.14735600 | 4.48255700 | 0.10243800 |
| H | 2.01669700 | 5.49091500 | 2.16407300 |
| H | -1.11547600 | 3.61581300 | 4.40963000 |
| H | -1.97417000 | 2.58467100 | 2.35454600 |
| H | -1.40591800 | 5.40116100 | -0.68353800 |
| H | -1.07422800 | 6.67116000 | -2.75568100 |
| H | 0.35731900 | 3.12959700 | -4.69849000 |
| H | 0.03675400 | 1.85936900 | -2.62836400 |
| H | 0.94249600 | -6.45828100 | -5.35153600 |
| H | -0.79570000 | -6.41161800 | -5.06870300 |
| H | -0.02758400 | -5.13078300 | -6.01143800 |
| H | -0.56792000 | -6.28280200 | 4.84181500 |
| H | -0.78169100 | -4.69698000 | 5.58404200 |
| H | -2.10402700 | -5.43528900 | 4.66363900 |
| H | 0.57149900 | 6.28490300 | 4.83924000 |
| H | 0.77890700 | 4.69940900 | 5.58405800 |
| H | 2.10504900 | 5.43211000 | 4.66463800 |
| H | -0.94652300 | 6.45340200 | -5.35495100 |
| H | 0.79103700 | 6.41671200 | -5.06697700 |
| H | 0.03275300 | 5.13064300 | -6.01067800 |
| H | -8.72646000 | 4.60535000 | -0.88811400 |
| H | -6.10829900 | 4.62907900 | -0.85114300 |
| H | 8.72633800 | -4.60533700 | -0.88855500 |
| H | 6.10817600 | -4.62900800 | -0.85149400 |
| H | -10.62106600 | 3.03287700 | -0.86642700 |
| H | 10.62098500 | -3.03289200 | -0.86683200 |
| H | -14.29509300 | -0.52757000 | -1.91077200 |
| H | -11.06154800 | -3.01368400 | 1.00090600 |
| H | 14.29510000 | 0.52754700 | -1.91088200 |
| H | 11.06172200 | 3.01345000 | 1.00115900 |
| H | -3.25755200 | 4.79340800 | 1.81708400 |

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|---|-------------|-------------|------------|
| H | -4.19475400 | 6.05402000 | 0.96741600 |
| H | -5.01550800 | 4.57932600 | 1.54841600 |
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ITOC-F

| | | | |
|-----|--------------|-------------|-------------|
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| C | -1.04164900 | -0.92187300 | -0.01396600 |
| C | -1.29433000 | 0.47108700 | 0.02222100 |
| C | -0.25424900 | 1.40560300 | 0.05751600 |
| C | 1.04242900 | 0.92467800 | 0.06497000 |
| C | 1.29508900 | -0.46823900 | 0.02762600 |
| C | 0.25503700 | -1.40276400 | -0.00751900 |
| C | -2.34894200 | -1.72785500 | -0.03456400 |
| C | 2.34975800 | 1.73053200 | 0.08861500 |
| C | -2.72743900 | 0.63099600 | 0.02555800 |
| C | -3.36224700 | -0.59559600 | 0.01217800 |
| C | -4.75868000 | -0.48827800 | 0.00811300 |
| C | -5.18697000 | 0.83370800 | 0.02639400 |
| S | -3.82479100 | 1.94795300 | 0.03138100 |
| C | 2.72817100 | -0.62821100 | 0.02543600 |
| C | 3.36308600 | 0.59827700 | 0.04178500 |
| C | 4.75952700 | 0.49080700 | 0.04743300 |
| C | 5.18759600 | -0.83125500 | 0.03027400 |
| S | 3.82533600 | -1.94521200 | 0.01188800 |
| C | -2.38631100 | -2.63014100 | 1.20365400 |
| C | -2.56310400 | -2.50914900 | -1.33741600 |
| C | 2.38930800 | 2.63444900 | -1.14834800 |
| C | -1.81042000 | -3.90390500 | 1.16991500 |
| C | -1.76379200 | -4.69693600 | 2.31122700 |
| C | -2.29217300 | -4.25189400 | 3.52608200 |
| C | -2.86188800 | -2.97691500 | 3.55604400 |
| C | -2.90839100 | -2.17847600 | 2.41741400 |
| C | -3.59226900 | -3.45530600 | -1.41338700 |
| C | -3.86419100 | -4.12192900 | -2.60102800 |
| C | -3.12054800 | -3.87203600 | -3.75945400 |
| C | -2.10145200 | -2.92236000 | -3.68120700 |
| C | -1.82549900 | -2.24997200 | -2.49262700 |
| C | 1.81355600 | 3.90825100 | -1.11382300 |
| C | 1.76815600 | 4.70246000 | -2.25433600 |
| C | 2.29775200 | 4.25856200 | -3.46908000 |
| C | 2.86749100 | 2.98362300 | -3.49973400 |
| C | 2.91270800 | 2.18391000 | -2.36195300 |
| C | -2.27510600 | -5.12553800 | 4.74846000 |
| C | -3.39714000 | -4.61971500 | -5.03305900 |
| C | 2.28140200 | 5.13327300 | -4.69068800 |
| C | 3.39191600 | 4.61368100 | 5.09355600 |
| C | 3.59130000 | 3.45555200 | 1.47214500 |
| C | 3.86174200 | 4.12006100 | 2.66127400 |
| C | 3.11643200 | 3.86840200 | 3.81829300 |
| C | 2.09712700 | 2.91925300 | 3.73692900 |
| C | 1.82263300 | 2.24899400 | 2.54673400 |
| C | 2.56196400 | 2.50978300 | 1.39299700 |
| C | -9.03924300 | 1.49191200 | 0.06927600 |
| C | -8.37218200 | 2.73300400 | 0.09402600 |
| C | -6.97123500 | 2.62333300 | 0.09000800 |
| C | -6.53829200 | 1.30128800 | 0.03947800 |
| S | -7.87101300 | 0.18690800 | 0.02912600 |
| C | -10.44269600 | 1.45818600 | 0.01869400 |
| C | -11.36761200 | 0.43420700 | -0.01443900 |
| C | -11.05918100 | -0.99921500 | 0.08742000 |
| C | -12.35558500 | -1.71180300 | 0.11106100 |
| C | -13.39791500 | -0.77838500 | 0.01362600 |
| C | -12.81303300 | 0.57585900 | -0.09402300 |
| O | -9.95770100 | -1.52577800 | 0.15502300 |
| C | -13.54769800 | 1.73384200 | -0.27181500 |
| C | -12.56697000 | -3.07367500 | 0.21662100 |
| C | -13.89056200 | -3.49288000 | 0.22574300 |
| C | -14.95606400 | -2.60170300 | 0.13495600 |
| C | -14.71833200 | -1.23432700 | 0.02652000 |
| C | 9.03969000 | -1.49207400 | 0.01543600 |
| C | 8.37213200 | -2.73261800 | 0.05538100 |
| C | 6.97135200 | -2.62174400 | 0.06947200 |
| C | 6.53878700 | -1.29948800 | 0.02285600 |
| S | 7.87190100 | -0.18626100 | -0.01360900 |
| O | 6.10675200 | -3.66833100 | 0.10772500 |

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| C | 10.44216000 | -1.45986200 | -0.05718100 |
| C | 11.36730100 | -0.43705700 | -0.11370000 |
| C | 11.06126600 | 0.99762600 | -0.02315200 |
| C | 12.35809800 | 1.70980400 | -0.03154800 |
| C | 13.39815500 | 0.77467300 | -0.13642400 |
| C | 12.81110100 | -0.58057900 | -0.21595400 |
| O | 9.96130000 | 1.52554200 | 0.05736300 |
| C | 13.54272700 | -1.74112400 | -0.38976400 |
| C | 12.57184800 | 3.07282100 | 0.05250100 |
| C | 13.89548500 | 3.49141700 | 0.03122100 |
| C | 14.95883000 | 2.59860700 | -0.06827700 |
| C | 14.71869000 | 1.23006400 | -0.15443800 |
| O | -9.05869500 | 3.88714400 | 0.16064900 |
| O | -6.10652100 | 3.67014900 | 0.11347500 |
| O | 9.05903700 | -3.88641400 | 0.11985500 |
| C | -8.80997100 | 4.82896100 | -0.89339500 |
| C | -6.12140700 | 4.41854700 | 1.33618300 |
| C | 6.12670300 | -4.40210100 | 1.33948400 |
| C | 8.79292600 | -4.83828500 | -0.92058700 |
| C | -12.98125000 | 3.02960400 | -0.43827500 |
| N | -12.57545300 | 4.11059300 | -0.58740300 |
| C | -14.96979600 | 1.75758300 | -0.33207200 |
| N | -16.13019400 | 1.83101700 | -0.38632200 |
| C | 14.96359800 | -1.76598900 | -0.47365900 |
| N | 16.12289500 | -1.84049800 | -0.54677200 |
| C | 12.97403500 | -3.03922000 | -0.52776100 |
| N | 12.56655300 | -4.12245000 | -0.65435200 |
| H | -0.45854600 | 2.47197100 | 0.07695200 |
| H | 0.45937800 | -2.46911300 | -0.02775200 |
| H | -5.44539200 | -1.32762400 | -0.00785600 |
| H | 5.44642900 | 1.32991200 | 0.06766400 |
| H | -1.40360800 | -4.28673300 | 0.23819100 |
| H | -1.31005600 | -5.68367300 | 2.25508600 |
| H | -3.27860100 | -2.59956000 | 4.48695900 |
| H | -3.35586300 | -1.19067400 | 2.47804400 |
| H | -4.18288800 | -3.67999700 | -0.52933000 |
| H | -4.67029500 | -4.85133100 | -2.62962300 |
| H | -1.50901500 | -2.70020200 | -4.56564400 |
| H | -1.02699000 | -1.51505300 | -2.47258100 |
| H | 1.40549300 | 4.29006700 | -0.18222300 |
| H | 1.31401100 | 5.68897700 | -2.19781700 |
| H | 3.28486600 | 2.60701600 | -4.43063600 |
| H | 3.35976100 | 1.19597600 | -2.42343600 |
| H | -3.18425800 | -5.73564600 | 4.80818500 |
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| H | -2.22310400 | -4.53011400 | 5.66425900 |
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| H | -3.01780900 | -4.07871100 | -5.90399500 |
| H | -2.91623900 | -5.60504700 | -5.02330300 |
| H | 3.18880000 | 5.74629800 | -4.74734000 |
| H | 2.23371000 | 4.53847100 | -5.60709800 |
| H | 1.42782500 | 5.81677600 | -4.68107200 |
| H | 4.46457300 | 4.77148200 | 5.23956200 |
| H | 2.91859800 | 5.60264300 | 5.08160900 |
| H | 3.00421400 | 4.07524900 | 5.96239100 |
| H | 4.18316700 | 3.68158500 | 0.58928100 |
| H | 4.66801100 | 4.84918100 | 2.69218900 |
| H | 1.50337200 | 2.69582600 | 4.62019700 |
| H | 1.02380800 | 1.51446600 | 2.52410900 |
| H | -10.83420900 | 2.47195000 | 0.01490600 |
| H | -11.74516700 | -3.77767200 | 0.28908300 |
| H | -15.56311200 | -0.56164000 | -0.04160800 |
| H | 10.83270600 | -2.47399800 | -0.05998100 |
| H | 11.75175600 | 3.77813100 | 0.13133400 |
| H | 15.56190100 | 0.55619900 | -0.22991300 |
| H | -9.43299200 | 5.69367700 | -0.66927000 |
| H | -7.75653900 | 5.11656600 | -0.92621200 |
| H | -9.10836300 | 4.39978200 | -1.85420300 |
| H | -7.11030900 | 4.84904300 | 1.51846400 |
| H | -5.83601300 | 3.78096400 | 2.17867700 |
| H | -5.38804600 | 5.21532400 | 1.21221400 |
| H | 7.11669300 | -4.82997400 | 1.52235900 |
| H | 5.84453200 | -3.75445000 | 2.17524800 |
| H | 5.39319400 | -5.20060100 | 1.22809400 |
| H | 9.41928200 | -5.70099000 | -0.69805500 |
| H | 7.73910100 | -5.12571500 | -0.93363600 |
| H | 9.07602500 | -4.41882400 | -1.89031800 |
| H | 15.97144500 | 2.98685400 | -0.07736800 |
| H | -15.96846200 | -2.99033200 | 0.15010500 |
| F | 14.16354200 | 4.79675800 | 0.10998400 |

F -14.15644200 -4.79715600 0.32637300

ITOIC-2F

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C 2.37699300 -1.69328500 -0.08793700
C -2.71691100 -0.67486400 -0.03346700
C -3.37141200 0.54153700 -0.01850400
C -4.76571100 0.41155600 -0.01479800
C -5.17246300 -0.91736200 -0.03539500
S -3.79242500 -2.00945800 -0.04233700
C 2.71735100 0.67124800 -0.02259000
C 3.37200300 -0.54503200 -0.03910500
C 4.76631800 -0.41483400 -0.04443400
C 5.17277400 0.91421000 -0.02696300
S 3.79261400 2.00594600 -0.00852000
C -2.42627900 2.59293900 -1.20639000
C -2.60436000 2.46610200 1.33422800
C 2.42849600 -2.59718300 1.14860900
C -1.86565000 3.87350100 -1.17119400
C -1.82915800 4.66862800 -2.31134600
C -2.35306600 4.21905000 -3.52652400
C -2.90778500 2.93756200 -3.55785200
C -2.94395900 2.13690100 -2.42033800
C -3.64556900 3.39906000 1.40883800
C -3.92887600 4.06050200 2.59674900
C -3.18521700 3.81820400 3.75674100
C -2.15427100 2.88123600 3.67990300
C -1.86676500 2.21419300 2.49109200
C 1.86780200 -3.87770800 1.11335300
C 1.83206000 -4.67318900 2.25324900
C 2.35688700 -4.22396700 3.46816300
C 2.91184100 -2.94259100 3.49945200
C 2.94721200 -2.14148200 2.36223400
C -2.34683300 5.09449700 -4.74770900
C -3.47418300 4.56069700 5.03062100
C 2.35085400 -5.09960700 4.68919400
C 3.47103800 -4.55928700 -5.09162100
C 3.64475400 -3.40147400 -1.46877600
C 3.92712800 -4.06170300 -2.65754700
C 3.18255100 -3.81826900 -3.81676300
C 2.15156400 -2.88154200 -3.73808400
C 1.86497300 -2.21571900 -2.54829000
C 2.60355900 -2.46859200 -1.39227600
C -9.01311700 -1.63761000 -0.07496000
C -8.32590000 -2.86810200 -0.10557000
C -6.92713400 -2.73570400 -0.10322500
C -6.51577200 -1.40666900 -0.04848300
S -7.86627500 -0.31392800 -0.03157300
C -10.41621100 -1.62726100 -0.02227800
C -11.35819800 -0.61861600 0.01815700
C -11.07409200 0.82148500 -0.07244700
C -12.38028200 1.51127400 -0.08241400
C -13.40603900 0.56151000 0.01057600
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O -9.98177200 1.36651000 -0.14092200
C -13.51828000 -1.95526700 0.26292600
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C -14.97583100 2.34791700 -0.08035800
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C 6.92662500 2.73370800 -0.07008900
C 6.51589700 1.40433900 -0.02037500
S 7.86691000 0.31292700 0.01797200
O 6.04484300 3.76572800 -0.11105000
C 10.41540800 1.62892000 0.05428700
C 11.35804100 0.62167600 0.11161400
C 11.07638400 -0.81941700 0.02993200
C 12.38324200 -1.50794600 0.04137100

| | | | |
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| C | 13.40690300 | -0.55632500 | 0.13832500 |
| C | 12.79741700 | 0.79152200 | 0.20861600 |
| O | 9.98538500 | -1.36614100 | -0.04565500 |
| C | 13.51407100 | 1.96268600 | 0.36902800 |
| C | 12.62317400 | -2.87001600 | -0.03380700 |
| C | 13.94488100 | -3.27824100 | -0.01209700 |
| C | 14.97939200 | -2.34180600 | 0.08200700 |
| C | 14.73649400 | -0.97974500 | 0.15974100 |
| F | -14.25744900 | 4.57096300 | -0.25471900 |
| F | -16.22679300 | 2.80187100 | -0.08582500 |
| F | 14.26524600 | -4.56707500 | -0.08129400 |
| F | 16.23077000 | -2.79443500 | 0.09560500 |
| O | -8.99457900 | -4.03203800 | -0.17590100 |
| O | -6.04531600 | -3.76794900 | -0.13235200 |
| O | 8.99409000 | 4.03117000 | -0.12585700 |
| C | -8.72619500 | -4.97777100 | 0.86994700 |
| C | -6.04811500 | -4.51000800 | -1.35911300 |
| C | 6.04957700 | 4.49347500 | -1.34665100 |
| C | 8.71006900 | 4.98584500 | 0.90741200 |
| C | -12.93415600 | -3.24563600 | 0.40913300 |
| N | -12.51239200 | -4.32260700 | 0.54109400 |
| C | -14.93989200 | -1.99589600 | 0.32384400 |
| N | -16.09969300 | -2.07789100 | 0.37714900 |
| C | 14.93483600 | 2.00517000 | 0.44616000 |
| N | 16.09382800 | 2.08899600 | 0.51265000 |
| C | 12.92748400 | 3.25395500 | 0.49613200 |
| N | 12.50359200 | 4.33183700 | 0.61302400 |
| H | -0.41936100 | -2.47938500 | -0.08300200 |
| H | 0.41992200 | 2.47566000 | 0.02935600 |
| H | -5.46599200 | 1.23956800 | 0.00276100 |
| H | 5.46684300 | -1.24256700 | -0.06537400 |
| H | -1.46281600 | 4.25978700 | -0.23916300 |
| H | -1.38708200 | 5.66057200 | -2.25410000 |
| H | -3.32073000 | 2.55665800 | -4.48900000 |
| H | -3.37971300 | 1.14395800 | -2.48220900 |
| H | -4.23668700 | 3.61758900 | 0.52358200 |
| H | -4.74399500 | 4.77985100 | 2.62428200 |
| H | -1.56151900 | 2.66513400 | 4.56562000 |
| H | -1.05916200 | 1.48924000 | 2.47213100 |
| H | 1.46393300 | -4.26358600 | 0.18159000 |
| H | 1.38942100 | -5.66488100 | 2.19618800 |
| H | 3.32522800 | -2.56184400 | 4.43044900 |
| H | 3.38270400 | -1.14844500 | 2.42438300 |
| H | -3.26256800 | 5.69485600 | -4.80557100 |
| H | -1.50294900 | 5.78989600 | -4.73633200 |
| H | -2.28941600 | 4.50093300 | -5.66438800 |
| H | -4.54855400 | 4.71450000 | 5.16780500 |
| H | -3.09175800 | 4.02250100 | 5.90194300 |
| H | -3.00407500 | 5.55124800 | 5.02397500 |
| H | 3.26490100 | -5.70275900 | 4.74487400 |
| H | 2.29723500 | -4.50597100 | 5.60603100 |
| H | 1.50477500 | -5.79235800 | 4.67960900 |
| H | 4.54591500 | -4.70494200 | -5.23383700 |
| H | 3.00880200 | -5.55350200 | -5.08217200 |
| H | 3.08046500 | -4.02452100 | -5.96143100 |
| H | 4.23653700 | -3.62085600 | -0.58419200 |
| H | 4.74225100 | -4.78099000 | -2.68640900 |
| H | 1.55807000 | -2.66466300 | -4.62315000 |
| H | 1.05721500 | -1.49095300 | -2.52773900 |
| H | -10.79112100 | -2.64728100 | -0.02283400 |
| H | -11.80848700 | 3.59160000 | -0.24240400 |
| H | -15.58517800 | 0.31959400 | 0.07823100 |
| H | 10.78918000 | 2.64935600 | 0.05337900 |
| H | 11.81540900 | -3.59020400 | -0.10712800 |
| H | 15.58484900 | -0.31155300 | 0.23008100 |
| H | -9.33441000 | -5.85150700 | 0.64040400 |
| H | -7.66783800 | -5.24691000 | 0.89782200 |
| H | -9.02941500 | -4.56137900 | 1.83484600 |
| H | -7.02946800 | -4.95681500 | -1.54295700 |
| H | -5.77472500 | -3.86300300 | -2.19835700 |
| H | -5.30076900 | -5.29439500 | -1.23990100 |
| H | 7.03163500 | 4.93749300 | -1.53380900 |
| H | 5.77702600 | 3.83674000 | -2.17847500 |
| H | 5.30254900 | 5.27966800 | -1.23773500 |
| H | 9.32235900 | 5.85720300 | 0.67972000 |
| H | 7.65166000 | 5.25572500 | 0.91672600 |
| H | 8.99825900 | 4.57779000 | 1.88048300 |

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|-----|--------------|-------------|-------------|
| 0 1 | | | |
| C | 1.12281500 | 0.82504000 | -0.01410400 |
| C | 1.24604300 | -0.58443800 | 0.05565600 |
| C | 0.12416100 | -1.42033700 | 0.06661800 |
| C | -1.12278400 | -0.82499800 | 0.01454600 |
| C | -1.24601600 | 0.58448100 | -0.05519400 |
| C | -0.12413300 | 1.42038000 | -0.06616600 |
| C | 2.49855800 | 1.50841100 | 0.00598600 |
| C | -2.49852100 | -1.50837700 | -0.00560400 |
| C | 2.65629600 | -0.87355500 | 0.11048400 |
| C | 3.40229900 | 0.28943400 | 0.09818000 |
| C | 4.78126500 | 0.05518200 | 0.14345100 |
| C | 5.08663800 | -1.30158800 | 0.19578100 |
| S | 3.62651500 | -2.28441200 | 0.18319200 |
| C | -2.65627200 | 0.87359200 | -0.11001900 |
| C | -3.40226600 | -0.28939900 | -0.09775000 |
| C | -4.78123900 | -0.05515900 | -0.14302000 |
| C | -5.08662100 | 1.30160500 | -0.19531700 |
| S | -3.62651100 | 2.28444600 | -0.18266600 |
| C | 2.57415800 | 2.41511900 | 1.23979200 |
| C | 2.83006400 | 2.25744300 | -1.29051800 |
| C | -2.57408700 | -2.41501300 | -1.23945800 |
| C | 2.08611000 | 3.72475200 | 1.18459200 |
| C | 2.07190300 | 4.52983600 | 2.31780700 |
| C | 2.54776200 | 4.06201300 | 3.54614400 |
| C | 3.03072600 | 2.75281300 | 3.59708200 |
| C | 3.04345900 | 1.94149700 | 2.46625300 |
| C | 3.93417800 | 3.11778900 | -1.32641000 |
| C | 4.30942600 | 3.75065900 | -2.50417500 |
| C | 3.59838700 | 3.55126800 | -3.69256300 |
| C | 2.50452000 | 2.68612500 | -3.65415000 |
| C | 2.12480100 | 2.04757800 | -2.47537800 |
| C | -2.08608600 | -3.72463900 | -1.18433800 |
| C | -2.07184600 | -4.52964600 | -2.31764000 |
| C | -2.54763000 | -4.06172800 | -3.54593900 |
| C | -3.03057100 | -2.75248600 | -3.59679800 |
| C | -3.04332900 | -1.94127600 | -2.46592700 |
| C | 2.56665100 | 4.94706400 | 4.76029200 |
| C | 3.98866300 | 4.26428700 | -4.95634500 |
| C | -2.56656400 | -4.94655700 | -4.76024700 |
| C | -3.98911400 | -4.26437200 | 4.95652100 |
| C | -3.93421900 | -3.11780700 | 1.32666700 |
| C | -4.30949400 | -3.75076100 | 2.50434600 |
| C | -3.59846400 | -3.55146700 | 3.69278700 |
| C | -2.50456200 | -2.68640900 | 3.65444600 |
| C | -2.12479700 | -2.04775700 | 2.47571300 |
| C | -2.83005700 | -2.25747600 | 1.29085700 |
| C | 8.85938700 | -2.30609300 | 0.27817100 |
| C | 8.10241500 | -3.47651900 | 0.34373600 |
| C | 6.72416400 | -3.24558200 | 0.34337600 |
| C | 6.38754300 | -1.88632900 | 0.24483100 |
| S | 7.81671400 | -0.91492400 | 0.17378800 |
| C | 10.26527800 | -2.29134700 | 0.14548500 |
| C | 11.20776300 | -1.29252500 | 0.09036400 |
| C | 12.48910400 | -1.59973500 | -0.60660600 |
| C | 13.10747200 | -0.28944300 | -0.91116400 |
| C | 12.32763400 | 0.73418600 | -0.34578000 |
| C | 11.22924300 | 0.11326500 | 0.42656500 |
| O | 12.90995900 | -2.70153300 | -0.91179100 |
| C | 10.54169800 | 0.72169700 | 1.45976300 |
| C | 14.25054800 | -0.02427900 | -1.64623800 |
| C | 14.61204500 | 1.30846600 | -1.83689200 |
| C | 13.83471700 | 2.33415000 | -1.29479700 |
| C | 12.69265300 | 2.06484300 | -0.53902300 |
| C | -8.85937500 | 2.30605300 | -0.27809600 |
| C | -8.10242800 | 3.47650700 | -0.34334500 |
| C | -6.72416300 | 3.24559800 | -0.34279300 |
| C | -6.38753100 | 1.88633900 | -0.24445000 |
| S | -7.81669900 | 0.91489400 | -0.17382200 |
| C | -10.26529300 | 2.29126500 | -0.14561800 |
| C | -11.20778400 | 1.29243300 | -0.09079000 |
| C | -12.48924300 | 1.59953600 | 0.60602100 |
| C | -13.10761900 | 0.28919400 | 0.91034600 |
| C | -12.32767200 | -0.73435000 | 0.34496100 |
| C | -11.22919200 | -0.11332500 | -0.42716100 |
| O | -12.91019000 | 2.70129200 | 0.91123100 |
| C | -10.54149600 | -0.72160600 | -1.46034300 |

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| C | -14.25079800 | 0.02391700 | 1.64522000 |
| C | -14.61229200 | -1.30885600 | 1.83566200 |
| C | -13.83486600 | -2.33446100 | 1.29355300 |
| C | -12.69269700 | -2.06504000 | 0.53798300 |
| C | 9.81842900 | -0.02387900 | 2.43204300 |
| N | 9.27017000 | -0.61078500 | 3.27399400 |
| C | 10.63098800 | 2.11405300 | 1.74020000 |
| N | 10.66924300 | 3.25080000 | 1.98656200 |
| C | -10.63070900 | -2.11393100 | -1.74095400 |
| N | -10.66892100 | -3.25064800 | -1.98746000 |
| C | -9.81814100 | 0.02413000 | -2.43243800 |
| N | -9.26980900 | 0.61117800 | -3.27424200 |
| H | 0.23213100 | -2.49995900 | 0.11265000 |
| H | -0.23210400 | 2.50000100 | -0.11220400 |
| H | 5.54252100 | 0.82765400 | 0.14182200 |
| H | -5.54248200 | -0.82764300 | -0.14140100 |
| H | 1.72304100 | 4.12535600 | 0.24222000 |
| H | 1.68612800 | 5.54403700 | 2.24510300 |
| H | 3.40590200 | 2.35753500 | 4.53811600 |
| H | 3.42360400 | 0.92718300 | 2.54390300 |
| H | 4.50172000 | 3.30171000 | -0.41817700 |
| H | 5.17118000 | 4.41411200 | -2.50090900 |
| H | 1.93454000 | 2.50482100 | -4.56231200 |
| H | 1.27024800 | 1.37830600 | -2.48621600 |
| H | -1.72306200 | -4.12533300 | -0.24198700 |
| H | -1.68610200 | -5.54386100 | -2.24500300 |
| H | -3.40568400 | -2.35711700 | -4.53782300 |
| H | -3.42343500 | -0.92694300 | -2.54350600 |
| H | 3.50182800 | 5.51679200 | 4.81683700 |
| H | 1.74663100 | 5.67040100 | 4.74001100 |
| H | 2.48584700 | 4.36314700 | 5.68131000 |
| H | 5.07597400 | 4.30830500 | -5.07017000 |
| H | 3.57262800 | 3.77032200 | -5.83834300 |
| H | 3.62259500 | 5.29779400 | -4.95440700 |
| H | -3.50437800 | -5.51157700 | -4.82024800 |
| H | -2.47964900 | -4.36292200 | -5.68090800 |
| H | -1.75019200 | -5.67389900 | -4.73717300 |
| H | -5.07632900 | -4.30143200 | 5.07395000 |
| H | -3.62999400 | -5.30028900 | 4.95133500 |
| H | -3.56693000 | -3.77480900 | 5.83803400 |
| H | -4.50172400 | -3.30166300 | 0.41839700 |
| H | -5.17124100 | -4.41422700 | 2.50098800 |
| H | -1.93455500 | -2.50525600 | 4.56261800 |
| H | -1.27018200 | -1.37856500 | 2.48661700 |
| H | 8.56467500 | -4.45477400 | 0.39231200 |
| H | 10.68743700 | -3.27261000 | -0.08019700 |
| H | 14.83627200 | -0.84003500 | -2.05828800 |
| H | 12.11043900 | 2.88334700 | -0.13401600 |
| H | -8.56469300 | 4.45476300 | -0.39182300 |
| H | -10.68750200 | 3.27249500 | 0.08011900 |
| H | -14.83659800 | 0.83961500 | 2.05727800 |
| H | -12.11041500 | -2.88348100 | 0.13294700 |
| O | 5.73921900 | -4.15623500 | 0.41264900 |
| O | -5.73923400 | 4.15630200 | -0.41170500 |
| C | 6.12352200 | -5.52061800 | 0.49817300 |
| C | -6.12359400 | 5.52065100 | -0.49748600 |
| H | 5.19761900 | -6.09185100 | 0.55012900 |
| H | 6.69161100 | -5.82374500 | -0.38802500 |
| H | 6.71790600 | -5.70336300 | 1.39988800 |
| H | -6.69201900 | 5.82382300 | 0.38848200 |
| H | -5.19770900 | 6.09194200 | -0.54914700 |
| H | -6.71767300 | 5.70327500 | -1.39942700 |
| H | 14.12301500 | 3.36726600 | -1.46268700 |
| H | 15.49904700 | 1.55409000 | -2.41249100 |
| H | -14.12317300 | -3.36760300 | 1.46127100 |
| H | -15.49937200 | -1.55457000 | 2.41110300 |

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|-----|-------------|-------------|-------------|
| 0 1 | | | |
| C | 1.41940100 | -0.31831100 | -0.11217900 |
| C | 0.61461900 | 0.82423800 | -0.16332200 |
| C | -0.75625200 | 0.64455900 | -0.14023700 |
| C | -1.30891400 | -0.65697400 | -0.05986600 |
| C | -0.50415900 | -1.79971200 | -0.01214400 |
| C | 0.86677700 | -1.62001600 | -0.03430100 |
| C | -1.85258600 | 1.72012200 | -0.16544000 |
| C | -3.09089000 | 0.84322500 | -0.07211600 |

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| C | -2.73989600 | -0.49154100 | -0.03245100 |
| C | 1.96338600 | -2.69559800 | -0.00595700 |
| C | 3.20269200 | -1.81789700 | -0.07796100 |
| C | 2.85043000 | -0.48269500 | -0.12603500 |
| C | -4.47817300 | 1.05029800 | -0.05832500 |
| C | -5.18331300 | -0.14476400 | 0.00559800 |
| S | -4.10340600 | -1.52721700 | 0.03960000 |
| C | 4.58833800 | -2.02200500 | -0.07910600 |
| C | 5.29499200 | -0.82629500 | -0.13341100 |
| S | 4.21243300 | 0.55434200 | -0.16560400 |
| C | 1.78860400 | -3.59998200 | -1.23155600 |
| C | 2.01020800 | -3.48652300 | 1.30725400 |
| C | -1.66486000 | 2.63787000 | 1.04788700 |
| C | -1.91371300 | 2.49848200 | -1.48586500 |
| C | 0.92155400 | -4.69634600 | -1.18268800 |
| C | 0.68793200 | -5.47241200 | -2.31208100 |
| C | 1.31266600 | -5.18797600 | -3.52992700 |
| C | 2.17496000 | -4.09054900 | -3.57433000 |
| C | 2.40941000 | -3.30820800 | -2.44738600 |
| C | 2.78458700 | -4.64992500 | 1.38520400 |
| C | 2.91456200 | -5.34251600 | 2.58217600 |
| C | 2.27741600 | -4.90268300 | 3.74720600 |
| C | 1.51373900 | -3.73758100 | 3.66638000 |
| C | 1.38114200 | -3.03850900 | 2.46898000 |
| C | -0.79388600 | 3.73003500 | 0.97779500 |
| C | -0.54855300 | 4.51997300 | 2.09484300 |
| C | -1.16579400 | 4.25453800 | 3.32083700 |
| C | -2.03246400 | 3.16176500 | 3.38625500 |
| C | -2.27819400 | 2.36503400 | 2.27173300 |
| C | -2.69465700 | 3.65741000 | -1.56713100 |
| C | -2.83771200 | 4.33909600 | -2.76867000 |
| C | -2.20690100 | 3.89302400 | -3.93491300 |
| C | -1.43576000 | 2.73327700 | -3.85028100 |
| C | -1.29049500 | 2.04449800 | -2.64823700 |
| C | 1.08513100 | -6.04986500 | -4.73943000 |
| C | 2.39352100 | -5.67327700 | 5.03175400 |
| C | -2.33841000 | 4.65224000 | -5.22471600 |
| C | -0.92613800 | 5.13222200 | 4.51654000 |
| C | -6.60269100 | -0.31581300 | 0.05550700 |
| C | 6.71322300 | -0.64785700 | -0.15346700 |
| S | -7.37271600 | -1.80841900 | -0.35637100 |
| C | -8.98661200 | -1.20990100 | -0.06375100 |
| C | -8.91070300 | 0.13138600 | 0.35691900 |
| C | -7.57703100 | 0.61351700 | 0.41269900 |
| S | 7.78040900 | -1.96225800 | 0.20825700 |
| C | 9.23105000 | -1.01022900 | 0.01614400 |
| C | 8.87665600 | 0.30385800 | -0.33992900 |
| C | 7.47175100 | 0.48958500 | -0.42525600 |
| C | 9.59148200 | 1.47103300 | -0.73494100 |
| C | 8.74630300 | 2.49113400 | -1.06309800 |
| S | 7.05267500 | 2.09648800 | -0.93413700 |
| C | -9.83974900 | 1.09030100 | 0.85477300 |
| C | -9.21755300 | 2.24497000 | 1.23285400 |
| S | -7.48582500 | 2.23272700 | 1.02763200 |
| C | 10.47391100 | -1.66366500 | 0.13252000 |
| C | -10.05560900 | -2.12077700 | -0.17587900 |
| C | 11.75550200 | -1.19365100 | 0.31296300 |
| C | -11.41869800 | -1.95274300 | -0.27214500 |
| C | 12.87274500 | -2.09444900 | -0.09405900 |
| C | 14.09345900 | -1.25994400 | -0.08811800 |
| C | 13.77345600 | 0.02163600 | 0.39046700 |
| C | 12.34584900 | 0.03671800 | 0.78607100 |
| C | -12.27174400 | -3.11394600 | 0.11507600 |
| C | -13.65055600 | -2.59083800 | 0.22144800 |
| C | -13.66425800 | -1.24304400 | -0.17509800 |
| C | -12.30428500 | -0.86905100 | -0.62845000 |
| C | 15.37362600 | -1.60084600 | -0.49045800 |
| C | 16.36223700 | -0.62014600 | -0.42792500 |
| C | 16.05290300 | 0.66219700 | 0.02984400 |
| C | 14.76497600 | 0.99902500 | 0.44971900 |
| C | -14.79170700 | -3.24710200 | 0.65052000 |
| C | -15.98237500 | -2.52422500 | 0.70093700 |
| C | -16.00552100 | -1.17954300 | 0.32525800 |
| C | -14.85696300 | -0.52447600 | -0.12226200 |
| O | 12.78295600 | -3.26816200 | -0.40761700 |
| C | 11.77033200 | 0.95872600 | 1.64144700 |
| C | -12.00742800 | 0.21283100 | -1.43736800 |
| O | -11.89464000 | -4.25058900 | 0.33819000 |
| C | 9.08484200 | 3.85567800 | -1.50543800 |
| O | 8.24978300 | 4.69292600 | -1.77814700 |

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| O | 10.40233600 | 4.04551400 | -1.56613100 |
| C | 10.81123300 | 5.35271600 | -1.98337300 |
| C | -9.82082400 | 3.47173800 | 1.78327800 |
| O | -9.17391800 | 4.45194600 | 2.08888800 |
| O | -11.14384500 | 3.36496200 | 1.90060000 |
| C | -11.80513800 | 4.52204300 | 2.42384400 |
| C | 10.51148300 | 0.74286100 | 2.26672800 |
| N | 9.50698900 | 0.57355600 | 2.82907800 |
| C | 12.43759000 | 2.13651900 | 2.08157300 |
| N | 12.94596100 | 3.11628300 | 2.45029700 |
| C | -10.77210100 | 0.33235500 | -2.13155500 |
| N | -9.79046300 | 0.43259900 | -2.74817000 |
| C | -12.95132000 | 1.22847700 | -1.75921100 |
| N | -13.69148500 | 2.08440800 | -2.03098300 |
| H | 1.05300500 | 1.81634300 | -0.21543000 |
| H | -0.94239400 | -2.79193200 | 0.04058000 |
| H | -4.95943800 | 2.01865100 | -0.13154100 |
| H | 5.07359300 | -2.99154700 | -0.05376400 |
| H | 0.43101600 | -4.95425000 | -0.24831200 |
| H | 0.00772200 | -6.31820700 | -2.24482300 |
| H | 2.67354500 | -3.84022300 | -4.50775100 |
| H | 3.08272700 | -2.45922400 | -2.52070300 |
| H | 3.28530400 | -5.02355500 | 0.49612200 |
| H | 3.52291600 | -6.24342700 | 2.61267300 |
| H | 1.01170700 | -3.36479700 | 4.55596300 |
| H | 0.78283200 | -2.13307700 | 2.44751600 |
| H | -0.30979300 | 3.97380300 | 0.03625000 |
| H | 0.13449200 | 5.36198000 | 2.01123800 |
| H | -2.52626000 | 2.92701500 | 4.32621900 |
| H | -2.95524300 | 1.52057200 | 2.36125700 |
| H | -3.19008500 | 4.03621000 | -0.67726100 |
| H | -3.45158700 | 5.23609800 | -2.80178700 |
| H | -0.93751400 | 2.35664200 | -4.74038800 |
| H | -0.68619000 | 1.14311800 | -2.62377500 |
| H | 0.07539500 | -6.46985900 | -4.74595800 |
| H | 1.22698700 | -5.48471100 | -5.66467400 |
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| H | 3.39046100 | -6.10838800 | 5.14728300 |
| H | 2.19561600 | -5.03681500 | 5.89829100 |
| H | 1.67403400 | -6.50018800 | 5.06078200 |
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| H | -1.64296300 | 5.49938300 | -5.25527100 |
| H | -2.11854500 | 4.01644500 | -6.08639700 |
| H | 0.08875800 | 5.53972100 | 4.51537500 |
| H | -1.61786000 | 5.98298900 | 4.52462000 |
| H | -1.07387500 | 4.58344900 | 5.45066700 |
| H | 10.66660800 | 1.56694400 | -0.78838800 |
| H | -10.90724400 | 0.94939000 | 0.94719300 |
| H | 10.45244500 | -2.74429900 | -0.02603300 |
| H | -9.78114700 | -3.17481100 | -0.09152200 |
| H | 15.58524800 | -2.60506600 | -0.84417200 |
| H | 17.37659300 | -0.84932800 | -0.73917500 |
| H | 16.83084200 | 1.41879500 | 0.06204500 |
| H | 14.56089500 | 2.00395100 | 0.79757600 |
| H | -14.74469900 | -4.29280100 | 0.93804400 |
| H | -16.89638300 | -3.00410600 | 1.03653800 |
| H | -16.93819100 | -0.62663000 | 0.38028500 |
| H | -14.91104400 | 0.51949200 | -0.40460800 |
| H | 11.89950000 | 5.33598700 | -1.97355100 |
| H | 10.43894400 | 5.56511800 | -2.98776500 |
| H | 10.43310200 | 6.10766400 | -1.29105200 |
| H | -12.86245800 | 4.26550600 | 2.45545800 |
| H | -11.43494100 | 4.75168700 | 3.42522300 |
| H | -11.63898600 | 5.38191400 | 1.77162400 |

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|-----|-------------|-------------|-------------|
| O 1 | | | |
| C | 1.14813200 | 0.78878200 | 0.03514800 |
| C | 1.22623900 | -0.62576000 | 0.04596300 |
| C | 0.07870800 | -1.42535900 | 0.00672100 |
| C | -1.14799000 | -0.78892300 | -0.03517900 |
| C | -1.22609800 | 0.62562000 | -0.04598500 |
| C | -0.07856600 | 1.42521700 | -0.00675600 |
| C | 2.54364300 | 1.42697900 | 0.10146500 |
| C | -2.54350300 | -1.42712100 | -0.10147900 |
| C | 2.62557700 | -0.96162300 | 0.10916500 |
| C | 3.40728700 | 0.17731000 | 0.15961700 |

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| C | 4.77681400 | -0.10179100 | 0.21573700 |
| C | 5.03966200 | -1.46890200 | 0.21138500 |
| S | 3.55044300 | -2.40405400 | 0.13238400 |
| C | -2.62543500 | 0.96148100 | -0.10916500 |
| C | -3.40714900 | -0.17745300 | -0.15959800 |
| C | -4.77668100 | 0.10164900 | -0.21553500 |
| C | -5.03953500 | 1.46876200 | -0.21107000 |
| S | -3.55030300 | 2.40391100 | -0.13215800 |
| C | 2.62863800 | 2.28485800 | 1.36900900 |
| C | 2.91966800 | 2.21129000 | -1.16175800 |
| C | -2.62851000 | -2.28498900 | -1.36902800 |
| C | 2.19609500 | 3.61478600 | 1.35308500 |
| C | 2.19070000 | 4.37771000 | 2.51525000 |
| C | 2.62013600 | 3.84550700 | 3.73441900 |
| C | 3.04670000 | 2.51584800 | 3.74603800 |
| C | 3.05046600 | 1.74674500 | 2.58612400 |
| C | 4.05833900 | 3.02576700 | -1.15288200 |
| C | 4.47348200 | 3.68697900 | -2.30148200 |
| C | 3.76931700 | 3.56294300 | -3.50396600 |
| C | 2.63989600 | 2.74372500 | -3.51009100 |
| C | 2.22021300 | 2.07697400 | -2.36100700 |
| C | -2.19591600 | -3.61491000 | -1.35312600 |
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| C | 2.64902700 | 4.68402300 | 4.98097500 |
| C | 4.20240200 | 4.30701600 | -4.73545300 |
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| C | -4.20226200 | -4.30721000 | 4.73541200 |
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| C | 7.98284900 | -3.74268400 | 0.28515900 |
| C | 6.61353500 | -3.46850900 | 0.27784100 |
| C | 6.32060200 | -2.09480300 | 0.25254600 |
| S | 7.77986600 | -1.16664100 | 0.26228000 |
| C | 10.18338000 | -2.61517500 | 0.19161800 |
| C | 11.15490100 | -1.64117900 | 0.22192500 |
| C | 12.43482400 | -1.93059900 | -0.48015800 |
| C | 13.09878500 | -0.61957700 | -0.66272200 |
| C | 12.34358200 | 0.37622900 | -0.02410900 |
| C | 11.20958600 | -0.26960200 | 0.67193700 |
| O | 12.83170300 | -3.01245600 | -0.87378300 |
| C | 10.51620600 | 0.27995300 | 1.73389300 |
| C | 14.26570300 | -0.34206100 | -1.35618600 |
| C | 14.66485100 | 0.98177800 | -1.41500900 |
| C | 13.91403200 | 1.98527700 | -0.79327100 |
| C | 12.75589900 | 1.70638000 | -0.08455200 |
| C | -8.77703200 | 2.59451900 | -0.29988200 |
| C | -7.98268200 | 3.74259600 | -0.28382900 |
| C | -6.61338200 | 3.46840200 | -0.27661600 |
| C | -6.32046800 | 2.09467200 | -0.25210100 |
| S | -7.77973800 | 1.16653300 | -0.26255400 |
| C | -10.18323200 | 2.61514100 | -0.19102900 |
| C | -11.15487600 | 1.64126700 | -0.22171600 |
| C | -12.43474300 | 1.93060900 | 0.48049200 |
| C | -13.09892500 | 0.61962100 | 0.66251600 |
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| C | -11.20975600 | 0.26987800 | -0.67223900 |
| O | -12.83145000 | 3.01236300 | 0.87457700 |
| C | -10.51638100 | -0.27940000 | -1.73434500 |
| C | -14.26594900 | 0.34205500 | 1.35578500 |
| C | -14.66537800 | -0.98172400 | 1.41399800 |
| C | -13.91472900 | -1.98510200 | 0.79185000 |
| C | -12.75649300 | -1.70614300 | 0.08333200 |
| C | 9.74713700 | -0.51424500 | 2.62915800 |
| N | 9.16062000 | -1.14766800 | 3.40926100 |
| C | 10.64043900 | 1.64444100 | 2.11716700 |
| N | 10.71234600 | 2.76019200 | 2.44017600 |
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| N | -10.71256400 | -2.75943600 | -2.44134100 |
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| H | 0.15152900 | -2.50886800 | 0.00727100 |
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| H | 5.56109000 | 0.64599200 | 0.25929700 |
| H | -5.56095700 | -0.64614000 | -0.25900300 |
| H | 1.86997000 | 4.06416300 | 0.41924000 |
| H | 1.84902200 | 5.40929200 | 2.47286200 |
| H | 3.38417600 | 2.07090400 | 4.67911800 |
| H | 3.38567100 | 0.71479000 | 2.63330500 |
| H | 4.62224700 | 3.15132900 | -0.23246000 |
| H | 5.36202200 | 4.31296800 | -2.26357500 |
| H | 2.07358700 | 2.62086200 | -4.43028500 |
| H | 1.33883700 | 1.44502600 | -2.40720200 |
| H | -1.86974600 | -4.06427700 | -0.41929300 |
| H | -1.84881900 | -5.40939500 | -2.47291700 |
| H | -3.38415200 | -2.07105000 | -4.67911200 |
| H | -3.38564000 | -0.71494400 | -2.63328500 |
| H | 3.60231200 | 5.21787400 | 5.07358300 |
| H | 1.85512900 | 5.43618800 | 4.97459500 |
| H | 2.53202500 | 4.06994100 | 5.87815400 |
| H | 5.29275200 | 4.35336600 | -4.81110400 |
| H | 3.81637600 | 3.83570900 | -5.64321100 |
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| H | -3.60141300 | -5.21953300 | -5.07260700 |
| H | -2.53374600 | -4.06990300 | -5.87827500 |
| H | -1.85380500 | -5.43509900 | -4.97541600 |
| H | -5.29262700 | -4.35009000 | 4.81305000 |
| H | -3.83869900 | -5.34152500 | 4.71855000 |
| H | -3.81304100 | -3.83817200 | 5.64297100 |
| H | -4.62202400 | -3.15159100 | 0.23243500 |
| H | -5.36172600 | -4.31329900 | 2.26352500 |
| H | -2.07341800 | -2.62098700 | 4.43027100 |
| H | -1.33872200 | -1.44509800 | 2.40719200 |
| H | 8.41325800 | -4.73644000 | 0.28392400 |
| H | 10.58108900 | -3.59097000 | -0.09384200 |
| H | 14.84650300 | -1.12240900 | -1.83600900 |
| H | 12.21808500 | 2.52541600 | 0.37634100 |
| H | -8.41307700 | 4.73635700 | -0.28199900 |
| H | -10.58085500 | 3.59084700 | 0.09485100 |
| H | -14.84659900 | 1.12233100 | 1.83590500 |
| H | -12.21883000 | -2.52509100 | -0.37789400 |
| O | 5.59988400 | -4.34896900 | 0.27929000 |
| O | -5.59971700 | 4.34884700 | -0.27752300 |
| C | 5.93946000 | -5.72814400 | 0.28824700 |
| C | -5.93928100 | 5.72803300 | -0.28529200 |
| H | 4.99513600 | -6.27076800 | 0.29350600 |
| H | 6.51115700 | -5.99622600 | -0.60686800 |
| H | 6.51373200 | -5.98300900 | 1.18547200 |
| H | -6.51085800 | 5.99537200 | 0.61012200 |
| H | -4.99495300 | 6.27065000 | -0.29023400 |
| H | -6.51367300 | 5.98364900 | -1.18222700 |
| F | -15.76890300 | -1.33556600 | 2.06658400 |
| F | -14.34390400 | -3.23988300 | 0.89638900 |
| F | 15.76826100 | 1.33554900 | -2.06783200 |
| F | 14.34292400 | 3.24010200 | -0.89840000 |

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| 0 1 | | | |
| C | -1.15301600 | 0.88298000 | -0.06132100 |
| C | -1.36819000 | -0.51610300 | -0.03340900 |
| C | -0.30748400 | -1.42707000 | -0.01338200 |
| C | 0.97615700 | -0.91387100 | -0.03054100 |
| C | 1.19139400 | 0.48531000 | -0.05119800 |
| C | 0.13066800 | 1.39636600 | -0.06265600 |
| C | 2.30344200 | -1.68473200 | -0.00302300 |
| C | 3.28283000 | -0.52551200 | -0.00272500 |
| C | 2.61898100 | 0.68461500 | -0.04587000 |
| C | -2.48063600 | 1.65424000 | -0.06055600 |
| C | -3.45983900 | 0.49540200 | -0.02130600 |
| C | -2.79573800 | -0.71529800 | -0.02140400 |
| C | -4.85340200 | 0.30954200 | -0.02129200 |
| C | -5.22074500 | -1.05234800 | -0.00991300 |
| S | -3.82682400 | -2.10417800 | -0.01514000 |
| S | -6.24257900 | 1.31435700 | -0.01762700 |
| C | -7.31854600 | -0.09318700 | 0.00563100 |
| C | -6.59407000 | -1.28619800 | 0.00394400 |
| C | 4.67625500 | -0.34028100 | -0.01461500 |

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| C | 5.04450000 | 1.02077100 | -0.05533100 |
| S | 3.65076200 | 2.07227800 | -0.09404600 |
| S | 6.06482600 | -1.34552700 | 0.01717400 |
| C | 7.14172300 | 0.06082800 | -0.02010400 |
| C | 6.41814900 | 1.25370100 | -0.05945100 |
| C | -2.72932600 | 2.44330400 | -1.35496300 |
| C | -2.53005400 | 2.53439900 | 1.19414200 |
| C | 2.35044900 | -2.52649500 | 1.27789000 |
| C | 2.55430500 | -2.51333600 | -1.27203800 |
| C | -8.70460300 | 0.19983800 | 0.00376000 |
| C | 8.52730900 | -0.23365300 | -0.02861800 |
| C | -9.83313100 | -0.58987200 | 0.05287900 |
| C | 9.65651400 | 0.55619000 | -0.01407500 |
| C | 11.02870800 | 0.05154700 | -0.03254100 |
| C | 11.93305600 | 1.20313100 | 0.17513900 |
| C | 11.16097000 | 2.37080300 | 0.24129700 |
| C | 9.73053400 | 2.03237400 | 0.10766000 |
| C | -11.20653100 | -0.08749500 | 0.03873300 |
| C | -12.10781700 | -1.23877500 | 0.26229600 |
| C | -11.33292600 | -2.40347100 | 0.34356100 |
| C | -9.90380800 | -2.06378800 | 0.20136600 |
| C | 13.32053800 | 1.29782200 | 0.29645200 |
| C | 13.88670400 | 2.55974300 | 0.47590300 |
| C | 13.10302300 | 3.71471900 | 0.53198100 |
| C | 11.71815400 | 3.62656300 | 0.41390600 |
| C | -13.49494600 | -1.33563600 | 0.38682400 |
| C | -14.05751500 | -2.59637900 | 0.58475500 |
| C | -13.27075300 | -3.74837700 | 0.65660800 |
| C | -11.88634600 | -3.65812600 | 0.53528600 |
| C | -2.05086000 | 2.13759800 | -2.53609200 |
| C | -2.33449900 | 2.79396900 | -3.73700800 |
| C | -3.33316500 | 3.77060300 | -3.74342400 |
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| C | -3.04286100 | 2.85684400 | 3.53257300 |
| C | -2.45229600 | 4.11320600 | 3.50222200 |
| C | -1.88960400 | 4.60441900 | 2.31870800 |
| C | -1.93902400 | 3.80315700 | 1.17824600 |
| C | 1.76461500 | -3.79659700 | 1.30122400 |
| C | 1.72935200 | -4.52686900 | 2.48351200 |
| C | 2.27854600 | -4.00474700 | 3.65121400 |
| C | 2.87233300 | -2.74143400 | 3.65137200 |
| C | 2.89412100 | -2.01503600 | 2.45635000 |
| C | 3.55936000 | -3.48458500 | -1.26975700 |
| C | 3.89303700 | -4.20263200 | -2.42116500 |
| C | 3.18657600 | -3.93681200 | -3.59633500 |
| C | 2.18358000 | -2.97292400 | -3.61398800 |
| C | 1.86800000 | -2.25941300 | -2.46177800 |
| C | -1.56126200 | 2.47209200 | -4.98538300 |
| C | -1.25661600 | 5.96737600 | 2.27970000 |
| C | 3.49940500 | -2.17853800 | 4.89614400 |
| C | 4.99952600 | -5.21934600 | -2.38848500 |
| O | 8.82019700 | 2.84758800 | 0.11468300 |
| O | -8.99202500 | -2.87724800 | 0.21978000 |
| C | 11.45810400 | -1.24314200 | -0.24897700 |
| C | -11.64090000 | 1.20513800 | -0.18022300 |
| C | -13.01393900 | 1.58526100 | -0.16822300 |
| N | -14.11663400 | 1.95679300 | -0.16906500 |
| C | -10.79192700 | 2.31241300 | -0.46786100 |
| N | -10.14992700 | 3.25223400 | -0.71185000 |
| C | 12.83002900 | -1.62719300 | -0.24140600 |
| N | 13.93196000 | -2.00094000 | -0.24502400 |
| C | 10.60314000 | -2.34666600 | -0.53358000 |
| N | 9.95471300 | -3.28234500 | -0.77653000 |
| H | -0.48710700 | -2.49733900 | 0.01830100 |
| H | 0.31035100 | 2.46705100 | -0.06860500 |
| H | -7.08852800 | -2.24856100 | 0.01448300 |
| H | 6.91343100 | 2.21531200 | -0.08779800 |
| H | -8.89596000 | 1.26821200 | -0.03325900 |
| H | 8.71786400 | -1.30281500 | -0.03682300 |
| H | 13.96441400 | 0.42911800 | 0.26096900 |
| H | 14.96475300 | 2.64153600 | 0.57410200 |
| H | 13.57829400 | 4.68088600 | 0.66986900 |
| H | 11.08035300 | 4.50392300 | 0.45509000 |
| H | -14.14152000 | -0.46956500 | 0.33938700 |
| H | -15.13526400 | -2.67957000 | 0.68508800 |
| H | -13.74324800 | -4.71371700 | 0.80907700 |
| H | -11.24596900 | -4.53297700 | 0.58820800 |
| H | -1.28032200 | 1.37157600 | -2.52930000 |

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|---|-------------|-------------|-------------|
| H | -3.57145300 | 4.28902700 | -4.66880100 |
| H | -4.79915100 | 4.84086000 | -2.59009200 |
| H | -4.25769000 | 3.68908300 | -0.47740500 |
| H | -3.54079600 | 1.08247300 | 2.42522400 |
| H | -3.47984800 | 2.48514200 | 4.45500200 |
| H | -2.42893700 | 4.72400500 | 4.40141800 |
| H | -1.52134400 | 4.18549300 | 0.25015800 |
| H | 1.34833400 | -4.21944700 | 0.39178700 |
| H | 1.27095200 | -5.51167300 | 2.49356700 |
| H | 2.24859300 | -4.58372400 | 4.57079100 |
| H | 3.34380200 | -1.02520200 | 2.45328800 |
| H | 4.08629700 | -3.70599000 | -0.34450100 |
| H | 3.42300200 | -4.49101300 | -4.50111800 |
| H | 1.63806000 | -2.77642900 | -4.53265100 |
| H | 1.08362200 | -1.51005000 | -2.49040700 |
| H | -1.17095900 | 1.45105000 | -4.96272800 |
| H | -2.18313700 | 2.58145500 | -5.87822800 |
| H | -0.70493400 | 3.14703300 | -5.10113800 |
| H | -1.98951600 | 6.74939400 | 2.50600400 |
| H | -0.45654600 | 6.05320500 | 3.02257700 |
| H | -0.82961100 | 6.18261000 | 1.29710100 |
| H | 3.06188800 | -2.61788300 | 5.79652200 |
| H | 4.57589000 | -2.38509700 | 4.92000400 |
| H | 3.37654600 | -1.09309700 | 4.94990600 |
| H | 5.98044200 | -4.73013700 | -2.40259400 |
| H | 4.95662900 | -5.82764400 | -1.48008000 |
| H | 4.95216700 | -5.88885800 | -3.25111100 |

IT-DM

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|---|-------------|-------------|-------------|
| C | 1.01917300 | 0.95060700 | 0.05453300 |
| C | 1.30308400 | -0.43625700 | 0.05599100 |
| C | 0.28871600 | -1.39876800 | 0.05125000 |
| C | -1.01906900 | -0.95024900 | 0.05702400 |
| C | -1.30299400 | 0.43660700 | 0.05395300 |
| C | -0.28861900 | 1.39909900 | 0.04668700 |
| C | -2.30707400 | -1.78638500 | 0.04337700 |
| C | -3.34232600 | -0.67642700 | 0.03070000 |
| C | -2.73892600 | 0.56507500 | 0.05062000 |
| C | 2.30722100 | 1.78666700 | 0.03883000 |
| C | 3.34245000 | 0.67665200 | 0.03026200 |
| C | 2.73901000 | -0.56476300 | 0.05383900 |
| C | -2.32296300 | -2.64188500 | -1.22801900 |
| C | -2.50492500 | -2.61459500 | 1.32067100 |
| C | -1.66651300 | -3.87727900 | -1.25484600 |
| C | -1.60430200 | -4.62615400 | -2.42348500 |
| C | -2.19744900 | -4.17505200 | -3.60696800 |
| C | -2.84792500 | -2.94057900 | -3.57580900 |
| C | -2.91030200 | -2.18447700 | -2.40829100 |
| C | -3.43948900 | -3.65527500 | 1.34141800 |
| C | -3.69944800 | -4.35859100 | 2.51216500 |
| C | -3.03644100 | -4.05280500 | 3.70387100 |
| C | -2.10945500 | -3.00848100 | 3.67967200 |
| C | -1.84753600 | -2.29924100 | 2.51134000 |
| C | 2.50446200 | 2.61906900 | 1.31348600 |
| C | 2.32375100 | 2.63811400 | -1.23528000 |
| C | 1.84663800 | 2.30752000 | 2.50492900 |
| C | 2.10807500 | 3.02055300 | 3.67104400 |
| C | 3.03500300 | 4.06501200 | 3.69220500 |
| C | 3.69839800 | 4.36700800 | 2.49976300 |
| C | 3.43889500 | 3.65989900 | 1.33118900 |
| C | 2.91248300 | 2.17750500 | -2.41357600 |
| C | 2.85055700 | 2.92997200 | -3.58350800 |
| C | 2.19918200 | 4.16381100 | -3.61908800 |
| C | 1.60472300 | 4.61819800 | -2.43748200 |
| C | 1.66649400 | 3.87301000 | -1.26650600 |
| C | 3.29204700 | 4.85370200 | 4.94482600 |
| C | 2.16068500 | 4.99065700 | -4.87294600 |
| C | -3.29400400 | -4.83750700 | 4.95888800 |
| C | -2.15877400 | -5.00584200 | -4.85820700 |
| C | -4.74371600 | -0.56001900 | 0.03808000 |
| C | -5.17850200 | 0.78112100 | 0.05500200 |
| S | -3.83856200 | 1.90052400 | 0.07530100 |

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|---|--------------|-------------|-------------|
| C | 4.74383500 | 0.56022400 | 0.03889300 |
| C | 5.17856500 | -0.78086500 | 0.06047100 |
| S | 3.83858500 | -1.90015300 | 0.08359300 |
| S | -6.08221100 | -1.63213100 | 0.01561100 |
| C | -7.22675800 | -0.27946000 | 0.02507100 |
| C | -6.56241200 | 0.94662300 | 0.04903700 |
| S | 6.08238400 | 1.63222000 | 0.01377900 |
| C | 7.22686700 | 0.27955200 | 0.02824500 |
| C | 6.56247800 | -0.94642300 | 0.05591500 |
| C | -8.59812400 | -0.64163300 | 0.01444900 |
| C | 8.59827900 | 0.64155800 | 0.01743600 |
| C | -9.76432800 | 0.09035900 | 0.00144700 |
| C | 9.76434800 | -0.09066600 | 0.00629800 |
| C | -11.11310300 | -0.48024300 | -0.01340900 |
| C | -12.07030000 | 0.64027000 | -0.09671000 |
| C | -11.35623400 | 1.84267500 | -0.10050300 |
| C | -9.91103600 | 1.56799300 | -0.03330000 |
| C | 11.11317300 | 0.47975800 | -0.00939000 |
| C | 12.07008600 | -0.64071200 | -0.09612500 |
| C | 11.35593700 | -1.84307700 | -0.09859900 |
| C | 9.91089600 | -1.56833300 | -0.02803900 |
| C | 13.46256100 | -0.68895800 | -0.16699400 |
| C | 14.11593600 | -1.92277200 | -0.23705000 |
| C | 13.37654900 | -3.12999300 | -0.23421900 |
| C | 11.98398100 | -3.07364700 | -0.16388700 |
| C | -13.46296800 | 0.68851500 | -0.16376000 |
| C | -14.11657600 | 1.92233000 | -0.23157700 |
| C | -13.37722700 | 3.12957300 | -0.23047800 |
| C | -11.98448200 | 3.07324400 | -0.16382100 |
| O | -9.03813000 | 2.42397900 | -0.01669900 |
| O | 9.03799800 | -2.42427500 | -0.00918100 |
| C | -11.48001400 | -1.81109600 | 0.05378300 |
| C | 11.48028800 | 1.81036900 | 0.06113200 |
| C | 14.07818200 | -4.45243800 | -0.30690700 |
| C | -14.07909200 | 4.45201100 | -0.30101900 |
| C | 15.61382600 | -1.95957300 | -0.31600100 |
| C | -15.61468900 | 1.95909400 | -0.30622700 |
| C | 12.83418400 | 2.25276500 | 0.03468100 |
| N | 13.91793200 | 2.67640000 | 0.01698700 |
| C | 10.57610600 | 2.90428500 | 0.18090700 |
| N | 9.88879700 | 3.83848000 | 0.28213900 |
| C | -12.83391600 | -2.25355100 | 0.02843700 |
| N | -13.91762200 | -2.67732500 | 0.01145100 |
| C | -10.57562900 | -2.90546400 | 0.16774200 |
| N | -9.88818100 | -3.84008900 | 0.26396800 |
| H | 0.52159900 | -2.45912900 | 0.04085400 |
| H | -0.52152700 | 2.45941200 | 0.03284000 |
| H | -1.20929800 | -4.26569500 | -0.34906900 |
| H | -1.08713200 | -5.58271500 | -2.41533300 |
| H | -3.31673300 | -2.56024600 | -4.48009800 |
| H | -3.41933800 | -1.22517500 | -2.42352200 |
| H | -3.96106600 | -3.93111500 | 0.42915400 |
| H | -4.43244000 | -5.16152500 | 2.49773300 |
| H | -1.58093900 | -2.74196300 | 4.59189200 |
| H | -1.12292000 | -1.49107100 | 2.53296400 |
| H | 1.12207100 | 1.49937200 | 2.52888700 |
| H | 1.57924900 | 2.75696100 | 4.58393300 |
| H | 4.43134200 | 5.16993900 | 2.48301800 |
| H | 3.96073900 | 3.93283800 | 0.41820600 |
| H | 3.42226100 | 1.21855000 | -2.42542000 |
| H | 3.32047500 | 2.54721000 | -4.48619400 |
| H | 1.08688600 | 5.57442300 | -2.43272500 |
| H | 1.20830300 | 4.26392200 | -0.36230000 |
| H | 3.10892400 | 4.25261700 | 5.83967100 |
| H | 4.32225100 | 5.21857100 | 4.98168800 |
| H | 2.63460500 | 5.72956900 | 4.99967900 |
| H | 2.30373100 | 4.37261600 | -5.76326400 |
| H | 1.20880300 | 5.52032000 | -4.97266100 |
| H | 2.95369000 | 5.74776800 | -4.86817300 |
| H | -4.32500500 | -5.19993200 | 4.99777200 |
| H | -2.63853800 | -5.71474500 | 5.01540900 |
| H | -3.10861700 | -4.23443200 | 5.85191700 |
| H | -1.20931200 | -5.54069100 | -4.95299600 |
| H | -2.95574300 | -5.75879100 | -4.85399100 |
| H | -2.29556500 | -4.38975600 | -5.75087200 |
| H | -7.10516700 | 1.88252500 | 0.05973600 |
| H | 7.10519100 | -1.88230800 | 0.06996400 |
| H | -8.73413500 | -1.71887700 | 0.00973900 |
| H | 8.73447700 | 1.71877200 | 0.01011200 |
| H | 14.06487200 | 0.21053800 | -0.17234700 |

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|---|--------------|-------------|-------------|
| H | 11.38878300 | -3.98262000 | -0.16075800 |
| H | -14.06529300 | -0.21097300 | -0.16760900 |
| H | -11.38929700 | 3.98222900 | -0.16196600 |
| H | 14.68170100 | -4.53337400 | -1.21812000 |
| H | 14.76388300 | -4.58597300 | 0.53756000 |
| H | 13.36427400 | -5.27850100 | -0.29825400 |
| H | -14.68481700 | 4.53319700 | -1.21074500 |
| H | -14.76274900 | 4.58524900 | 0.54514800 |
| H | -13.36520600 | 5.27810900 | -0.29385500 |
| H | 16.03579500 | -0.95273300 | -0.30862700 |
| H | 16.04268800 | -2.51424700 | 0.52629900 |
| H | 15.95127800 | -2.46303600 | -1.22910700 |
| H | -16.03657400 | 0.95222400 | -0.29821600 |
| H | -16.04116400 | 2.51325900 | 0.53762200 |
| H | -15.95478800 | 2.46306100 | -1.21806800 |

IT-M

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|---|--------------|-------------|-------------|
| C | 1.03402400 | 0.93419700 | 0.01519600 |
| C | 1.29600100 | -0.45703500 | 0.01790900 |
| C | 0.26643500 | -1.40322700 | 0.01368100 |
| C | -1.03394400 | -0.93379700 | 0.01884400 |
| C | -1.29593300 | 0.45743100 | 0.01475000 |
| C | -0.26636100 | 1.40359100 | 0.00681500 |
| C | -2.33482600 | -1.74961600 | 0.00570500 |
| C | -3.35236000 | -0.62352600 | -0.00601900 |
| C | -2.72962500 | 0.60859900 | 0.01239400 |
| C | 2.33493700 | 1.74993100 | -0.00086100 |
| C | 3.35246700 | 0.62378800 | -0.00662500 |
| C | 2.72968800 | -0.60822000 | 0.01731500 |
| C | -2.36398000 | -2.60426200 | -1.26611200 |
| C | -2.54522200 | -2.57531100 | 1.28263000 |
| C | -1.72561100 | -3.84908700 | -1.29328700 |
| C | -1.67408100 | -4.59837600 | -2.46212300 |
| C | -2.26050600 | -4.13827900 | -3.64553200 |
| C | -2.89322800 | -2.89465300 | -3.61390600 |
| C | -2.94470500 | -2.13801900 | -2.44614600 |
| C | -3.49463700 | -3.60241100 | 1.30248600 |
| C | -3.76500200 | -4.30254300 | 2.47286100 |
| C | -3.09813900 | -4.00685800 | 3.66489500 |
| C | -2.15642000 | -2.97568300 | 3.64163000 |
| C | -1.88392600 | -2.26977100 | 2.47376800 |
| C | 2.54443800 | 2.58153900 | 1.27238700 |
| C | 2.36500400 | 2.59881800 | -1.27649300 |
| C | 1.88251300 | 2.28139500 | 2.46453800 |
| C | 2.15430700 | 2.99269000 | 3.62930100 |
| C | 3.09590700 | 4.02404800 | 3.64835100 |
| C | 3.76334700 | 4.31438800 | 2.45531500 |
| C | 3.49367100 | 3.60888200 | 1.28802300 |
| C | 2.94758700 | 2.12783800 | -2.45371900 |
| C | 2.89683800 | 2.87923700 | -3.62490400 |
| C | 2.26304000 | 4.12212600 | -3.66285900 |
| C | 1.67485200 | 4.58702300 | -2.48219300 |
| C | 1.72568000 | 3.84300600 | -1.30997900 |
| C | 3.36390800 | 4.81143500 | 4.89948500 |
| C | 2.23638100 | 4.94720800 | -4.91817200 |
| C | -3.36680300 | -4.78853400 | 4.91946600 |
| C | -2.23325500 | -4.96903900 | -4.89707800 |
| C | -4.75144800 | -0.48525400 | 0.00542000 |
| C | -5.16539400 | 0.86280600 | 0.02332000 |
| S | -3.80795800 | 1.96130900 | 0.03933500 |
| C | 4.75154900 | 0.48552600 | 0.00653100 |
| C | 5.16542500 | -0.86244200 | 0.03139200 |
| S | 3.80795000 | -1.96081400 | 0.05180100 |
| S | -6.10573700 | -1.53683000 | -0.01083500 |
| C | -7.22962100 | -0.16688500 | 0.00347700 |
| C | -6.54629000 | 1.04946000 | 0.02302800 |
| S | 6.10590200 | 1.53695700 | -0.01405800 |
| C | 7.22970800 | 0.16704200 | 0.00766300 |
| C | 6.54631100 | -1.04915200 | 0.03293800 |
| C | -8.60529300 | -0.50912900 | 0.00139600 |
| C | 8.60542900 | 0.50908100 | 0.00497900 |
| C | -9.76193200 | 0.23918300 | 0.00258500 |
| C | 9.76188400 | -0.23950600 | 0.00887200 |
| C | -11.11848400 | -0.31205400 | 0.00020700 |
| C | -12.06182600 | 0.82237400 | -0.03916700 |
| C | -11.33169400 | 2.01678900 | -0.04118500 |

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| C | -9.88713300 | 1.71736700 | -0.01283900 |
| C | 11.11851500 | 0.31148400 | 0.00504900 |
| C | 12.06156400 | -0.82295900 | -0.03977300 |
| C | 11.33128400 | -2.01729400 | -0.03973700 |
| C | 9.88685500 | -1.71772400 | -0.00607900 |
| C | 13.45653900 | -0.89337300 | -0.07950200 |
| C | 14.05942300 | -2.14689600 | -0.11437400 |
| C | 13.32476200 | -3.34402300 | -0.10835100 |
| C | 11.93016300 | -3.26402800 | -0.07274900 |
| C | -13.45697400 | 0.89269700 | -0.07280000 |
| C | -14.06013200 | 2.14617300 | -0.10413800 |
| C | -13.32556500 | 3.34337400 | -0.10060100 |
| C | -11.93083300 | 3.26348800 | -0.07094800 |
| O | -9.00309900 | 2.56140700 | -0.00734400 |
| O | 9.00276700 | -2.56167500 | 0.00276100 |
| C | -11.50425700 | -1.63860300 | 0.03921000 |
| C | 11.50453900 | 1.63778200 | 0.04918700 |
| C | 14.02968200 | -4.66764100 | -0.12396300 |
| C | -14.03071300 | 4.66691100 | -0.11244900 |
| C | 12.86579800 | 2.05766800 | 0.03942700 |
| N | 13.95712900 | 2.46161300 | 0.03348800 |
| C | 10.61527400 | 2.74810100 | 0.11867400 |
| N | 9.94003500 | 3.69459800 | 0.17795100 |
| C | -12.86548700 | -2.05863500 | 0.03167500 |
| N | -13.95674400 | -2.46280500 | 0.02733400 |
| C | -10.61476600 | -2.74929900 | 0.09915800 |
| N | -9.93938800 | -3.69617700 | 0.15026000 |
| H | 0.48203200 | -2.46718100 | 0.00454500 |
| H | -0.48198500 | 2.46747900 | -0.00753500 |
| H | -1.27430000 | -4.24438800 | -0.38754900 |
| H | -1.17078800 | -5.56230600 | -2.45423000 |
| H | -3.35654600 | -2.50735900 | -4.51806500 |
| H | -3.43975900 | -1.17140700 | -2.46125200 |
| H | -4.01974200 | -3.87039600 | 0.38989000 |
| H | -4.50925700 | -5.09502400 | 2.45779300 |
| H | -1.62456300 | -2.71715700 | 4.55420300 |
| H | -1.14782900 | -1.47204400 | 2.49606600 |
| H | 1.14648600 | 1.48370100 | 2.49009500 |
| H | 1.62199200 | 2.73830700 | 4.54276800 |
| H | 4.50751500 | 5.10688300 | 2.43702900 |
| H | 4.01915000 | 3.87278000 | 0.37445700 |
| H | 3.44352500 | 1.16161800 | -2.46392900 |
| H | 3.36160600 | 2.48835500 | -4.52677300 |
| H | 1.17074300 | 5.55055500 | -2.47917400 |
| H | 1.27304700 | 4.24197300 | -0.40651500 |
| H | 3.17982400 | 4.21223200 | 5.79541300 |
| H | 4.39691500 | 5.16863000 | 4.93203600 |
| H | 2.71311000 | 5.69210700 | 4.95647100 |
| H | 2.37107400 | 4.32571600 | -5.80737700 |
| H | 1.29194700 | 5.48981400 | -5.01905800 |
| H | 3.03977100 | 5.69329100 | -4.91443300 |
| H | -4.39937900 | -5.14692400 | 4.95236700 |
| H | -2.71490300 | -5.66804200 | 4.98158000 |
| H | -3.18469700 | -4.18477200 | 5.81273700 |
| H | -1.28970700 | -5.51391500 | -4.99389400 |
| H | -3.03810400 | -5.71353800 | -4.89137900 |
| H | -2.36524100 | -4.35130000 | -5.78930100 |
| H | -7.07391700 | 1.99391100 | 0.03572100 |
| H | 7.07387800 | -1.99355900 | 0.05058400 |
| H | -8.75670000 | -1.58432900 | -0.00528300 |
| H | 8.75709200 | 1.58422100 | -0.00582400 |
| H | 14.08038500 | -0.00946400 | -0.08806400 |
| H | 15.14438300 | -2.20066800 | -0.14893600 |
| H | 11.31356400 | -4.15856500 | -0.07219300 |
| H | -14.08078900 | 0.00875200 | -0.07902300 |
| H | -15.14524200 | 2.19985300 | -0.13379700 |
| H | -11.31433400 | 4.15809100 | -0.07240700 |
| H | 14.48700900 | -4.87257300 | 0.85074200 |
| H | 13.34050200 | -5.48485600 | -0.34769500 |
| H | 14.83370800 | -4.67911900 | -0.86569200 |
| H | -14.83639400 | 4.67948100 | -0.85237100 |
| H | -14.48593600 | 4.87015900 | 0.86359200 |
| H | -13.34217100 | 5.48460100 | -0.33639700 |

ITCPTC

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|-----|--------------|-------------|-------------|
| 0 1 | | | |
| C | -1.27988400 | -0.50047900 | 0.06082800 |
| C | -1.06424400 | 0.89894800 | 0.06401300 |
| C | -0.21939300 | -1.41201700 | 0.05738300 |
| C | 1.06425600 | -0.89893000 | 0.06414400 |
| C | 1.27989600 | 0.50049900 | 0.06073400 |
| C | 0.21940500 | 1.41203700 | 0.05715200 |
| C | 2.39103700 | -1.67133700 | 0.04688900 |
| C | 3.37053600 | -0.51232700 | 0.02368400 |
| C | 2.70740400 | 0.69904600 | 0.04811700 |
| C | 4.76359300 | -0.32761100 | 0.01857200 |
| C | 5.13266400 | 1.03438900 | 0.02981600 |
| S | 3.73956300 | 2.08718800 | 0.06110400 |
| S | 6.15080200 | -1.33422000 | -0.01530400 |
| C | 7.22892600 | 0.07242200 | -0.01817800 |
| C | 6.50551000 | 1.26672100 | 0.01000800 |
| C | -2.39102400 | 1.67135300 | 0.04665500 |
| C | -3.37052500 | 0.51233600 | 0.02361900 |
| C | -2.70739100 | -0.69903100 | 0.04824100 |
| C | -4.76358300 | 0.32761700 | 0.01857500 |
| C | -5.13265000 | -1.03438300 | 0.03006100 |
| S | -3.73954400 | -2.08717500 | 0.06149500 |
| S | -6.15079400 | 1.33421200 | -0.01547700 |
| C | -7.22891600 | -0.07243200 | -0.01810400 |
| C | -6.50549500 | -1.26672100 | 0.01028900 |
| C | -2.63689500 | 2.48134800 | 1.32748100 |
| C | -2.44014700 | 2.53227200 | -1.22017200 |
| C | 2.63690600 | -2.48115300 | 1.32783300 |
| C | 2.44016500 | -2.53245300 | -1.21979800 |
| C | -3.62709600 | 3.46918900 | 1.34965200 |
| C | -3.92692900 | 4.15364700 | 2.52213400 |
| C | -3.25037400 | 3.88063900 | 3.71409000 |
| C | -2.26826800 | 2.88786300 | 3.68866000 |
| C | -1.96576700 | 2.19799900 | 2.51862800 |
| C | -1.85602700 | 3.80326000 | -1.23171000 |
| C | -1.82058600 | 4.56083800 | -2.39613800 |
| C | -2.36972200 | 4.08270200 | -3.58988100 |
| C | -2.94788600 | 2.81212000 | -3.57382000 |
| C | -2.98287400 | 2.04747800 | -2.41104900 |
| C | 3.62705000 | -3.46906300 | 1.35010500 |
| C | 3.92688400 | -4.15336900 | 2.52266400 |
| C | 3.25038800 | -3.88014100 | 3.71461700 |
| C | 2.26835500 | -2.88731200 | 3.68908200 |
| C | 1.96584800 | -2.19759000 | 2.51895500 |
| C | 1.85580000 | -3.80335900 | -1.23118300 |
| C | 1.82034300 | -4.56112300 | -2.39545800 |
| C | 2.36973000 | -4.08329100 | -3.58923800 |
| C | 2.94816900 | -2.81286300 | -3.57332000 |
| C | 2.98314900 | -2.04799400 | -2.41066600 |
| C | -3.55058400 | 4.64687000 | 4.97101500 |
| C | -2.36280800 | 4.92077900 | -4.83677200 |
| C | 3.55064100 | -4.64624700 | 4.97160800 |
| C | 2.36260400 | -4.92165700 | -4.83593400 |
| C | 8.61298700 | -0.22250700 | -0.04668700 |
| C | -8.61297700 | 0.22249000 | -0.04659300 |
| C | 9.74872100 | 0.56053200 | -0.05514900 |
| C | -9.74872400 | -0.56053400 | -0.05497500 |
| C | 11.11077600 | 0.02294800 | -0.08892500 |
| C | 12.02308300 | 1.16721100 | -0.07429800 |
| C | 11.26469800 | 2.37193400 | -0.03762600 |
| C | 9.82899000 | 2.05089700 | -0.02612500 |
| C | -11.11076900 | -0.02291900 | -0.08875500 |
| C | -12.02309900 | -1.16716500 | -0.07433300 |
| C | -11.26474100 | -2.37190500 | -0.03767200 |
| C | -9.82902700 | -2.05089900 | -0.02598900 |
| C | 13.37504500 | 1.39705500 | -0.08685000 |
| S | 13.69148200 | 3.08834600 | -0.05316400 |
| C | 12.02123400 | 3.50401900 | -0.02240700 |
| C | -13.37506400 | -1.39698500 | -0.08705600 |
| S | -13.69153400 | -3.08827400 | -0.05354400 |
| C | -12.02129700 | -3.50397900 | -0.02262600 |
| O | 8.91312200 | 2.85821000 | 0.00204100 |
| O | -8.91318100 | -2.85823100 | 0.00227000 |
| C | -11.54514500 | 1.28858300 | -0.13016600 |
| C | 11.54517400 | -1.28853900 | -0.13055000 |
| C | -10.70652300 | 2.43652000 | -0.15213200 |
| N | -10.05868300 | 3.40369300 | -0.17170900 |
| C | -12.93446900 | 1.59510200 | -0.15701900 |
| N | -14.06838600 | 1.85616600 | -0.17908200 |
| C | 10.70656200 | -2.43647400 | -0.15285900 |

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|---|--------------|-------------|-------------|
| N | 10.05872100 | -3.40364100 | -0.17273900 |
| C | 12.93450400 | -1.59503400 | -0.15732700 |
| N | 14.06843600 | -1.85603800 | -0.17936200 |
| H | -0.39923200 | -2.48266600 | 0.04440700 |
| H | 0.39923700 | 2.48268600 | 0.04400200 |
| H | 7.00198700 | 2.22810700 | 0.01450100 |
| H | -7.00196100 | -2.22811200 | 0.01493900 |
| H | -4.16151500 | 3.71955300 | 0.43738700 |
| H | -4.70213900 | 4.91587600 | 2.50877500 |
| H | -1.72779700 | 2.64741800 | 4.60110200 |
| H | -1.19798200 | 1.43070400 | 2.53932100 |
| H | -1.43492000 | 4.21203000 | -0.31753200 |
| H | -1.35970900 | 5.54554200 | -2.37610600 |
| H | -3.38055500 | 2.40997900 | -4.48665900 |
| H | -3.43407300 | 1.05980500 | -2.43845500 |
| H | 4.16141600 | -3.71958400 | 0.43785100 |
| H | 4.70204400 | -4.91565200 | 2.50938200 |
| H | 1.72793400 | -2.64670400 | 4.60151000 |
| H | 1.19811200 | -1.43024400 | 2.53957200 |
| H | 1.43452500 | -4.21189100 | -0.31697400 |
| H | 1.35926900 | -5.54573500 | -2.37530300 |
| H | 3.38107900 | -2.41100200 | -4.48616400 |
| H | 3.43456100 | -1.06042300 | -2.43819900 |
| H | -2.91832200 | 5.53949900 | 5.04695800 |
| H | -4.59094600 | 4.98256600 | 4.99455700 |
| H | -3.36547500 | 4.04065400 | 5.86206000 |
| H | -1.46855400 | 5.54810400 | -4.89104600 |
| H | -2.40111400 | 4.29970900 | -5.73572700 |
| H | -3.23100200 | 5.58985600 | -4.86411700 |
| H | 2.92011700 | -5.54019800 | 5.04643500 |
| H | 4.59165200 | -4.97986900 | 4.99624900 |
| H | 3.36326900 | -4.04074800 | 5.86266000 |
| H | 1.46461000 | -5.54334400 | -4.89366700 |
| H | 2.40843000 | -4.30111000 | -5.73487700 |
| H | 3.22657300 | -5.59631400 | -4.85952500 |
| H | 8.80264600 | -1.29216400 | -0.06614000 |
| H | -8.80263200 | 1.29214700 | -0.06613900 |
| H | 14.20052000 | 0.70044600 | -0.11285700 |
| H | 11.70687500 | 4.53838900 | 0.00429100 |
| H | -14.20052500 | -0.70036100 | -0.11310400 |
| H | -11.70695900 | -4.53835600 | 0.00402800 |

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|---|-------------|-------------|-------------|
| C | -0.09044500 | -1.42532800 | 0.04642500 |
| C | 1.14148100 | -0.76424300 | 0.01254700 |
| C | 1.23357000 | 0.64784000 | -0.03683400 |
| C | 0.09044900 | 1.42531700 | -0.04676900 |
| C | -1.14147800 | 0.76423100 | -0.01289700 |
| C | -1.23356700 | -0.64785200 | 0.03648800 |
| C | -2.49222200 | 1.26583900 | -0.02546400 |
| C | -3.40324400 | 0.22762300 | -0.00645800 |
| C | -2.69592800 | -1.11467900 | 0.05301900 |
| C | 2.49222500 | -1.26584900 | 0.02512800 |
| C | 3.40324600 | -0.22763200 | 0.00613400 |
| C | 2.69592900 | 1.11466900 | -0.05335300 |
| C | -2.94688900 | -1.98442800 | -1.18384200 |
| C | -3.09393100 | -1.80945600 | 1.36259800 |
| C | 2.94688900 | 1.98444300 | 1.18348600 |
| C | 3.09393100 | 1.80942600 | -1.36295000 |
| C | -2.66051200 | -3.35333200 | -1.15707600 |
| C | -2.80859500 | -4.13473500 | -2.29690200 |
| C | -3.25098300 | -3.58277000 | -3.50292600 |
| C | -3.53045400 | -2.21506800 | -3.52548000 |
| C | -3.38060900 | -1.42729500 | -2.38788800 |
| C | -2.35982900 | -1.64381000 | 2.53829100 |
| C | -2.79137800 | -2.21166900 | 3.73364800 |
| C | -3.96863900 | -2.95959900 | 3.80030000 |
| C | -4.70550400 | -3.11452800 | 2.62263800 |
| C | -4.27780000 | -2.55256200 | 1.42553400 |
| C | 2.66052400 | 3.35334300 | 1.15669700 |
| C | 2.80861300 | 4.13476800 | 2.29651600 |
| C | 3.25099600 | 3.58282300 | 3.50254400 |
| C | 3.53044900 | 2.21511200 | 3.52512400 |
| C | 3.38059800 | 1.42732400 | 2.38755100 |
| C | 4.27780800 | 2.55249000 | -1.42591500 |

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|----|--------------|-------------|-------------|
| C | 4.70549800 | 3.11445600 | -2.62304000 |
| C | 3.96860200 | 2.95956200 | -3.80066800 |
| C | 2.79131600 | 2.21164300 | -3.73399100 |
| C | 2.35979100 | 1.64379400 | -2.53863700 |
| S | -3.19808200 | 2.84544800 | -0.05481500 |
| C | -4.78372400 | 2.11544800 | -0.04744100 |
| C | -4.72526200 | 0.70799000 | -0.01484100 |
| C | -6.07989900 | 2.61371800 | -0.07174800 |
| C | -7.04586500 | 1.59722500 | -0.05991700 |
| S | -6.29637400 | -0.00143400 | -0.01446600 |
| S | 3.19808700 | -2.84545900 | 0.05453900 |
| C | 4.78372900 | -2.11545300 | 0.04722300 |
| C | 4.72526500 | -0.70799600 | 0.01457900 |
| C | 6.07990300 | -2.61372000 | 0.07160200 |
| C | 7.04587000 | -1.59722700 | 0.05978900 |
| S | 6.29637800 | 0.00143200 | 0.01424500 |
| C | -8.41660500 | 1.94382700 | -0.08060500 |
| C | 8.41660800 | -1.94382800 | 0.08058100 |
| C | -9.58747300 | 1.21879600 | -0.07494500 |
| C | 9.58747800 | -1.21880000 | 0.07500100 |
| C | -10.94198700 | 1.75848000 | -0.09871800 |
| C | -11.87551100 | 0.61107000 | -0.07338700 |
| C | -11.13149300 | -0.57565900 | -0.03992900 |
| C | -9.68950100 | -0.25100800 | -0.04027500 |
| C | 10.94199100 | -1.75848000 | 0.09895600 |
| C | 11.87551300 | -0.61106100 | 0.07403400 |
| C | 11.13149800 | 0.57566600 | 0.04046300 |
| C | 9.68950800 | 0.25100700 | 0.04041200 |
| C | -13.26935600 | 0.53242100 | -0.07797000 |
| C | -13.87255800 | -0.72225200 | -0.04943600 |
| C | -13.10013800 | -1.88537200 | -0.01700200 |
| C | -11.70922300 | -1.83114600 | -0.01163500 |
| C | 13.26935600 | -0.53240300 | 0.07907900 |
| C | 13.87255900 | 0.72227700 | 0.05085200 |
| C | 13.10014200 | 1.88539400 | 0.01826500 |
| C | 11.70922900 | 1.83116000 | 0.01245800 |
| O | -8.77846200 | -1.06352900 | -0.01637500 |
| O | 8.77847100 | 1.06352500 | 0.01631500 |
| C | 11.33642500 | -3.08168400 | 0.13956800 |
| C | -11.33641000 | 3.08167900 | -0.13959100 |
| C | -4.41569300 | -3.59789100 | 5.08478300 |
| C | -3.44677000 | -4.43808900 | -4.72244100 |
| C | 3.44682400 | 4.43813800 | 4.72205600 |
| C | 4.41554600 | 3.59788300 | -5.08517500 |
| Cl | -13.89384600 | -3.42637100 | 0.01733200 |
| Cl | 13.89384900 | 3.42640100 | -0.01569000 |
| C | 12.69930800 | -3.49433800 | 0.15906600 |
| N | 13.79510200 | -3.88550000 | 0.17641500 |
| C | 10.44120700 | -4.18876000 | 0.16881500 |
| N | 9.75129900 | -5.12595000 | 0.19452700 |
| C | -12.69928900 | 3.49435600 | -0.15888000 |
| N | -13.79507400 | 3.88555000 | -0.17603800 |
| C | -10.44117400 | 4.18872600 | -0.16938300 |
| N | -9.75124300 | 5.12588600 | -0.19555900 |
| H | -0.14457000 | -2.50931900 | 0.07781100 |
| H | 0.14457500 | 2.50930800 | -0.07814700 |
| H | -2.33121800 | -3.81835600 | -0.23213300 |
| H | -2.57904600 | -5.19646800 | -2.24714500 |
| H | -3.87341200 | -1.75463000 | -4.44887300 |
| H | -3.60189400 | -0.36540300 | -2.44408500 |
| H | -1.44170700 | -1.06449300 | 2.52849600 |
| H | -2.19817500 | -2.06731800 | 4.63348300 |
| H | -5.63107600 | -3.68481600 | 2.64033500 |
| H | -4.86827100 | -2.70610000 | 0.52661900 |
| H | 2.33123600 | 3.81835700 | 0.23174800 |
| H | 2.57907400 | 5.19650200 | 2.24674000 |
| H | 3.87339600 | 1.75468900 | 4.44853000 |
| H | 3.60186600 | 0.36543100 | 2.44376400 |
| H | 4.86831200 | 2.70601600 | -0.52701900 |
| H | 5.63108200 | 3.68472300 | -2.64075300 |
| H | 2.19809300 | 2.06730100 | -4.63381500 |
| H | 1.44165500 | 1.06449900 | -2.52881300 |
| H | -6.35010400 | 3.66332400 | -0.09693600 |
| H | 6.35010800 | -3.66332500 | 0.09683200 |
| H | -8.52978400 | 3.02312200 | -0.10646000 |
| H | 8.52978200 | -3.02312200 | 0.10649000 |
| H | -13.90015000 | 1.41108700 | -0.10253000 |
| H | -14.95410200 | -0.80054600 | -0.05233400 |
| H | -11.09786800 | -2.72657900 | 0.01344400 |
| H | 13.90014600 | -1.41106800 | 0.10377800 |

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|---|-------------|-------------|-------------|
| H | 14.95410100 | 0.80057800 | 0.05411500 |
| H | 11.09787500 | 2.72659100 | -0.01272900 |
| H | -4.06436500 | -4.63444200 | 5.15135300 |
| H | -4.02298400 | -3.06361700 | 5.95406400 |
| H | -5.50652500 | -3.62047800 | 5.16032900 |
| H | -2.72672700 | -5.26069600 | -4.75351200 |
| H | -4.44891200 | -4.88285200 | -4.73259600 |
| H | -3.34015200 | -3.85436000 | -5.64079700 |
| H | 2.72750900 | 5.26139800 | 4.75258900 |
| H | 3.33913900 | 3.85462700 | 5.64042900 |
| H | 4.44937000 | 4.88197800 | 4.73275700 |
| H | 5.50639000 | 3.62250500 | -5.15981100 |
| H | 4.02459300 | 3.06230900 | -5.95445400 |
| H | 4.06225400 | 4.63370400 | -5.15272600 |

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|-----|--------------|-------------|-------------|
| 0 1 | | | |
| C | -0.15391100 | -1.41930700 | 0.05902700 |
| C | 1.10631100 | -0.81437900 | 0.01680100 |
| C | 1.26123500 | 0.59173900 | -0.04482200 |
| C | 0.15391900 | 1.41929300 | -0.05961200 |
| C | -1.10630400 | 0.81436500 | -0.01737700 |
| C | -1.26122700 | -0.59175300 | 0.04423500 |
| C | -2.43335200 | 1.37569700 | -0.03132300 |
| C | -3.38965400 | 0.37936800 | -0.00155700 |
| C | -2.74289500 | -0.99257300 | 0.06765700 |
| C | 2.43335900 | -1.37570800 | 0.03079400 |
| C | 3.38966300 | -0.37938000 | 0.00103100 |
| C | 2.74290100 | 0.99255800 | -0.06823800 |
| C | -3.03558600 | -1.86116700 | -1.16069500 |
| C | -3.16834100 | -1.65741300 | 1.38418900 |
| C | 3.03558800 | 1.86121000 | 1.16007200 |
| C | 3.16834800 | 1.65734400 | -1.38479900 |
| C | -2.80518100 | -3.24039000 | -1.12298100 |
| C | -2.99118200 | -4.02515000 | -2.25483300 |
| C | -3.41737400 | -3.46615800 | -3.46353600 |
| C | -3.64110900 | -2.08850000 | -3.49700700 |
| C | -3.45310400 | -1.29740000 | -2.36729400 |
| C | -2.42618400 | -1.51154200 | 2.55744600 |
| C | -2.87933700 | -2.04933200 | 3.75868700 |
| C | -4.08656200 | -2.74698400 | 3.83370900 |
| C | -4.83111800 | -2.88193700 | 2.65840700 |
| C | -4.38228600 | -2.34949100 | 1.45553700 |
| C | 2.80523700 | 3.24044800 | 1.12227200 |
| C | 2.99124100 | 4.02526300 | 2.25407600 |
| C | 3.41738000 | 3.46631900 | 3.46283100 |
| C | 3.64105600 | 2.08866300 | 3.49638700 |
| C | 3.45304900 | 1.29750000 | 2.36670800 |
| C | 4.38232100 | 2.34936100 | -1.45618700 |
| C | 4.83114800 | 2.88177400 | -2.65907700 |
| C | 4.08655200 | 2.74684900 | -3.83435300 |
| C | 2.87929300 | 2.04925200 | -3.75929100 |
| C | 2.42614900 | 1.51149600 | -2.55803500 |
| S | -3.06839600 | 2.98480300 | -0.07333400 |
| C | -4.68499500 | 2.32630300 | -0.05649200 |
| C | -4.68902100 | 0.91806700 | -0.01160800 |
| C | -5.95790700 | 2.88158100 | -0.08289600 |
| C | -6.96803900 | 1.90902200 | -0.06111100 |
| S | -6.28978900 | 0.27902400 | -0.00279900 |
| S | 3.06839800 | -2.98481400 | 0.07289200 |
| C | 4.68500000 | -2.32631500 | 0.05609600 |
| C | 4.68902900 | -0.91808100 | 0.01114500 |
| C | 5.95790800 | -2.88159300 | 0.08264100 |
| C | 6.96804300 | -1.90903700 | 0.06088900 |
| S | 6.28979800 | -0.27904100 | 0.00242900 |
| C | -8.32243300 | 2.31492800 | -0.08296600 |
| C | 8.32243600 | -2.31494200 | 0.08286300 |
| C | -9.52346700 | 1.64086000 | -0.07284100 |
| C | 9.52347000 | -1.64087400 | 0.07283400 |
| C | -10.85364300 | 2.23782600 | -0.10062900 |
| C | -11.83533700 | 1.13114500 | -0.08146000 |
| C | -11.14247300 | -0.08616000 | -0.04294400 |
| C | -9.68816000 | 0.17672300 | -0.03514400 |
| C | 10.85364300 | -2.23783800 | 0.10082000 |
| C | 11.83533400 | -1.13114600 | 0.08219600 |
| C | 11.14247400 | 0.08615800 | 0.04358900 |
| C | 9.68816600 | -0.17673300 | 0.03529300 |

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| C | -13.23131100 | 1.11224200 | -0.09512700 |
| C | -13.88701500 | -0.11613500 | -0.07033400 |
| C | -13.16551100 | -1.31052300 | -0.03245200 |
| C | -11.77421600 | -1.31560200 | -0.01790700 |
| C | 13.23130200 | -1.11223500 | 0.09641500 |
| C | 13.88700600 | 0.11615000 | 0.07203900 |
| C | 13.16550700 | 1.31053700 | 0.03402100 |
| C | 11.77421800 | 1.31560800 | 0.01894500 |
| O | -8.81264400 | -0.67369500 | -0.00422200 |
| O | 8.81265500 | 0.67368200 | 0.00416800 |
| C | 11.19139800 | -3.57677700 | 0.13745800 |
| C | -11.19139300 | 3.57675600 | -0.13764700 |
| C | -4.55811300 | -3.35394200 | 5.12459500 |
| C | -3.65471200 | -4.32366600 | -4.67409800 |
| C | 3.65467700 | 4.32393100 | 4.67332700 |
| C | 4.55806700 | 3.35378400 | -5.12526300 |
| Br | -14.10021300 | -2.94573000 | -0.00050700 |
| Br | 14.10021200 | 2.94575300 | 0.00264200 |
| C | 12.53531300 | -4.04725300 | 0.16263700 |
| N | 13.61322700 | -4.48508100 | 0.18448700 |
| C | 10.24971400 | -4.64485900 | 0.15471900 |
| N | 9.52035400 | -5.55191200 | 0.17030700 |
| C | -12.53530900 | 4.04724200 | -0.16257400 |
| N | -13.61321400 | 4.48510400 | -0.18423100 |
| C | -10.24969900 | 4.64481700 | -0.15564300 |
| N | -9.52034100 | 5.55186100 | -0.17182000 |
| H | -0.25643400 | -2.49936000 | 0.10029500 |
| H | 0.25644200 | 2.49934700 | -0.10087100 |
| H | -2.49009000 | -3.71002500 | -0.19542000 |
| H | -2.80490600 | -5.09489400 | -2.19669600 |
| H | -3.97015600 | -1.62259200 | -4.42271500 |
| H | -3.63148600 | -0.22795200 | -2.43184100 |
| H | -1.48455900 | -0.97139700 | 2.54131900 |
| H | -2.27936200 | -1.92108500 | 4.65648400 |
| H | -5.77976800 | -3.41271700 | 2.68262600 |
| H | -4.98011800 | -2.48636800 | 0.55876600 |
| H | 2.49019200 | 3.71004000 | 0.19467300 |
| H | 2.80501100 | 5.09501300 | 2.19586900 |
| H | 3.97006400 | 1.62279800 | 4.42212900 |
| H | 3.63138800 | 0.22804900 | 2.43132400 |
| H | 4.98018600 | 2.48622200 | -0.55943500 |
| H | 5.77982400 | 3.41250400 | -2.68332800 |
| H | 2.27928800 | 1.92102000 | -4.65707000 |
| H | 1.48450100 | 0.97139100 | -2.54187700 |
| H | -6.18078100 | 3.94196500 | -0.11661900 |
| H | 6.18077700 | -3.94197600 | 0.11643500 |
| H | -8.38902700 | 3.39792200 | -0.11614100 |
| H | 8.38902600 | -3.39793400 | 0.11609700 |
| H | -13.82425800 | 2.01676000 | -0.12435600 |
| H | -14.97074500 | -0.14701800 | -0.08055900 |
| H | -11.20187200 | -2.23618300 | 0.01152700 |
| H | 13.82424400 | -2.01675300 | 0.12577400 |
| H | 14.97073200 | 0.14704100 | 0.08270400 |
| H | 11.20187900 | 2.23619000 | -0.01058600 |
| H | -4.25583900 | -4.40539700 | 5.19776800 |
| H | -4.13729600 | -2.83230700 | 5.98835700 |
| H | -5.64851700 | -3.32443100 | 5.20414600 |
| H | -2.96296400 | -5.17021600 | -4.70629900 |
| H | -4.67114800 | -4.73480800 | -4.67005900 |
| H | -3.53857600 | -3.75086800 | -5.59812700 |
| H | 2.96143100 | 5.16922200 | 4.70660800 |
| H | 3.54071500 | 3.75068800 | 5.59734400 |
| H | 4.67034300 | 4.73695300 | 4.66811300 |
| H | 5.64850700 | 3.32492400 | -5.20452700 |
| H | 4.13779100 | 2.83168200 | -5.98900900 |
| H | 4.25515200 | 4.40503100 | -5.19877600 |

NFBDT

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|-----|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.98020900 | -0.96876600 | -0.00779400 |
| C | 1.34193100 | 0.41636000 | 0.00415100 |
| C | 3.50827200 | 2.51746200 | 1.34186400 |
| C | 3.69136000 | 2.62593800 | -1.21461300 |
| C | -3.69369400 | -2.62568700 | 1.21956300 |
| C | 2.76329900 | 3.69670500 | 1.37381700 |
| C | 2.50854500 | 4.34716300 | 2.57955900 |
| C | 2.98524100 | 3.84458500 | 3.79008800 |

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| C | 3.72398600 | 2.65649300 | 3.75318400 |
| C | 3.97992700 | 2.00424100 | 2.55473700 |
| C | 2.95605400 | 2.28231300 | -2.34726200 |
| C | 2.99401000 | 3.07919400 | -3.49101000 |
| C | 3.76596600 | 4.23854900 | -3.54252000 |
| C | 4.50720800 | 4.57701000 | -2.40338900 |
| C | 4.47231700 | 3.78844100 | -1.26261400 |
| C | -2.96359100 | -2.27866600 | 2.35507100 |
| C | -3.00401900 | -3.07377600 | 3.49938800 |
| C | -3.77235200 | -4.23621600 | 3.54878200 |
| C | -4.50930500 | -4.57691900 | 2.40812900 |
| C | -4.47221900 | -3.78936100 | 1.26617900 |
| C | 2.73333300 | 4.55534300 | 5.08946200 |
| C | 3.80080200 | 5.10650200 | -4.76833300 |
| C | -3.79693900 | -5.10856600 | 4.77166400 |
| C | -2.72743500 | -4.55922000 | -5.08110900 |
| C | -3.97288800 | -2.00184000 | -2.55036800 |
| C | -3.71278000 | -2.65288700 | -3.74923100 |
| C | -2.97645000 | -3.84178100 | -3.78493100 |
| C | -2.50389300 | -4.34637900 | -2.57289000 |
| C | -2.76217100 | -3.69735600 | -1.36780700 |
| C | -3.50650400 | -2.51701500 | -1.33692900 |
| C | 8.63447400 | 0.27186000 | 0.03669400 |
| C | 9.68573800 | -0.61900100 | 0.01948800 |
| C | 11.10527700 | -0.29113400 | 0.04592700 |
| C | 11.85514400 | -1.56819100 | 0.01016100 |
| C | 10.93782400 | -2.62841800 | -0.03440600 |
| C | 9.56580000 | -2.08701200 | -0.02994000 |
| C | 11.69418600 | 0.95779700 | 0.09726100 |
| O | 8.53664500 | -2.74673700 | -0.06157300 |
| C | 13.22127200 | -1.85305600 | 0.01486300 |
| C | 13.62212900 | -3.18884100 | -0.02526400 |
| C | 12.69528200 | -4.23237500 | -0.06936900 |
| C | 11.32995200 | -3.95529200 | -0.07430400 |
| C | -8.63502200 | -0.27221300 | -0.04122400 |
| C | -9.68644200 | 0.61849900 | -0.02573700 |
| C | -11.10588700 | 0.29043300 | -0.05482500 |
| C | -11.85600200 | 1.56737400 | -0.02022500 |
| C | -10.93892100 | 2.62772400 | 0.02620500 |
| C | -9.56681300 | 2.08651700 | 0.02415500 |
| C | -11.69455800 | -0.95855900 | -0.10739100 |
| O | -8.53782000 | 2.74639600 | 0.05781900 |
| C | -13.22216100 | 1.85203600 | -0.02733000 |
| C | -13.62328700 | 3.18775400 | 0.01235200 |
| C | -12.69667400 | 4.23141500 | 0.05833100 |
| C | -11.33131300 | 3.95453200 | 0.06566300 |
| C | -2.75875400 | -0.56749300 | 0.01704700 |
| C | -3.42171600 | 0.64057100 | 0.02996000 |
| S | -2.38607100 | 2.02625300 | 0.03348800 |
| C | -3.73420200 | -1.74056000 | -0.02946000 |
| C | -5.05290400 | -0.97008500 | -0.03260700 |
| C | -4.83001300 | 0.40662800 | 0.01376300 |
| C | 2.75807900 | 0.56769600 | -0.01043400 |
| C | 3.42097800 | -0.64040600 | -0.02409900 |
| S | 2.38533300 | -2.02606900 | -0.02606400 |
| C | 3.73371900 | 1.74068600 | 0.03422200 |
| C | 5.05239400 | 0.97013100 | 0.03509500 |
| C | 4.82929700 | -0.40657500 | -0.01051400 |
| C | -6.40519400 | -1.27278100 | -0.04943600 |
| C | -7.22974700 | -0.13206300 | -0.02094200 |
| S | -6.25851900 | 1.34158700 | 0.03628500 |
| C | 6.40476800 | 1.27267500 | 0.04911200 |
| C | 7.22914600 | 0.13186800 | 0.01916300 |
| S | 6.25765500 | -1.34168800 | -0.03581700 |
| C | -0.33542900 | -1.39221600 | -0.00631800 |
| C | -1.34261200 | -0.41616300 | 0.00405700 |
| C | -0.98091400 | 0.96895900 | 0.01625500 |
| C | 0.33472300 | 1.39240600 | 0.01489800 |
| C | -13.10343700 | -1.16511700 | -0.13129700 |
| N | -14.24412600 | -1.39457200 | -0.15297200 |
| C | -10.97513700 | -2.18692200 | -0.14516500 |
| N | -10.43429000 | -3.21726600 | -0.17813300 |
| C | 13.10312600 | 1.16423200 | 0.11845600 |
| N | 14.24386300 | 1.39364600 | 0.13791400 |
| C | 10.97494400 | 2.18622500 | 0.13626700 |
| N | 10.43419400 | 3.21658600 | 0.17025400 |
| H | 2.38811900 | 4.12693500 | 0.44999300 |
| H | 1.92845000 | 5.26670800 | 2.57336300 |
| H | 4.10736800 | 2.23581900 | 4.67979200 |
| H | 4.55626100 | 1.08321300 | 2.56298300 |

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|---|--------------|-------------|-------------|
| H | 2.34703800 | 1.38379800 | -2.34909400 |
| H | 2.40823500 | 2.78745500 | -4.35920700 |
| H | 5.12184000 | 5.47403600 | -2.41144000 |
| H | 5.04967600 | 4.08743500 | -0.39194100 |
| H | -2.35825400 | -1.37765100 | 2.35845000 |
| H | -2.42388900 | -2.77827800 | 4.37016000 |
| H | -5.12334500 | -5.47431200 | 2.41582500 |
| H | -5.04751500 | -4.08968600 | 0.39459600 |
| H | 1.99708900 | 5.35440800 | 4.97181300 |
| H | 2.36721300 | 3.86472200 | 5.85574300 |
| H | 3.65431300 | 5.00591200 | 5.47665500 |
| H | 3.25389000 | 4.64957600 | -5.59674800 |
| H | 3.35249400 | 6.08666900 | -4.57102100 |
| H | 4.82934900 | 5.28540300 | -5.09836300 |
| H | -3.17841500 | -6.00237100 | 4.62921700 |
| H | -3.41437400 | -4.57891900 | 5.64781800 |
| H | -4.81150200 | -5.45183900 | 4.99552700 |
| H | -2.54814800 | -3.85489600 | -5.89866500 |
| H | -1.86481300 | -5.22685700 | -5.00905400 |
| H | -3.59294400 | -5.16980900 | -5.36415000 |
| H | -4.54677300 | -1.07928500 | -2.55986000 |
| H | -4.09028200 | -2.22950100 | -4.67694100 |
| H | -1.92385600 | -5.26604600 | -2.56584000 |
| H | -2.38936700 | -4.12808400 | -0.44326300 |
| H | 8.90475900 | 1.32279500 | 0.07147500 |
| H | 13.97323000 | -1.07589300 | 0.04821400 |
| H | 14.68329900 | -3.41790700 | -0.02203100 |
| H | 13.04342400 | -5.26009600 | -0.09978100 |
| H | 10.58406000 | -4.74318500 | -0.10806900 |
| H | -8.90510000 | -1.32317200 | -0.07680300 |
| H | -13.97394100 | 1.07476500 | -0.06218900 |
| H | -14.68448300 | 3.41666400 | 0.00726500 |
| H | -13.04502200 | 5.25907900 | 0.08832900 |
| H | -10.58559700 | 4.74252700 | 0.10092700 |
| H | -6.82695200 | -2.27132800 | -0.08309900 |
| H | 6.82671500 | 2.27117400 | 0.08170200 |
| H | -0.59198600 | -2.44543100 | -0.01776400 |
| H | 0.59128100 | 2.44561700 | 0.02615400 |

ITIC2

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|-----|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.71237300 | -1.11293100 | 0.29763900 |
| C | -1.43693400 | 0.10297800 | 0.06921700 |
| C | -0.67933400 | 1.27738700 | -0.14396200 |
| C | 0.70874900 | 1.14431600 | -0.13904100 |
| C | 1.43360700 | -0.07245200 | 0.08551300 |
| C | 0.67582900 | -1.24543600 | 0.30591800 |
| S | 1.75559500 | 2.51729500 | -0.44650200 |
| C | 3.12554500 | 1.49779500 | -0.23944200 |
| C | 2.84892300 | 0.17457300 | 0.04537300 |
| S | -1.76001700 | -2.48456200 | 0.60883800 |
| C | -3.12941900 | -1.46717500 | 0.38981700 |
| C | -2.85196500 | -0.14538700 | 0.10057600 |
| C | 4.53342700 | 1.71222700 | -0.26580800 |
| C | 5.17475800 | 0.50693100 | -0.00569400 |
| C | 4.15547100 | -0.60010600 | 0.28715400 |
| S | 5.61397000 | 2.99754300 | -0.54989900 |
| C | 6.98764500 | 1.91287600 | -0.35442100 |
| C | 6.56118000 | 0.61230000 | -0.06658400 |
| C | -4.53781200 | -1.67734200 | 0.42910100 |
| C | -5.17799100 | -0.47906800 | 0.13552600 |
| C | -4.15752200 | 0.63159600 | -0.13792600 |
| S | -5.61910700 | -2.95451100 | 0.74482100 |
| C | -6.99253200 | -1.88689100 | 0.47130300 |
| C | -6.56508200 | -0.59407000 | 0.15202500 |
| C | 4.35253500 | -0.96714800 | 1.76627700 |
| C | 4.35026300 | -1.74464700 | -0.72003700 |
| C | -4.35365800 | 1.75210400 | 0.89842500 |
| C | -4.34572500 | 1.03364500 | -1.60787900 |
| C | 5.51346900 | -1.63692900 | 2.17690100 |
| C | 5.75620400 | -1.89962200 | 3.51846400 |
| C | 4.85921500 | -1.49347100 | 4.51225500 |
| C | 3.71636700 | -0.80625100 | 4.10448500 |
| C | 3.46675300 | -0.54576300 | 2.75832800 |

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| C | 4.54616100 | -3.07371500 | -0.35808800 |
| C | 4.78010500 | -4.04801400 | -1.32862400 |
| C | 4.81012800 | -3.73415500 | -2.68535300 |
| C | 4.58841300 | -2.39905500 | -3.04565000 |
| C | 4.36866900 | -1.42479600 | -2.08414800 |
| C | -4.34547700 | 1.40364300 | 2.25626500 |
| C | -4.56435800 | 2.35310100 | 3.24235100 |
| C | -4.81132600 | 3.69269900 | 2.91454500 |
| C | -4.80786200 | 4.03530500 | 1.56480900 |
| C | -4.57413500 | 3.08564300 | 0.56949400 |
| C | -3.45126000 | 0.63818000 | -2.60232500 |
| C | -3.69035700 | 0.93166600 | -3.94350700 |
| C | -4.83148500 | 1.62573700 | -4.34365900 |
| C | -5.73793200 | 2.00513000 | -3.34805800 |
| C | -5.50558700 | 1.70902100 | -2.01195500 |
| C | 5.11701500 | -1.79981400 | 5.96008700 |
| C | 5.07832800 | -4.77983300 | -3.73042100 |
| C | -5.06543100 | 4.71387900 | 3.98717800 |
| C | -5.08202400 | 1.96152900 | -5.78608100 |
| C | 1.22496100 | -2.60300000 | 0.49477700 |
| C | -1.22991500 | 2.63731300 | -0.31179500 |
| C | -1.65196600 | 3.27485200 | -1.44837500 |
| C | -1.95056500 | 4.64948700 | -1.24021900 |
| C | -1.74454800 | 5.06699500 | 0.04744100 |
| S | -1.18099100 | 3.75548700 | 1.02251200 |
| C | 1.64575800 | -3.21831200 | 1.64425400 |
| C | 1.93581400 | -4.59868700 | 1.46520500 |
| C | 1.72495800 | -5.04199000 | 0.18677300 |
| S | 1.16808900 | -3.74834900 | -0.81526500 |
| C | 8.28343500 | 2.47984500 | -0.37653000 |
| C | -8.28707500 | -2.39816200 | 0.72532300 |
| C | 9.54101900 | 1.92765900 | -0.36410700 |
| C | -9.54422800 | -1.88451300 | 0.51983800 |
| C | 10.65522300 | 2.80050600 | 0.10907600 |
| C | 11.78399000 | 1.89326400 | 0.40866800 |
| C | 11.43243300 | 0.58186500 | 0.04693400 |
| C | 10.09384500 | 0.60827400 | -0.58423500 |
| C | -10.64934700 | -2.45084600 | 1.34700400 |
| C | -11.76983300 | -1.49150800 | 1.24034000 |
| C | -11.42329200 | -0.47233800 | 0.33702600 |
| C | -10.09857000 | -0.78626600 | -0.24272400 |
| C | 13.00916800 | 2.19975700 | 0.97671700 |
| C | 13.90342500 | 1.15581900 | 1.20627100 |
| C | 13.55827000 | -0.15447500 | 0.86758000 |
| C | 12.32958000 | -0.45897000 | 0.28040000 |
| C | -12.98479800 | -1.50826000 | 1.90446900 |
| C | -13.87331800 | -0.46073200 | 1.66951500 |
| C | -13.53302000 | 0.56718400 | 0.78710600 |
| C | -12.31486700 | 0.57394200 | 0.10652300 |
| O | 10.61943200 | 4.00802400 | 0.26359500 |
| C | 9.59439400 | -0.37046400 | -1.42132900 |
| O | -10.61248100 | -3.46963200 | 2.01335900 |
| C | -9.61176000 | -0.27782700 | -1.43124200 |
| C | -8.53115200 | -0.88228400 | -2.13016900 |
| N | -7.67777500 | -1.38329000 | -2.74185600 |
| C | -10.22668500 | 0.79792200 | -2.13213700 |
| N | -10.68845700 | 1.68729300 | -2.72370500 |
| C | 8.48833500 | -0.14321000 | -2.28527200 |
| N | 7.61372100 | 0.03064000 | -3.03254800 |
| C | 10.22285000 | -1.63492700 | -1.60480600 |
| N | 10.70004700 | -2.68354100 | -1.76793100 |
| H | 7.25715700 | -0.19404500 | 0.12652400 |
| H | -7.25994800 | 0.22083500 | -0.00598600 |
| H | 6.23983400 | -1.96527200 | 1.43974500 |
| H | 6.66566300 | -2.42510800 | 3.80009200 |
| H | 3.00427100 | -0.46174500 | 4.85053900 |
| H | 2.56787400 | -0.00106200 | 2.48859500 |
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| H | 4.94001900 | -5.07661000 | -1.01391900 |
| H | 4.60153100 | -2.11686300 | -4.09559200 |
| H | 4.21881200 | -0.39456600 | -2.39700500 |
| H | -4.16732300 | 0.37010600 | 2.54364500 |
| H | -4.55135900 | 2.05004300 | 4.28677800 |
| H | -4.98796700 | 5.06784100 | 1.27485400 |
| H | -4.55283600 | 3.40417900 | -0.46579600 |
| H | -2.55403000 | 0.08761500 | -2.33923900 |
| H | -2.97232900 | 0.60553500 | -4.69204400 |
| H | -6.64882100 | 2.53105400 | -3.62421500 |
| H | -6.24162200 | 2.01417600 | -1.27433600 |
| H | 4.90126600 | -2.85098900 | 6.18432700 |

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| H | 6.16408100 | -1.62326100 | 6.22456800 |
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| H | 4.30920700 | -4.76934500 | -4.50965500 |
| H | 6.03967500 | -4.60484600 | -4.22642300 |
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| H | -5.21644300 | 5.70965800 | 3.56240600 |
| H | -5.95523600 | 4.46079400 | 4.57411300 |
| H | -4.91986200 | 3.02880800 | -5.97660400 |
| H | -4.41557000 | 1.40193200 | -6.44726600 |
| H | -6.11407800 | 1.73694600 | -6.07248700 |
| H | -1.73827100 | 2.77346300 | -2.40479800 |
| H | -2.30381700 | 5.31425800 | -2.02141500 |
| H | 1.73572900 | -2.69680100 | 2.58962100 |
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| H | 8.31940500 | 3.56707500 | -0.27921900 |
| H | -8.31943600 | -3.33436100 | 1.28694200 |
| H | 13.25034100 | 3.22660500 | 1.23317700 |
| H | 14.87144100 | 1.35736300 | 1.65422200 |
| H | 14.26079700 | -0.95850000 | 1.06399300 |
| H | 12.09338600 | -1.48638600 | 0.03294800 |
| H | -13.22258500 | -2.31845000 | 2.58660100 |
| H | -14.83332800 | -0.43782700 | 2.17565200 |
| H | -14.23124900 | 1.38226600 | 0.62365900 |
| H | -12.08208000 | 1.38779200 | -0.56894100 |
| C | 1.93482300 | -6.41259300 | -0.36602200 |
| H | 1.01384600 | -6.82698600 | -0.78870600 |
| H | 2.69137400 | -6.41527900 | -1.15786000 |
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| C | -1.96360400 | 6.42442100 | 0.62839700 |
| H | -1.04579300 | 6.83602800 | 1.06065500 |
| H | -2.30553100 | 7.10804800 | -0.15254500 |
| H | -2.72130500 | 6.40606700 | 1.41897800 |

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| C | -0.16265400 | -1.41790900 | 0.05839200 |
| C | 1.10194200 | -0.82209100 | 0.01787000 |
| C | 1.26469000 | 0.58301300 | -0.04312500 |
| C | 0.16268700 | 1.41778500 | -0.05923000 |
| C | 2.42598500 | -1.39125700 | 0.03217200 |
| C | 3.38756500 | -0.40080300 | 0.00187600 |
| C | 2.74925500 | 0.97497100 | -0.06393300 |
| C | -2.42594900 | 1.39113900 | -0.03294400 |
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| C | 3.01320900 | 3.99652900 | 2.27148300 |
| C | 3.43855500 | 3.43059000 | 3.47732200 |
| C | 3.65631300 | 2.05187400 | 3.50455400 |
| C | 3.46339400 | 1.26636500 | 2.37167400 |
| C | 4.39665500 | 2.33133900 | -1.44357000 |
| C | 4.85154900 | 2.86359500 | -2.64452000 |
| C | 4.11183200 | 2.73000600 | -3.82283400 |
| C | 2.90309800 | 2.03403200 | -3.75291600 |
| C | 2.44406500 | 1.49678300 | -2.55387500 |
| C | -2.82226700 | -3.21741600 | -1.13755800 |
| C | -3.01320900 | -3.99651300 | -2.27245800 |
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| C | -3.65643700 | -2.05180800 | -3.50538500 |
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| C | -2.44399700 | -1.49702400 | 2.55302400 |
| C | -2.90300100 | -2.03437600 | 3.75205100 |
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| S | 3.05780200 | -3.00172100 | 0.07297000 |
| C | 4.67711500 | -2.35505600 | 0.05388800 |
| C | 4.68218500 | -0.94904200 | 0.00906400 |

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| C | 5.95215900 | -2.92772800 | 0.07908400 |
| C | 6.95364700 | -1.96278100 | 0.05473500 |
| S | 6.29295700 | -0.33251800 | -0.00396900 |
| S | -3.05776000 | 3.00160300 | -0.07365300 |
| C | -4.67707200 | 2.35495000 | -0.05446100 |
| C | -4.68214900 | 0.94893500 | -0.00967700 |
| C | -5.95211400 | 2.92763300 | -0.07951300 |
| C | -6.95360800 | 1.96269500 | -0.05508500 |
| S | -6.29293100 | 0.33242400 | 0.00350300 |
| C | 8.34612800 | -2.22657200 | 0.07283500 |
| C | -8.34608600 | 2.22651400 | -0.07299700 |
| C | 9.35870700 | -1.30268800 | 0.04964200 |
| C | -9.35869000 | 1.30266100 | -0.04969100 |
| C | 10.70404500 | -1.73301400 | 0.07860800 |
| C | -10.70401500 | 1.73304400 | -0.07840600 |
| C | 11.81763800 | -0.92082400 | 0.06234200 |
| C | -11.81764500 | 0.92091000 | -0.06189600 |
| C | 13.21549700 | -1.31647000 | 0.09327500 |
| C | 14.02830500 | -0.08067800 | 0.05416400 |
| C | 13.16855400 | 1.02421900 | 0.00226500 |
| C | 11.76469000 | 0.56009100 | 0.00523300 |
| C | -13.21549000 | 1.31663300 | -0.09247600 |
| C | -14.02835900 | 0.08089900 | -0.05279300 |
| C | -13.16865600 | -1.02404200 | -0.00105000 |
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| O | 10.78115100 | 1.28238400 | -0.03309100 |
| C | 13.73786000 | -2.59419700 | 0.14992100 |
| O | -10.78125300 | -1.28234800 | 0.03338900 |
| C | -13.73779200 | 2.59437500 | -0.14935000 |
| C | 15.40923200 | 0.12428300 | 0.06234500 |
| C | 15.86557600 | 1.43117700 | 0.01710100 |
| C | 14.99270500 | 2.52351400 | -0.03466700 |
| C | 13.62289600 | 2.33222700 | -0.04273700 |
| C | -15.40930200 | -0.12397700 | -0.06034400 |
| C | -15.86571000 | -1.43083300 | -0.01465300 |
| C | -14.99288500 | -2.52321600 | 0.03693900 |
| C | -13.62306100 | -2.33201400 | 0.04438400 |
| F | 15.51555100 | 3.74525200 | -0.07530200 |
| F | 17.17290100 | 1.67825700 | 0.02253400 |
| F | -17.17305200 | -1.67783200 | -0.01946600 |
| F | -15.51579000 | -3.74491400 | 0.07802900 |
| C | -4.58864400 | -3.33729100 | 5.11086100 |
| C | -3.68099300 | -4.28177400 | -4.69223300 |
| C | 4.58870500 | 3.33682300 | -5.11182000 |
| C | 3.68090600 | 4.28190800 | 4.69126700 |
| C | 15.13418400 | -2.87058000 | 0.17244600 |
| N | 16.26537900 | -3.14341300 | 0.19241000 |
| C | 12.94800200 | -3.77773600 | 0.19232500 |
| N | 12.34501300 | -4.77257900 | 0.22908800 |
| C | -15.13410600 | 2.87083900 | -0.17148300 |
| N | -16.26528700 | 3.14375300 | -0.19112300 |
| C | -12.94787300 | 3.77784900 | -0.19244200 |
| N | -12.34484400 | 4.77264700 | -0.22974100 |
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| H | 2.50778500 | 3.69228200 | 0.21154500 |
| H | 2.83139700 | 5.06730500 | 2.21815300 |
| H | 3.98427300 | 1.58054400 | 4.42791500 |
| H | 3.63685400 | 0.19582600 | 2.43142000 |
| H | 4.98990300 | 2.46840300 | -0.54368800 |
| H | 5.80068100 | 3.39375900 | -2.66468700 |
| H | 2.30675500 | 1.90691400 | -4.65331300 |
| H | 1.50152000 | 0.95812800 | -2.54118500 |
| H | -2.50768200 | -3.69236900 | -0.21253200 |
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| H | -3.98446500 | -1.58042700 | -4.42869500 |
| H | -3.63698900 | -0.19582100 | -2.43214300 |
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| H | -5.80052400 | -3.39417200 | 2.66376000 |
| H | -4.98981100 | -2.46864400 | 0.54281500 |
| H | 6.16472100 | -3.98990800 | 0.11342800 |
| H | -6.16467000 | 3.98981600 | -0.11379600 |
| H | 8.61149400 | -3.28307700 | 0.11100400 |
| H | -8.61143000 | 3.28302700 | -0.11109300 |
| H | 9.15225900 | -0.23755700 | 0.01064400 |
| H | -9.15227400 | 0.23752000 | -0.01076600 |
| H | 10.84921500 | -2.80895700 | 0.11827900 |
| H | -10.84914400 | 2.80899400 | -0.11803300 |
| H | 16.14039000 | -0.67255000 | 0.10144900 |

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| H | 12.93904800 | 3.17325000 | -0.08235300 |
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| H | -4.26612500 | -4.38180300 | 5.19618000 |
| H | -4.18983200 | -2.80116300 | 5.97624300 |
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| H | 4.19282000 | 2.79836200 | -5.97710800 |
| H | 4.26290400 | 4.38017100 | -5.19893200 |
| H | 4.69746300 | 4.69274000 | 4.68556900 |
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| C | -1.94533100 | -2.17433500 | 0.00887400 |
| C | 1.94533600 | 2.17433700 | -0.00887500 |
| C | -2.79737600 | 0.05781700 | 0.01577100 |
| C | -3.16652600 | -1.27160700 | -0.00011700 |
| C | 2.79738000 | -0.05781600 | -0.01578000 |
| C | 3.16653100 | 1.27160800 | 0.00010900 |
| C | -1.97922100 | -3.01612500 | 1.29172400 |
| C | -1.81386600 | -3.02182300 | -1.26138400 |
| C | 1.97922300 | 3.01614100 | -1.29171500 |
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| C | -1.51320100 | -3.30368400 | 3.65331000 |
| C | -2.21839800 | -4.50832300 | 3.68926500 |
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| C | -2.69463100 | -4.21813700 | 1.32475400 |
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| C | -2.27781300 | -3.39756800 | -3.61143300 |
| C | -1.42582900 | -4.50308900 | -3.64561000 |
| C | -0.76554200 | -4.84964900 | -2.46285100 |
| C | -0.95570700 | -4.12621200 | -1.29142600 |
| C | 2.69461900 | 4.21816100 | -1.32472700 |
| C | 2.81079000 | 4.94817100 | -2.50203800 |
| C | 2.21839100 | 4.50837000 | -3.68923600 |
| C | 1.51320800 | 3.30372100 | -3.65329900 |
| C | 1.39482400 | 2.56809800 | -2.47776100 |
| C | -2.31668000 | -5.31780200 | 4.95114800 |
| C | -1.24540700 | -5.30977600 | -4.90014500 |
| C | 2.31665600 | 5.31786700 | -4.95111000 |
| C | 1.24536000 | 5.30972200 | 4.90017200 |
| C | 0.95570900 | 4.12620100 | 1.29144400 |
| C | 0.76553800 | 4.84962300 | 2.46287200 |
| C | 1.42582300 | 4.50304800 | 3.64563500 |
| C | 2.27781000 | 3.39753500 | 3.61144700 |
| C | 2.46918400 | 2.66761900 | 2.44189800 |
| C | 1.81387200 | 3.02181100 | 1.26139300 |
| C | -10.50735800 | -0.62817900 | -0.03583600 |
| C | -11.46730600 | 0.35830600 | -0.03636900 |
| C | -11.20930400 | 1.81013900 | -0.01021600 |
| C | -12.52472100 | 2.47775000 | -0.01784800 |
| C | -13.53728500 | 1.50713900 | -0.04754000 |
| C | -12.91189100 | 0.16514300 | -0.06118100 |
| O | -10.12246100 | 2.36913300 | 0.01400000 |
| C | -13.61516200 | -1.02348000 | -0.09415500 |
| C | -12.79260600 | 3.83606600 | 0.00013700 |
| C | -14.12626500 | 4.23821200 | -0.01202300 |
| C | -15.14622900 | 3.28473900 | -0.04144400 |
| C | -14.87100000 | 1.91723200 | -0.05954100 |
| C | 10.50736300 | 0.62817700 | 0.03582700 |
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| C | 11.20930600 | -1.81014200 | 0.01020200 |
| C | 12.52472300 | -2.47775400 | 0.01781800 |
| C | 13.53728800 | -1.50714400 | 0.04751200 |
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| O | 10.12246200 | -2.36913400 | -0.01401000 |

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| C | 13.61516700 | 1.02347400 | 0.09417700 |
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| S | 4.12652200 | -1.16449600 | -0.03841100 |
| S | 5.65977200 | 2.76968800 | 0.01551400 |
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| C | -4.56616300 | -1.41419400 | 0.00854800 |
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| S | -4.12651800 | 1.16449700 | 0.03840100 |
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| C | 9.09342000 | 0.62281500 | 0.01763600 |
| S | 7.98130300 | -0.75009800 | -0.01324600 |
| C | -8.39812300 | -1.83968500 | -0.02744300 |
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| S | -7.98129900 | 0.75009700 | 0.01324000 |
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| N | -12.57139100 | -3.39093200 | -0.12712900 |
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| N | -16.19439400 | -1.21967000 | -0.13525600 |
| C | 13.01405500 | 2.31437900 | 0.11153800 |
| N | 12.57139800 | 3.39092600 | 0.12721900 |
| C | 15.03729400 | 1.09748300 | 0.11621400 |
| N | 16.19439900 | 1.21966200 | 0.13527000 |
| H | -0.95685200 | 2.32459600 | 0.01074300 |
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| H | 3.37281800 | 5.87904100 | -2.49674700 |
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| H | -2.17114700 | -4.69458700 | 5.83748400 |
| H | -3.28981000 | -5.81024000 | 5.03452300 |
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| H | -1.94803600 | -6.15100900 | -4.93060900 |
| H | -1.42327500 | -4.70432100 | -5.79301500 |
| H | -0.23676200 | -5.72758400 | -4.96454300 |
| H | 1.55255200 | 6.10388200 | -4.97409800 |
| H | 3.28969200 | 5.81051000 | -5.03436800 |
| H | 2.17136000 | 4.69462000 | -5.83746100 |
| H | 0.23640700 | 5.72672600 | 4.96500900 |
| H | 1.42413700 | 4.70450600 | 5.79302000 |
| H | 1.94731200 | 6.15153600 | 4.93020200 |
| H | 0.43891000 | 4.43307100 | 0.38656700 |
| H | 0.09166500 | 5.70308500 | 2.45698600 |
| H | 2.80323100 | 3.09898800 | 4.51542200 |
| H | 3.13374100 | 1.80857900 | 2.45502300 |
| H | -10.87607900 | -1.64902000 | -0.05380100 |
| H | -11.97725900 | 4.55228400 | 0.02296000 |
| H | -15.69188100 | 1.21275200 | -0.08207900 |
| H | 10.87608400 | 1.64901900 | 0.05378800 |
| H | 11.97725800 | -4.55228700 | -0.02300500 |
| H | 15.69188400 | -1.21275900 | 0.08203000 |
| H | 8.91314500 | 2.79349000 | 0.04603400 |
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| H | -14.37727000 | 5.29421100 | 0.00131900 |
| H | -16.18145200 | 3.61147100 | -0.05053200 |
| H | 16.18145300 | -3.61147800 | 0.05045300 |
| H | 14.37726900 | -5.29421600 | -0.00139500 |

INIC2

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| 01 | | | |
| C | -0.80430100 | -1.13674800 | 0.01003100 |

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|---|--------------|-------------|-------------|
| C | -1.36541100 | 0.16263300 | 0.01128100 |
| C | -0.56746200 | 1.31073100 | 0.00411000 |
| C | 0.80430300 | 1.13674700 | -0.00998500 |
| C | 1.36541200 | -0.16263300 | -0.01123700 |
| C | 0.56746300 | -1.31073100 | -0.00406600 |
| C | -1.89459900 | -2.21893300 | 0.00693900 |
| C | 1.89460100 | 2.21893300 | -0.00688800 |
| C | -2.79761400 | -0.00695000 | 0.01369900 |
| C | -3.13631400 | -1.34463000 | -0.00353800 |
| C | 2.79761600 | 0.00694900 | -0.01366200 |
| C | 3.13631600 | 1.34462900 | 0.00357400 |
| C | -1.91114300 | -3.06126500 | 1.28980300 |
| C | -1.74193100 | -3.06392100 | -1.26265100 |
| C | 1.91113800 | 3.06128100 | -1.28974100 |
| C | -1.33507300 | -2.60298100 | 2.47596300 |
| C | -1.43899300 | -3.34180200 | 3.65096400 |
| C | -2.12093700 | -4.55973800 | 3.68617400 |
| C | -2.70501600 | -5.00999600 | 2.49874000 |
| C | -2.60309600 | -4.27697200 | 1.32205700 |
| C | -2.40258900 | -2.72520600 | -2.44472500 |
| C | -2.19230600 | -3.45135300 | -3.61340400 |
| C | -1.31537400 | -4.53727000 | -3.64512100 |
| C | -0.65013000 | -4.86832900 | -2.46069200 |
| C | -0.85927900 | -4.14885000 | -1.29007500 |
| C | 2.60310100 | 4.27698100 | -1.32198800 |
| C | 2.70501300 | 5.01002000 | -2.49866400 |
| C | 2.12091500 | 4.55978100 | -3.68609600 |
| C | 1.43896300 | 3.34184800 | -3.65089300 |
| C | 1.33505200 | 2.60301500 | -2.47590100 |
| C | -2.20344100 | -5.37198100 | 4.94740700 |
| C | -1.11354700 | -5.34011700 | -4.89885400 |
| C | 2.20339900 | 5.37204000 | -4.94732000 |
| C | 1.11353100 | 5.34005100 | 4.89894500 |
| C | 0.85925800 | 4.14881200 | 1.29016700 |
| C | 0.65011100 | 4.86827300 | 2.46079000 |
| C | 1.31538700 | 4.53721700 | 3.64520800 |
| C | 2.19234700 | 3.45132900 | 3.61346200 |
| C | 2.40262900 | 2.72519600 | 2.44477000 |
| C | 1.74194000 | 3.06390300 | 1.26271500 |
| C | -10.48864300 | -0.86244700 | -0.03794100 |
| C | -11.46971100 | 0.10401500 | -0.03560200 |
| C | -11.24234900 | 1.56176800 | -0.00936300 |
| C | -12.56933200 | 2.20019700 | -0.01458700 |
| C | -13.56178600 | 1.20937100 | -0.04287200 |
| C | -12.90783700 | -0.12090000 | -0.05753800 |
| O | -10.16739100 | 2.14341200 | 0.01273700 |
| C | -13.58994100 | -1.32125200 | -0.08845300 |
| C | -12.86953400 | 3.55343400 | 0.00429300 |
| C | -14.20606100 | 3.93486700 | -0.00537500 |
| C | -15.18325400 | 2.94338300 | -0.03357700 |
| C | -14.90385300 | 1.58126400 | -0.05276500 |
| C | 10.48864600 | 0.86244700 | 0.03789300 |
| C | 11.46971400 | -0.10401400 | 0.03555000 |
| C | 11.24235400 | -1.56176800 | 0.00931200 |
| C | 12.56933700 | -2.20019500 | 0.01450700 |
| C | 13.56179100 | -1.20936800 | 0.04277700 |
| C | 12.90784000 | 0.12090200 | 0.05746700 |
| O | 10.16739600 | -2.14341300 | -0.01277000 |
| C | 13.58994300 | 1.32125500 | 0.08839200 |
| C | 12.86954100 | -3.55343100 | -0.00438600 |
| C | 14.20606800 | -3.93486300 | 0.00525200 |
| C | 15.18326000 | -2.94337800 | 0.03343700 |
| C | 14.90385800 | -1.58125900 | 0.05263900 |
| C | 4.53235500 | 1.51878800 | -0.00376300 |
| C | 5.22551600 | 0.29745400 | -0.01785800 |
| S | 4.15097800 | -1.06918500 | -0.03664500 |
| S | 5.59576000 | 2.89813700 | 0.02224300 |
| C | 6.97875400 | 1.82913100 | 0.01961800 |
| C | 6.62072800 | 0.46989300 | -0.00491500 |
| C | -4.53235300 | -1.51878900 | 0.00378900 |
| C | -5.22551400 | -0.29745500 | 0.01787800 |
| S | -4.15097700 | 1.06918400 | 0.03667800 |
| S | -5.59575800 | -2.89813800 | -0.02223400 |
| C | -6.97875200 | -1.82913200 | -0.01962700 |
| C | -6.62072600 | -0.46989400 | 0.00491500 |
| C | 8.35386700 | 2.02810700 | 0.03319700 |
| C | 9.07585500 | 0.82627600 | 0.02182800 |
| S | 7.99384300 | -0.57069300 | -0.00953100 |
| C | -8.35386500 | -2.02810800 | -0.03322500 |
| C | -9.07585300 | -0.82627700 | -0.02186000 |

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| S | -7.99384100 | 0.57069300 | 0.00951800 |
| C | -12.96475600 | -2.60067800 | -0.10507000 |
| N | -12.50045000 | -3.66794500 | -0.11976700 |
| C | -15.01062500 | -1.41802800 | -0.10836000 |
| N | -16.16628800 | -1.55276800 | -0.12566700 |
| C | 12.96475600 | 2.60067900 | 0.10504600 |
| N | 12.50045100 | 3.66794600 | 0.11977000 |
| C | 15.01062700 | 1.41803200 | 0.10827700 |
| N | 16.16629000 | 1.55277600 | 0.12556300 |
| H | -1.01042300 | 2.30217100 | 0.01128200 |
| H | 1.01042400 | -2.30217200 | -0.01124000 |
| H | -0.79980500 | -1.65856600 | 2.48880300 |
| H | -0.97879900 | -2.96068500 | 4.55942000 |
| H | -3.24892800 | -5.95155300 | 2.49282100 |
| H | -3.05549700 | -4.66541100 | 0.41378900 |
| H | -3.08629000 | -1.88133900 | -2.45986500 |
| H | -2.72235000 | -3.16531500 | -4.51872200 |
| H | 0.04276700 | -5.70639400 | -2.45285000 |
| H | -0.33804700 | -4.44374700 | -0.38375300 |
| H | 3.05551900 | 4.66540500 | -0.41372200 |
| H | 3.24893300 | 5.95157100 | -2.49274100 |
| H | 0.97875600 | 2.96074500 | -4.55934900 |
| H | 0.79977900 | 1.65860300 | -2.48874600 |
| H | -2.06858100 | -4.74704100 | 5.83420200 |
| H | -3.16736200 | -5.88215800 | 5.03105900 |
| H | -1.42530900 | -6.14414800 | 4.96889900 |
| H | -1.79649300 | -6.19736300 | -4.93058900 |
| H | -1.30316100 | -4.73929900 | -5.79242700 |
| H | -0.09539500 | -5.73459700 | -4.96062500 |
| H | 1.42511500 | 6.14405200 | -4.96889800 |
| H | 3.16722900 | 5.88240600 | -5.03086800 |
| H | 2.06875500 | 4.74707400 | -5.83413000 |
| H | 0.09507200 | 5.73366800 | 4.96119300 |
| H | 1.30411800 | 4.73951000 | 5.79249500 |
| H | 1.79574500 | 6.19789700 | 4.93020600 |
| H | 0.33800200 | 4.44370400 | 0.38385600 |
| H | -0.04280800 | 5.70632000 | 2.45296800 |
| H | 2.72241900 | 3.16529800 | 4.51876700 |
| H | 3.08635400 | 1.88134900 | 2.45989100 |
| H | -10.83597800 | -1.89084000 | -0.05639400 |
| H | -15.72809100 | 0.88103100 | -0.07397800 |
| H | 10.83597900 | 1.89084100 | 0.05633500 |
| H | 15.72809600 | -0.88102600 | 0.07383800 |
| H | 8.84801000 | 2.99282900 | 0.05213800 |
| H | -8.84800700 | -2.99283000 | -0.05217500 |
| H | -14.50744400 | 4.97641300 | 0.00827300 |
| H | 14.50745200 | -4.97640900 | -0.00840800 |
| H | 12.07214900 | -4.28911600 | -0.02614800 |
| H | -12.07214200 | 4.28911700 | 0.02606800 |
| F | 16.46447100 | -3.31902000 | 0.04256500 |
| F | -16.46446300 | 3.31902600 | -0.04273500 |

INIC1

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|-----|-------------|-------------|-------------|
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| C | -0.80582800 | -1.13570900 | 0.01013600 |
| C | -1.36512700 | 0.16445100 | 0.01031500 |
| C | -0.56570500 | 1.31152100 | 0.00300700 |
| C | 0.80583000 | 1.13570800 | -0.01012100 |
| C | 1.36512900 | -0.16445200 | -0.01030100 |
| C | 0.56570600 | -1.31152200 | -0.00299300 |
| C | -1.89760700 | -2.21641500 | 0.00679900 |
| C | 1.89761000 | 2.21641400 | -0.00677900 |
| C | -2.79753800 | -0.00308500 | 0.01209600 |
| C | -3.13810700 | -1.34038800 | -0.00440400 |
| C | 2.79754000 | 0.00308300 | -0.01208600 |
| C | 3.13810900 | 1.34038600 | 0.00441200 |
| C | -1.91574600 | -3.05863800 | 1.28969100 |
| C | -1.74545600 | -3.06170700 | -1.26267300 |
| C | 1.91574300 | 3.05865200 | -1.28966100 |
| C | -1.33986800 | -2.60084800 | 2.47613000 |
| C | -1.44501800 | -3.33957200 | 3.65107500 |
| C | -2.12804900 | -4.55690700 | 3.68593500 |
| C | -2.71198100 | -5.00663100 | 2.49822900 |
| C | -2.60883000 | -4.27370500 | 1.32159200 |
| C | -2.40549400 | -2.72254900 | -2.44496200 |
| C | -2.19544600 | -3.44897400 | -3.61351600 |
| C | -1.31936600 | -4.53558100 | -3.64488400 |

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|---|--------------|-------------|-------------|
| C | -0.65477000 | -4.86711800 | -2.46022100 |
| C | -0.86370100 | -4.14738500 | -1.28973100 |
| C | 2.60882100 | 4.27372200 | -1.32155000 |
| C | 2.71196600 | 5.00666300 | -2.49817900 |
| C | 2.12803000 | 4.55695100 | -3.68588700 |
| C | 1.44500600 | 3.33961000 | -3.65104000 |
| C | 1.33986400 | 2.60087300 | -2.47610500 |
| C | -2.21177600 | -5.36913500 | 4.94709600 |
| C | -1.11767800 | -5.33861200 | -4.89852500 |
| C | 2.21173800 | 5.36919600 | -4.94703900 |
| C | 1.11765700 | 5.33856400 | 4.89857100 |
| C | 0.86369600 | 4.14736300 | 1.28977700 |
| C | 0.65476600 | 4.86708200 | 2.46027000 |
| C | 1.31937500 | 4.53554000 | 3.64493000 |
| C | 2.19546800 | 3.44895000 | 3.61354500 |
| C | 2.40551600 | 2.72253400 | 2.44498000 |
| C | 1.74546400 | 3.06169100 | 1.26270400 |
| C | -10.48900300 | -0.84807600 | -0.03968700 |
| C | -11.47362500 | 0.11569000 | -0.03900900 |
| C | -11.24189200 | 1.57264700 | -0.01637000 |
| C | -12.57287400 | 2.20735400 | -0.02379100 |
| C | -13.56926100 | 1.21637300 | -0.04902000 |
| C | -12.90969300 | -0.11165400 | -0.06016200 |
| O | -10.16245400 | 2.14319500 | 0.00466500 |
| C | -13.58691400 | -1.31581800 | -0.08778600 |
| C | -12.91726700 | 3.54782600 | -0.00969500 |
| C | -14.25396000 | 3.92738400 | -0.01996300 |
| C | -15.23477200 | 2.93980000 | -0.04455700 |
| C | -14.91352600 | 1.58078100 | -0.05943500 |
| C | 10.48900600 | 0.84807400 | 0.03964900 |
| C | 11.47362800 | -0.11569100 | 0.03898200 |
| C | 11.24189600 | -1.57264900 | 0.01635000 |
| C | 12.57287800 | -2.20735500 | 0.02375700 |
| C | 13.56926500 | -1.21637300 | 0.04897400 |
| C | 12.90969600 | 0.11165400 | 0.06012700 |
| O | 10.16245800 | -2.14319700 | -0.00467400 |
| C | 13.58691600 | 1.31581800 | 0.08776400 |
| C | 12.91727200 | -3.54782700 | 0.00965800 |
| C | 14.25396600 | -3.92738400 | 0.01990800 |
| C | 15.23477700 | -2.93979900 | 0.04448700 |
| C | 14.91353100 | -1.58077900 | 0.05936900 |
| C | 4.53434000 | 1.51241600 | -0.00274800 |
| C | 5.22561500 | 0.28993700 | -0.01571600 |
| S | 4.14910900 | -1.07514100 | -0.03379700 |
| S | 5.59982200 | 2.89027700 | 0.02214900 |
| C | 6.98124200 | 1.81902600 | 0.02058300 |
| C | 6.62101500 | 0.46007100 | -0.00269000 |
| C | -4.53433800 | -1.51241800 | 0.00275000 |
| C | -5.22561300 | -0.28993900 | 0.01571800 |
| S | -4.14910700 | 1.07513900 | 0.03380800 |
| S | -5.59982000 | -2.89027900 | -0.02216500 |
| C | -6.98124000 | -1.81902800 | -0.02060600 |
| C | -6.62101300 | -0.46007300 | 0.00267800 |
| C | 8.35634200 | 2.01558500 | 0.03393500 |
| C | 9.07665900 | 0.81213300 | 0.02385900 |
| S | 7.99199300 | -0.58288100 | -0.00599200 |
| C | -8.35634000 | -2.01558700 | -0.03397200 |
| C | -9.07665700 | -0.81213500 | -0.02389000 |
| S | -7.99199100 | 0.58287800 | 0.00597900 |
| C | -12.95495100 | -2.59193600 | -0.10056400 |
| N | -12.48684600 | -3.65769400 | -0.11205600 |
| C | -15.00644400 | -1.42704300 | -0.10785800 |
| N | -16.15971700 | -1.58155400 | -0.12530200 |
| C | 12.95495200 | 2.59193500 | 0.10056800 |
| N | 12.48684800 | 3.65769300 | 0.11209000 |
| C | 15.00644600 | 1.42704400 | 0.10782700 |
| N | 16.15971900 | 1.58155700 | 0.12526300 |
| H | -1.00742600 | 2.30350900 | 0.00934000 |
| H | 1.00742800 | -2.30351100 | -0.00932900 |
| H | -0.80372800 | -1.65693300 | 2.48922500 |
| H | -0.98488200 | -2.95888400 | 4.55973800 |
| H | -3.25669400 | -5.94772400 | 2.49204500 |
| H | -3.06107200 | -4.66174500 | 0.41307200 |
| H | -3.08844500 | -1.87808200 | -2.46042000 |
| H | -2.72494900 | -3.16254100 | -4.51902700 |
| H | 0.03751200 | -5.70568300 | -2.45211000 |
| H | -0.34291600 | -4.44260700 | -0.38325900 |
| H | 3.06106800 | 4.66175200 | -0.41302700 |
| H | 3.25667600 | 5.94775700 | -2.49198600 |
| H | 0.98487000 | 2.95893000 | -4.55970600 |

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| H | 0.80373100 | 1.65695400 | -2.48920800 |
| H | -2.07693200 | -4.74431400 | 5.83397800 |
| H | -3.17609800 | -5.87864600 | 5.03023400 |
| H | -1.43417500 | -6.14182600 | 4.96895300 |
| H | -1.80109200 | -6.19548400 | -4.93040000 |
| H | -1.30671000 | -4.73771900 | -5.79217400 |
| H | -0.09972700 | -5.73365400 | -4.95999900 |
| H | 1.43397400 | 6.14172000 | -4.96899000 |
| H | 3.17596200 | 5.87890900 | -5.03006400 |
| H | 2.07712800 | 4.74434600 | -5.83393700 |
| H | 0.09940100 | 5.73275400 | 4.96051400 |
| H | 1.30764800 | 4.73794900 | 5.79220000 |
| H | 1.80034700 | 6.19603000 | 4.92997500 |
| H | 0.34290300 | 4.44258700 | 0.38331000 |
| H | -0.03752600 | 5.70564000 | 2.45217000 |
| H | 2.72498400 | 3.16251800 | 4.51904800 |
| H | 3.08847900 | 1.87807600 | 2.46042800 |
| H | -10.83517700 | -1.87676400 | -0.05639600 |
| H | -15.71017600 | 0.85007600 | -0.07832500 |
| H | 10.83517900 | 1.87676300 | 0.05634300 |
| H | 15.71018000 | -0.85007400 | 0.07824500 |
| H | 8.85216300 | 2.97948600 | 0.05182200 |
| H | -8.85216100 | -2.97948800 | -0.05186800 |
| H | -14.51005000 | 4.98117300 | -0.00870200 |
| H | -16.27889700 | 3.23543100 | -0.05235700 |
| H | 16.27890200 | -3.23542900 | 0.05227200 |
| H | 14.51005600 | -4.98117200 | 0.00864600 |
| F | -11.97171000 | 4.48422000 | 0.01358900 |
| F | 11.97171500 | -4.48422100 | -0.01361000 |

INIC3

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| 0 1 | | | |
| C | -0.77392400 | 1.15767800 | -0.01365300 |
| C | -1.36927000 | -0.12636300 | -0.00791200 |
| C | -0.60196800 | -1.29513600 | 0.00247800 |
| C | 0.77391700 | -1.15776100 | 0.01295200 |
| C | 1.36925700 | 0.12628300 | 0.00722600 |
| C | 0.60195900 | 1.29505500 | -0.00317200 |
| C | -1.83491500 | 2.26846000 | -0.01385000 |
| C | 1.83492400 | -2.26853300 | 0.01314600 |
| C | -2.79648100 | 0.08115600 | -0.00753800 |
| C | -3.09935600 | 1.42758100 | 0.00520800 |
| C | 2.79646900 | -0.08122000 | 0.00694500 |
| C | 3.09935800 | -1.42764100 | -0.00577100 |
| C | -1.83334200 | 3.10322100 | -1.30198800 |
| C | -1.65581200 | 3.11798800 | 1.24924700 |
| C | 1.83327700 | -3.10340100 | 1.30121700 |
| C | -1.27076200 | 2.62485800 | -2.48666900 |
| C | -1.35923300 | 3.35976200 | -3.66546700 |
| C | -2.01185700 | 4.59345800 | -3.70612900 |
| C | -2.58243000 | 5.06408600 | -2.52001900 |
| C | -2.49563000 | 4.33518700 | -1.33961600 |
| C | -2.32300400 | 2.80726800 | 2.43532800 |
| C | -2.08950200 | 3.53644800 | 3.59777500 |
| C | -1.18215200 | 4.59731500 | 3.61897800 |
| C | -0.51078100 | 4.90033100 | 2.43047000 |
| C | -0.74314200 | 4.17800300 | 1.26605000 |
| C | 2.49546300 | -4.33542200 | 1.33876500 |
| C | 2.58219100 | -5.06440800 | 2.51912100 |
| C | 2.01164700 | -4.59381600 | 3.70525700 |
| C | 1.35913400 | -3.36005700 | 3.66467700 |
| C | 1.27073400 | -2.62506700 | 2.48592900 |
| C | -2.07752100 | 5.40064700 | -4.97158500 |
| C | -0.95438700 | 5.40386300 | 4.86588100 |
| C | 2.07721300 | -5.40110300 | 4.97065600 |
| C | 0.95476800 | -5.40358800 | -4.86687800 |
| C | 0.74320000 | -4.17793900 | -1.26700500 |
| C | 0.51094000 | -4.90018400 | -2.43148700 |
| C | 1.18245900 | -4.59711900 | -3.61991100 |
| C | 2.08984400 | -3.53629800 | -3.59854000 |
| C | 2.32325100 | -2.80719600 | -2.43601500 |
| C | 1.65592100 | -3.11795700 | -1.25003500 |
| C | -10.46096300 | 1.13711300 | 0.04726300 |
| C | -11.46623400 | 0.19531300 | 0.04431100 |
| C | -11.27473400 | -1.26532400 | 0.01768800 |
| C | -12.62061300 | -1.86992800 | 0.01766900 |
| C | -13.58584800 | -0.85501000 | 0.04507500 |
| C | -12.89942800 | 0.45583800 | 0.06378800 |

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| O | -10.21911600 | -1.87996400 | -0.00136500 |
| C | -13.55064900 | 1.67332100 | 0.09605100 |
| C | -12.94044500 | -3.21761800 | -0.00514400 |
| C | -14.28433500 | -3.54459700 | 0.00016200 |
| C | -15.26218900 | -2.54395700 | 0.02794400 |
| C | -14.93932900 | -1.19714900 | 0.05047700 |
| C | 10.46097000 | -1.13706000 | -0.04669800 |
| C | 11.46622400 | -0.19524300 | -0.04367600 |
| C | 11.27469900 | 1.26538900 | -0.01693100 |
| C | 12.62057000 | 1.87001200 | -0.01665000 |
| C | 13.58582300 | 0.85511100 | -0.04408100 |
| C | 12.89942300 | -0.45574500 | -0.06303300 |
| O | 10.21907000 | 1.88001300 | 0.00202200 |
| C | 13.55066200 | -1.67321600 | -0.09542000 |
| C | 12.94037900 | 3.21770300 | 0.00638500 |
| C | 14.28426400 | 3.54470300 | 0.00128800 |
| C | 15.26213700 | 2.54408100 | -0.02651800 |
| C | 14.93930000 | 1.19727100 | -0.04927500 |
| C | 4.49025300 | -1.63868300 | -0.00095700 |
| C | 5.21531100 | -0.43588500 | 0.00742400 |
| S | 4.17779000 | 0.95882000 | 0.02339200 |
| S | 5.51690200 | -3.04566000 | -0.02399700 |
| C | 6.92761400 | -2.01351400 | -0.02664900 |
| C | 6.60519800 | -0.64514400 | -0.00653800 |
| C | -4.49024800 | 1.63864000 | 0.00052900 |
| C | -5.21532400 | 0.43585300 | -0.00777200 |
| S | -4.17782100 | -0.95886800 | -0.02385500 |
| S | -5.51687200 | 3.04563300 | 0.02382500 |
| C | -6.92759600 | 2.01350800 | 0.02670400 |
| C | -6.60520500 | 0.64513300 | 0.00648300 |
| C | 8.29691100 | -2.24822400 | -0.03982400 |
| C | 9.05003400 | -1.06528600 | -0.03193300 |
| S | 8.00415600 | 0.35944000 | -0.00516900 |
| C | -8.29688700 | 2.24824100 | 0.04011900 |
| C | -9.05003000 | 1.06531500 | 0.03232100 |
| S | -8.00418000 | -0.35942500 | 0.00535500 |
| F | -14.68183700 | -4.81269000 | -0.02082800 |
| F | -16.53797900 | -2.92003900 | 0.03202100 |
| F | 16.53792100 | 2.92018300 | -0.03039000 |
| F | 14.68174500 | 4.81279800 | 0.02250600 |
| C | -12.89417700 | 2.93673200 | 0.11686100 |
| N | -12.40470100 | 3.99262500 | 0.13492900 |
| C | -14.96859100 | 1.80262500 | 0.11362900 |
| N | -16.12153800 | 1.95928600 | 0.12911700 |
| C | 12.89420300 | -2.93663000 | -0.11646100 |
| N | 12.40474600 | -3.99252800 | -0.13471000 |
| C | 14.96860600 | -1.80250300 | -0.11289600 |
| N | 16.12155400 | -1.95916400 | -0.12830100 |
| H | -1.07115700 | -2.27437600 | 0.00043300 |
| H | 1.07114500 | 2.27429700 | -0.00110500 |
| H | -0.75843700 | 1.66777000 | -2.49560800 |
| H | -0.91003100 | 2.96290000 | -4.57268100 |
| H | -3.10337000 | 6.01855300 | -2.51809200 |
| H | -2.93656100 | 4.73965100 | -0.43270900 |
| H | -3.03024900 | 1.98320700 | 2.45866000 |
| H | -2.62522800 | 3.27275900 | 4.50651600 |
| H | 0.20535200 | 5.71849800 | 2.41456000 |
| H | -0.21637900 | 4.45113000 | 0.35609600 |
| H | 2.93637700 | -4.73985700 | 0.43183600 |
| H | 3.10305400 | -6.01891800 | 2.51713400 |
| H | 0.90996400 | -2.96321600 | 4.57191700 |
| H | 0.75849800 | -1.66793100 | 2.49493000 |
| H | -1.95912900 | 4.76801700 | -5.85526300 |
| H | -3.02928600 | 5.93298900 | -5.05625500 |
| H | -1.28145600 | 6.15413400 | -4.99850600 |
| H | -1.61242900 | 6.28054500 | 4.89234500 |
| H | -1.15884000 | 4.81576200 | 5.76462100 |
| H | 0.07477600 | 5.76952300 | 4.92214300 |
| H | 1.28090800 | -6.15433400 | 4.99762900 |
| H | 3.02881900 | -5.93375200 | 5.05517800 |
| H | 1.95912500 | -4.76848900 | 5.85438800 |
| H | -0.07470900 | -5.76827600 | -4.92378700 |
| H | 1.16037200 | -4.81578200 | -5.76554500 |
| H | 1.61198100 | -6.28090800 | -4.89279700 |
| H | 0.21633300 | -4.45110400 | -0.35712300 |
| H | -0.20523100 | -5.71832100 | -2.41571000 |
| H | 2.62568900 | -3.27257400 | -4.50720100 |
| H | 3.03053100 | -1.98316300 | -2.45922800 |
| H | -10.78319900 | 2.17361200 | 0.06398700 |
| H | -12.17584600 | -3.98661600 | -0.02642500 |

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| H | -15.74724100 | -0.47761400 | 0.07074000 |
| H | 10.78322500 | -2.17355400 | -0.06337300 |
| H | 12.17576500 | 3.98668600 | 0.02767400 |
| H | 15.74722500 | 0.47775200 | -0.06954500 |
| H | 8.76571000 | -3.22560800 | -0.05552400 |
| H | -8.76566800 | 3.22563200 | 0.05591900 |

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| C | 12.46777600 | 3.39962300 | -0.19575200 |
| C | 13.47026700 | 2.41900300 | -0.20742800 |
| C | 14.80723300 | 2.81522700 | -0.24050400 |
| C | 15.09634400 | 4.18059600 | -0.26053600 |
| C | 14.08635100 | 5.14406200 | -0.24861400 |
| C | 12.74855400 | 4.75471100 | -0.21581600 |
| C | 11.14542400 | 2.74285400 | -0.15845300 |
| C | 11.39074200 | 1.29125400 | -0.14676900 |
| C | 12.82816700 | 1.08302200 | -0.17865900 |
| C | 13.52408400 | -0.11366900 | -0.18345100 |
| O | 10.06504100 | 3.31588800 | -0.14036000 |
| C | -0.98010200 | 0.99660500 | 0.37733100 |
| C | -1.31776100 | -0.37456200 | 0.34662000 |
| C | -0.34802000 | -1.38199800 | 0.34944200 |
| C | 0.98010300 | -0.99663300 | 0.37728100 |
| C | 1.31776200 | 0.37453500 | 0.34666800 |
| C | 0.34802100 | 1.38197100 | 0.34954200 |
| C | -2.24468900 | 1.88229100 | 0.37846600 |
| C | 2.24468900 | -1.88232000 | 0.37838000 |
| C | -6.55627300 | -0.63065300 | -0.01537400 |
| C | -6.94217200 | 0.73012600 | -0.00670200 |
| C | -8.31718900 | 0.90720200 | -0.03924300 |
| C | -9.01342500 | -0.31489900 | -0.07452700 |
| S | -7.90494600 | -1.70092500 | -0.06711100 |
| N | -5.82794900 | 1.54337400 | 0.05780200 |
| C | -2.75204200 | -0.44522800 | 0.25529700 |
| C | -3.32315900 | 0.81290100 | 0.23184800 |
| C | -4.73087700 | 0.71289300 | 0.09531700 |
| C | -5.16462000 | -0.63782800 | 0.04279100 |
| S | -3.85602400 | -1.77339300 | 0.13368500 |
| C | -5.88442200 | 2.99777000 | 0.01823600 |
| C | 6.55627800 | 0.63064900 | -0.01525700 |
| C | 6.94217800 | -0.73013000 | -0.00666900 |
| C | 8.31719500 | -0.90720300 | -0.03921500 |
| C | 9.01343100 | 0.31490000 | -0.07442300 |
| S | 7.90495000 | 1.70092600 | -0.06692500 |
| N | 5.82795500 | -1.54338300 | 0.05777400 |
| C | 2.75204500 | 0.44520700 | 0.25537000 |
| C | 3.32316200 | -0.81292100 | 0.23184700 |
| C | 4.73088200 | -0.71290400 | 0.09533600 |
| C | 5.16462500 | 0.63782000 | 0.04289800 |
| S | 3.85602800 | 1.77337900 | 0.13384700 |
| C | 5.88443100 | -2.99777700 | 0.01812600 |
| C | -2.21863500 | 2.80844000 | -0.84927200 |
| C | -2.34249200 | 2.60616600 | 1.73185400 |
| C | 2.34246900 | -2.60627700 | 1.73172600 |
| C | -2.24233500 | 4.19873900 | -0.77965400 |
| C | -2.19094100 | 4.97394400 | -1.94062500 |
| C | -2.12641800 | 4.39119100 | -3.20381200 |
| C | -2.11494100 | 2.99131000 | -3.26995000 |
| C | -2.15538700 | 2.21845700 | -2.11998600 |
| C | -3.35951700 | 2.32728400 | 2.64639600 |
| C | -3.41068100 | 2.95906300 | 3.88840700 |
| C | -2.44768500 | 3.89058100 | 4.26957600 |
| C | -1.42118400 | 4.16421800 | 3.35849400 |
| C | -1.36720700 | 3.53622900 | 2.12225800 |
| C | 1.36714700 | -3.53632500 | 2.12207900 |
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| C | 2.44763200 | -3.89086200 | 4.26936300 |
| C | 3.41066700 | -2.95936800 | 3.88824200 |
| C | 3.35951500 | -2.32750200 | 2.64627200 |
| C | -2.06400800 | 5.22247600 | -4.45344900 |
| C | -2.50404700 | 4.58345200 | 5.60105300 |
| C | 2.50391900 | -4.58376500 | 5.60082600 |
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| C | -6.62579700 | 2.85877200 | -2.42616300 |
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| C | 6.62587200 | -2.85864800 | -2.42624600 |

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| C | 2.06406400 | -5.22223000 | -4.45372700 |
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| C | 2.12646700 | -4.39101500 | -3.20404400 |
| C | 2.11501800 | -2.99112900 | -3.27010300 |
| C | 2.15544800 | -2.21834100 | -2.12009500 |
| C | 2.21865200 | -2.80839600 | -0.84941400 |
| C | 10.42042100 | 0.30751300 | -0.10953100 |
| C | -10.42041600 | -0.30750600 | -0.10963300 |
| C | -12.46779900 | -3.39959600 | -0.19597400 |
| C | -13.47028100 | -2.41896600 | -0.20760000 |
| C | -14.80725100 | -2.81517600 | -0.24066700 |
| C | -15.09637400 | -4.18054200 | -0.26074100 |
| C | -14.08639000 | -5.14401800 | -0.24887000 |
| C | -12.74858900 | -4.75468100 | -0.21608100 |
| C | -11.14544000 | -2.74284100 | -0.15867200 |
| C | -11.39074300 | -1.29124000 | -0.14691900 |
| C | -12.82816700 | -1.08299300 | -0.17879200 |
| C | -13.52406800 | 0.11370700 | -0.18354100 |
| O | -10.06506200 | -3.31588700 | -0.14061200 |
| C | 12.91498800 | -1.39992100 | -0.15646100 |
| N | 12.46623600 | -2.47430000 | -0.13494300 |
| C | 14.94453400 | -0.19981200 | -0.21663300 |
| N | 16.10063500 | -0.33344900 | -0.24299400 |
| C | -5.35039300 | 8.36254900 | 0.57297300 |
| C | -6.05531500 | 7.44330000 | -0.41618300 |
| C | -5.58204400 | 5.99507500 | -0.32877700 |
| C | -6.29818700 | 5.08296400 | -1.32145100 |
| C | 5.35035100 | -8.36258500 | 0.57254700 |
| C | 6.05531100 | -7.44328300 | -0.41653200 |
| C | 5.58204000 | -5.99506100 | -0.32906500 |
| C | 6.29822100 | -5.08289900 | -1.32166400 |
| C | -12.91495400 | 1.39994900 | -0.15651700 |
| N | -12.46618200 | 2.47432000 | -0.13497700 |
| C | -14.94451800 | 0.19987100 | -0.21670600 |
| N | -16.10061700 | 0.33352900 | -0.24304900 |
| H | 15.62096400 | 2.10215200 | -0.25064200 |
| H | 11.94004000 | 5.47904300 | -0.20565300 |
| H | -0.64196200 | -2.42503400 | 0.29416200 |
| H | 0.64196500 | 2.42501100 | 0.29433900 |
| H | -8.84024800 | 1.85658000 | -0.03730300 |
| H | -6.82403400 | 3.28099600 | 0.50707100 |
| H | -5.07579400 | 3.38003000 | 0.64672900 |
| H | 8.84025500 | -1.85658100 | -0.03733400 |
| H | 6.82403100 | -3.28103000 | 0.50696700 |
| H | 5.07578800 | -3.38007400 | 0.64657700 |
| H | -2.31167400 | 4.69806700 | 0.18053800 |
| H | -2.20777900 | 6.05771400 | -1.85224800 |
| H | -2.07061900 | 2.50113500 | -4.23968600 |
| H | -2.14046600 | 1.13480100 | -2.20584400 |
| H | -4.12201500 | 1.59381900 | 2.40682100 |
| H | -4.21783400 | 2.71208800 | 4.57359300 |
| H | -0.64618200 | 4.87929600 | 3.62384300 |
| H | -0.55043200 | 3.78423200 | 1.45320600 |
| H | 0.55036100 | -3.78425600 | 1.45301400 |
| H | 0.64608600 | -4.87947000 | 3.62357300 |
| H | 4.21784700 | -2.71248600 | 4.57342900 |
| H | 4.12205000 | -1.59406200 | 2.40673400 |
| H | -2.19189200 | 6.28510300 | -4.23281600 |
| H | -1.10099100 | 5.09939500 | -4.96150300 |
| H | -2.84162600 | 4.92748900 | -5.16556400 |
| H | -2.73278600 | 5.64856000 | 5.48201000 |
| H | -3.27184300 | 4.14783600 | 6.24515000 |
| H | -1.54427600 | 4.51789100 | 6.12346100 |
| H | 2.73140300 | -5.64912900 | 5.48170100 |
| H | 3.27251100 | -4.14896600 | 6.24452300 |
| H | 1.54448600 | -4.51712000 | 6.12372600 |
| H | -4.76670900 | 3.61951500 | -1.70117200 |
| H | -6.51617500 | 3.33517500 | -3.40540400 |
| H | -6.29104600 | 1.82200000 | -2.52267700 |
| H | -7.69475000 | 2.84959900 | -2.18368100 |
| H | 4.76676200 | -3.61942000 | -1.70134800 |
| H | 6.51627600 | -3.33499900 | -3.40551600 |
| H | 6.29112700 | -1.82187000 | -2.52271500 |
| H | 7.69481900 | -2.84949100 | -2.18373300 |
| H | 2.19203700 | -6.28486100 | -4.23316200 |
| H | 1.10101200 | -5.09919300 | -4.96172700 |
| H | 2.84162500 | -4.92714200 | -5.16586100 |
| H | 2.31162900 | -4.69808200 | 0.18029400 |
| H | 2.20776300 | -6.05761400 | -1.85257000 |

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| H | 2.07073200 | -2.50090000 | -4.23981300 |
| H | 2.14055000 | -1.13467900 | -2.20589300 |
| H | 10.78877100 | -0.71353500 | -0.10451900 |
| H | -10.78876200 | 0.71354400 | -0.10456400 |
| H | -15.62097500 | -2.10209400 | -0.25076500 |
| H | -11.94008200 | -5.47902100 | -0.20595700 |
| H | -5.70964500 | 9.39303100 | 0.49061600 |
| H | -5.51624600 | 8.03392000 | 1.60495600 |
| H | -4.26820500 | 8.37280300 | 0.40095700 |
| H | -5.89831600 | 7.81163500 | -1.43892400 |
| H | -7.13965800 | 7.48023000 | -0.24523200 |
| H | -5.73192700 | 5.63799800 | 0.69931100 |
| H | -4.50051500 | 5.95528200 | -0.51176800 |
| H | -6.20048800 | 5.51215500 | -2.32762400 |
| H | -7.37620300 | 5.08431900 | -1.09868300 |
| H | 5.70960300 | -9.39306300 | 0.49014600 |
| H | 5.51616700 | -8.03401300 | 1.60455400 |
| H | 4.26816900 | -8.37282700 | 0.40049100 |
| H | 5.89834900 | -7.81156200 | -1.43930000 |
| H | 7.13964800 | -7.48022500 | -0.24554400 |
| H | 5.73188900 | -5.63804100 | 0.69904800 |
| H | 4.50051800 | -5.95525700 | -0.51209100 |
| H | 6.20055200 | -5.51203300 | -2.32786400 |
| H | 7.37623000 | -5.08427100 | -1.09886200 |
| H | -14.34728900 | -6.19766700 | -0.26515700 |
| H | -16.13481200 | -4.49630700 | -0.28615800 |
| H | 16.13477800 | 4.49637100 | -0.28595900 |
| H | 14.34723900 | 6.19771300 | -0.26486800 |

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| C | 12.64276000 | 2.67423600 | -0.03929300 |
| C | 13.58848100 | 1.64167600 | -0.01948900 |
| C | 14.94758000 | 1.95851900 | -0.02048400 |
| C | 15.29582900 | 3.29975400 | -0.04126500 |
| C | 14.33753300 | 4.31781900 | -0.06095800 |
| C | 12.98724700 | 4.01523500 | -0.06014900 |
| C | 11.28495700 | 2.09257600 | -0.03338100 |
| C | 11.45053700 | 0.63131000 | -0.01020500 |
| C | 12.87373900 | 0.34378700 | 0.00017100 |
| C | 13.50638300 | -0.88681900 | 0.02587700 |
| O | 10.24213000 | 2.73013400 | -0.04611400 |
| C | -0.91918800 | 1.05324900 | 0.27248300 |
| C | -1.33752600 | -0.29550200 | 0.24665100 |
| C | -0.42946300 | -1.35887900 | 0.24617100 |
| C | 0.91918800 | -1.05326000 | 0.27243200 |
| C | 1.33752600 | 0.29549200 | 0.24669100 |
| C | 0.42946400 | 1.35886900 | 0.24626300 |
| C | -2.12860700 | 2.01324000 | 0.27835700 |
| C | 2.12860600 | -2.01325200 | 0.27826800 |
| C | -6.58690200 | -0.24599100 | -0.00662500 |
| C | -6.89311900 | 1.13537000 | 0.00562200 |
| C | -8.25525900 | 1.39202000 | 0.00644100 |
| C | -9.02233300 | 0.21151200 | -0.00593900 |
| S | -7.99539800 | -1.23665600 | -0.02060300 |
| N | -5.73221600 | 1.88241900 | 0.03903300 |
| C | -2.77435600 | -0.28141200 | 0.17555400 |
| C | -3.27117000 | 1.00833900 | 0.15959400 |
| C | -4.68484300 | 0.98987700 | 0.05407500 |
| C | -5.19747900 | -0.33389700 | 0.01756700 |
| S | -3.95557000 | -1.54367200 | 0.08303100 |
| C | -5.70516300 | 3.33748500 | -0.00843000 |
| C | 6.58690600 | 0.24599700 | -0.00652800 |
| C | 6.89312400 | -1.13536400 | 0.00564200 |
| C | 8.25526300 | -1.39201300 | 0.00645900 |
| C | 9.02233700 | -0.21150500 | -0.00585000 |
| S | 7.99540100 | 1.23666400 | -0.02044500 |
| N | 5.73222000 | -1.88241600 | 0.03899700 |
| C | 2.77435800 | 0.28140600 | 0.17561500 |
| C | 3.27117200 | -1.00834300 | 0.15958600 |
| C | 4.68484600 | -0.98987600 | 0.05408400 |
| C | 5.19748300 | 0.33390100 | 0.01765800 |
| S | 3.95557200 | 1.54367200 | 0.08317700 |
| C | 5.70517100 | -3.33748000 | -0.00853400 |
| C | -2.06740900 | 2.91925700 | -0.96404300 |
| C | -2.16102900 | 2.76055700 | 1.62143100 |
| C | 2.16100300 | -2.76065200 | 1.62129600 |
| C | -2.02769300 | 4.31014400 | -0.91527800 |

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| C | -1.95137900 | 5.06540400 | -2.08784000 |
| C | -1.92425100 | 4.46215000 | -3.34270900 |
| C | -1.97780500 | 3.06249000 | -3.38798500 |
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IPIC-4CI

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References

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