

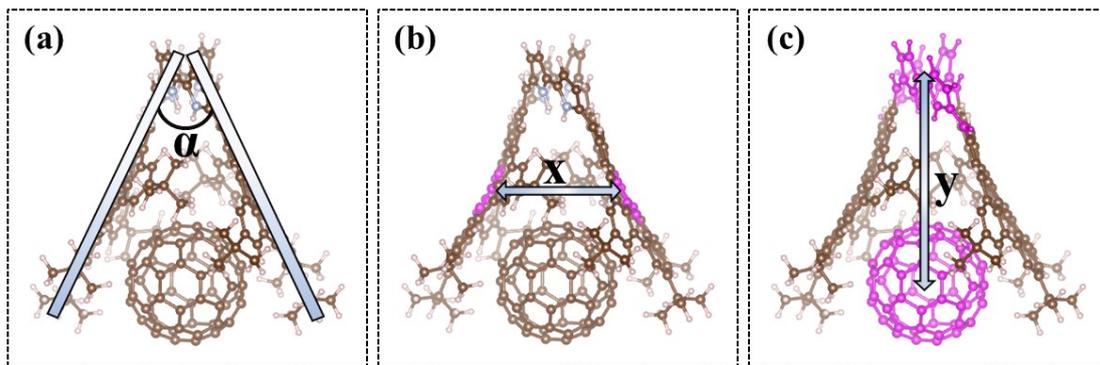
# **Quantum Simulation of Carrier Dynamics in Nanographene-fused Carbaporphyrin Tweezers@C60 Heterojunctions: Role of Dihedral Angle Engineering**

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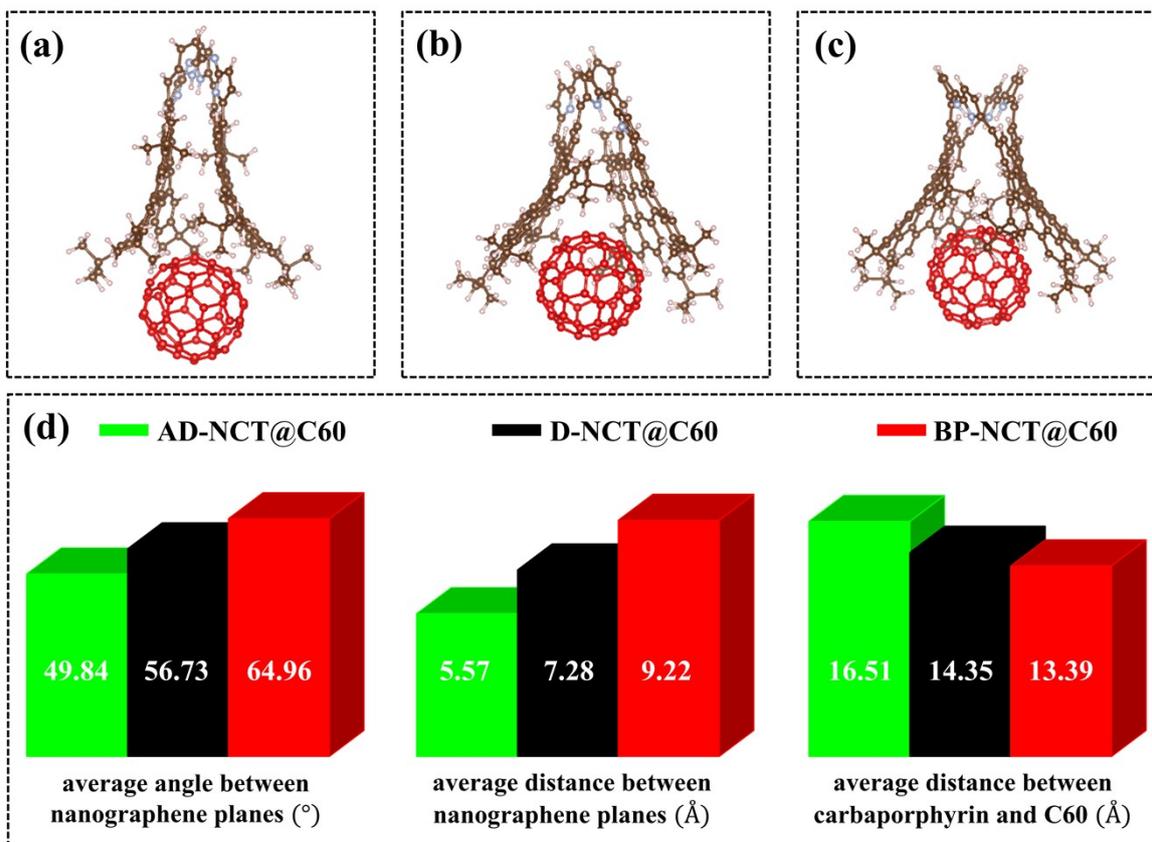
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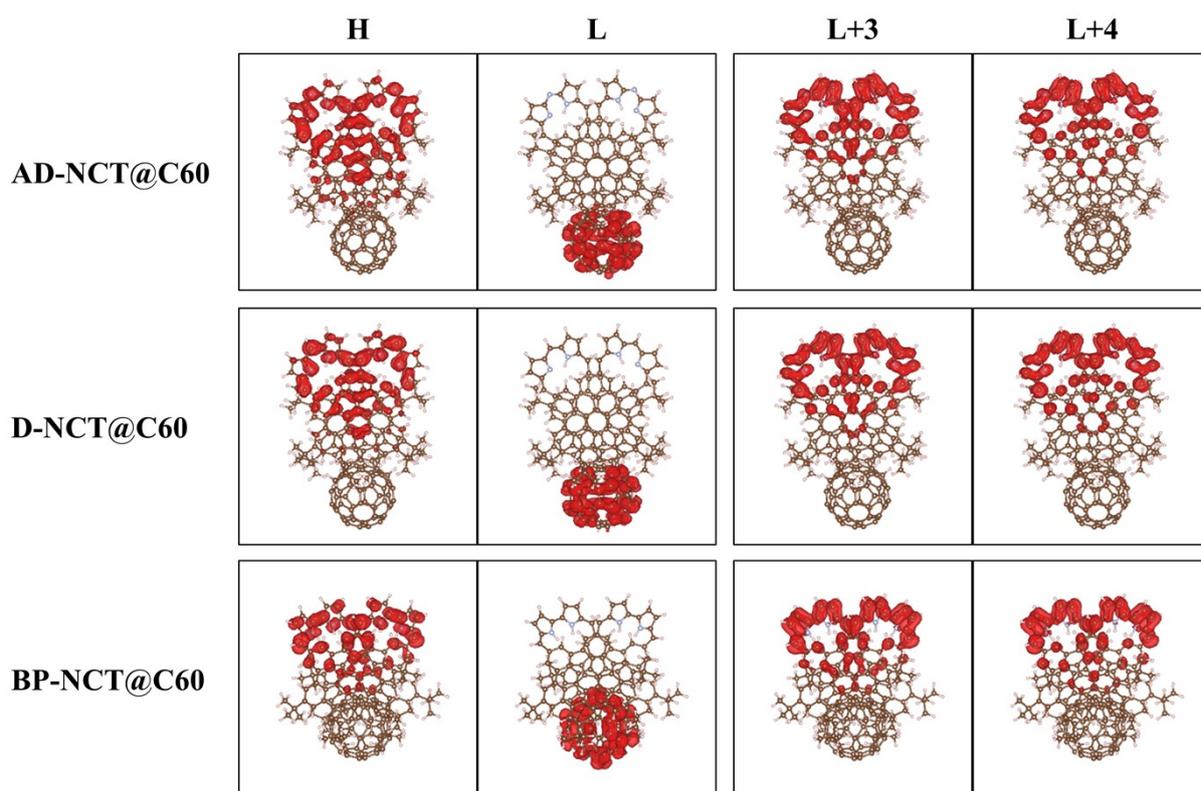
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sougatpal\_1979@yahoo.co.in



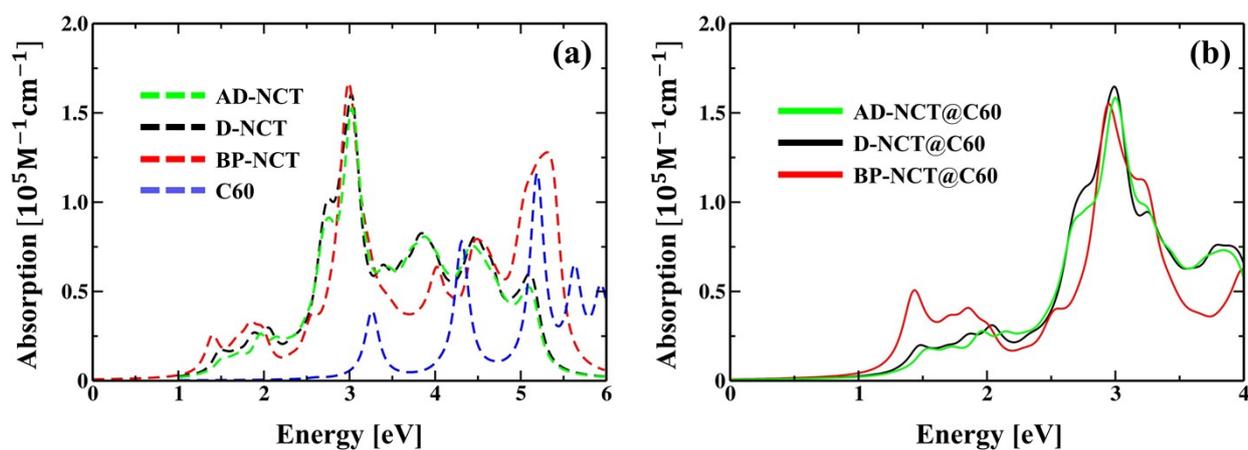
**Figure S1.** Schematic illustration of the geometrical parameters of the NCT@C60 hybrids with all values quantified as time average value at each fs-timestep throughout the MD trajectory. (a) average dihedral angle between nanographene planes obtained by assuming each nanographene as a rigid plane and calculating the inter-planar angle between them. (b) average interplanar distance simulated as the distances between atoms of the centroid benzene rings of two nanographene fragments. (c) average spatial separation computed from all atom-atom distances between carbaporphyrin linker and C60 molecule.



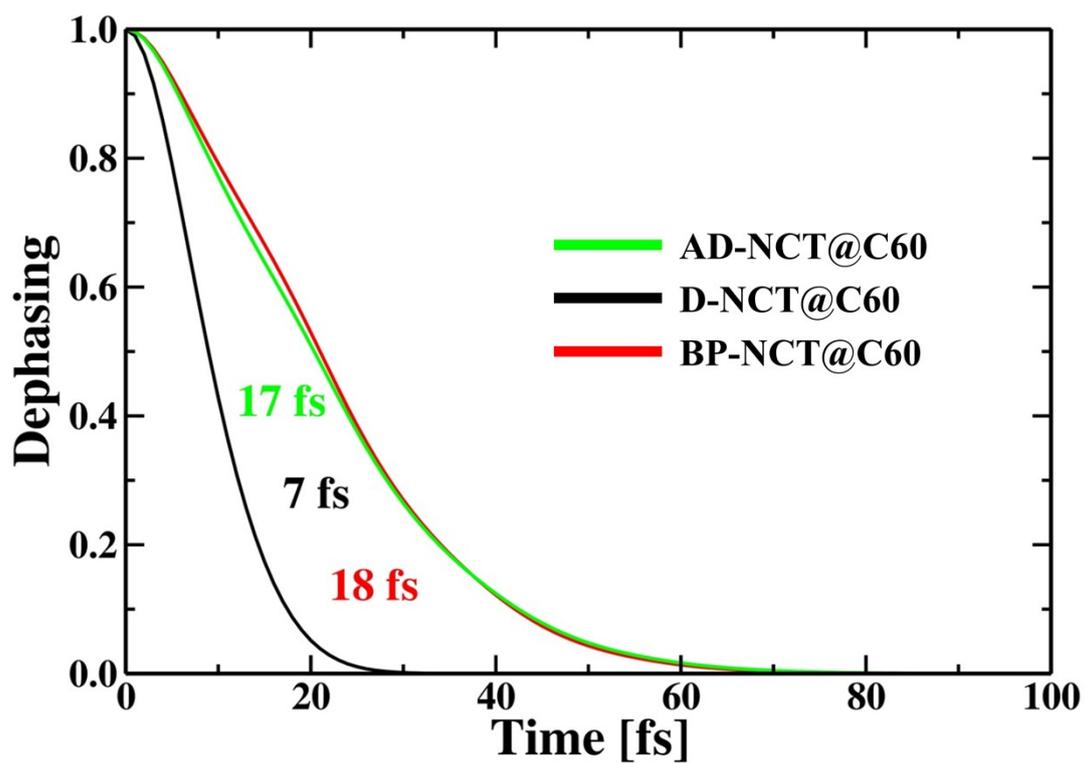
**Figure S2.** The geometries of the NCT@C60 composites at ambient temperature (300 K) are shown in (a) AD-NCT@C60, (b) D-NCT@C60 and (c) BP-NCT@C60 respectively. The C60 molecule encapsulated into the cavity of the tweezer molecule through  $\pi$ - $\pi$  van der Waals interaction, they all show stable geometries at room temperature. C atoms of the C60 are represented by red balls, while C, N, and H atoms of the NCT are denoted by the brown, light blue and light pink balls, respectively. (d) Relative column charts of the structural parameters at 300K temperature. Smaller dihedral angle between two nanographene planes and lower interplanar distance between them increases electronic repulsion, pushes C60 to the downward direction. Increasing spatial charge separation between carbaporphyrin and C60 in the AD-NCT@C60 composite gives weaker orbital overlap, indicating lower NA coupling.



**Figure S3.** Charge density distributions of the key orbitals participating in the ET and e-h recombination dynamics of the NCT@C60 composite are presented. The HOMO and donor state of all the composites distributed over the tweezer molecule specifically into the carbaporphyrin molecule whereas the LUMO is delocalized on the C60 molecule.



**Figure S4.** UV-Vis absorption spectra of the (a) individual molecule and (b) NCT@C60 hybrids are simulated utilizing time-dependent DFTB. The absorption spectra of the composite systems show that the NCT has a stronger light absorbing capacity than the C60 molecule at low energy. Constant highest absorption peak is shown throughout the hybrids.



*Figure S5. Pure-dephasing functions during the e-h recombination process in NCT@C60 composites.*

**Table S1.** Total energy, stabilisation energy and interaction energy per atom of the NCT@C60 composites.

| <b>system</b> | <b>total energy<br/>(eV)</b> | <b>stabilisationenergy<br/>(eV)</b> | <b>interaction energy<br/>(meV/atom)</b> |
|---------------|------------------------------|-------------------------------------|--|
| AD-NCT@C60    | -10656.1598                  | -0.3137                             | -1.005                                   |
| D-NCT@C60     | -10640.8918                  | -0.5094                             | -1.622                                   |
| BP-NCT@C60    | -10547.7161                  | -0.2609                             | -0.836                                   |

**Table S2.** Mulliken population of charges of NCT@C60 nanohybrids.

| <b>system</b> | <b>Mulliken charge</b> |                       |             |
|---------------|------------------------|-----------------------|-------------|
|               | <b>nanographene</b>    | <b>carbaporphyrin</b> | <b>C60</b>  |
| AD-NCT@C60    | 0.186846               | -0.178903             | -0.00794331 |
| D-NCT@C60     | 0.162364               | -0.154082             | -0.00828265 |
| BP-NCT@C60    | -0.155595              | 0.170608              | -0.01501350 |

## Optimized Cartesian coordinates of the AD-NCT@C60.

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| C | 19.75701479 | 11.31205100 | 23.63260780 |
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| C | 22.36549095 | 13.74675254 | 23.22712802 |
| C | 23.93466094 | 13.56420126 | 21.48391374 |
| C | 24.34332943 | 12.78779373 | 20.37910191 |
| C | 23.84586533 | 10.85578569 | 19.13220796 |
| C | 22.95926683 | 9.76247899  | 19.02952093 |
| C | 21.06949676 | 8.74430290  | 19.99707371 |
| C | 20.12275430 | 8.84967850  | 21.03892266 |
| C | 20.71662126 | 9.15827986  | 18.64719749 |
| C | 21.88415747 | 9.78843872  | 18.04915788 |
| C | 18.79309453 | 9.37255506  | 20.76351594 |
| C | 18.38165827 | 10.17745949 | 21.90435613 |
| C | 18.99210727 | 12.53309120 | 23.42469219 |
| C | 19.90517805 | 13.66130208 | 23.53135684 |
| C | 22.20107332 | 14.89684783 | 22.35153134 |
| C | 23.16944574 | 14.78099854 | 21.27466593 |
| C | 23.99105598 | 13.20272851 | 19.02879596 |
| C | 23.68447293 | 12.00854069 | 18.25769521 |
| C | 19.42679581 | 9.66462710  | 18.37932908 |
| C | 18.45096152 | 9.77361455  | 19.45386453 |
| C | 17.64000514 | 11.36110556 | 21.70248140 |
| C | 17.94901632 | 12.55690141 | 22.47387441 |
| C | 19.74909532 | 14.78113631 | 22.68435596 |
| C | 20.91584266 | 15.41321147 | 22.08636503 |
| C | 23.24465826 | 14.38243352 | 18.82697492 |
| C | 22.82849104 | 15.18265866 | 19.96667074 |
| C | 21.72760302 | 10.90674664 | 17.20149104 |
| C | 22.64121723 | 12.03488428 | 17.30659707 |
| C | 17.68674906 | 10.99360834 | 19.24452674 |
| C | 17.29099910 | 11.77408885 | 20.35212581 |
| C | 20.39792909 | 11.42899816 | 16.92478547 |
| C | 19.26550478 | 10.81682679 | 17.50507435 |
| C | 21.87635142 | 13.25522920 | 17.09566722 |
| C | 22.17565617 | 14.41551886 | 17.84261159 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 21.50762747 | 15.71965330 | 19.69012315 |
| C | 20.56489194 | 15.82902992 | 20.73581342 |
| C | 17.79077462 | 13.70937627 | 21.60050209 |
| C | 18.67726454 | 14.80271709 | 21.70246457 |
| C | 18.19070137 | 11.63804458 | 18.04067114 |
| C | 20.49023935 | 12.88014381 | 16.85872403 |
| C | 21.10184961 | 15.24108194 | 18.37648142 |
| C | 19.18266984 | 15.44761609 | 20.50005042 |
| C | 17.38666972 | 13.22365029 | 20.29019660 |
| C | 19.75973427 | 14.87254831 | 18.15022232 |
| C | 18.79418537 | 14.97147131 | 19.23123595 |
| C | 17.88487304 | 13.84430684 | 19.12658347 |
| C | 18.28508145 | 13.04478942 | 17.98122427 |
| C | 19.44849934 | 13.67737028 | 17.37920751 |

## Optimized Cartesian coordinates of the D-NCT@C60.

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 18.20290811 | 21.26699653 | 20.96419715 |
| C | 17.81291923 | 19.90721139 | 20.80984211 |
| C | 17.84243360 | 19.30113955 | 19.52473395 |
| C | 18.34800122 | 20.02529331 | 18.41242127 |
| C | 18.68314034 | 21.40047605 | 18.54896943 |
| C | 18.55614795 | 22.03786559 | 19.81812475 |
| C | 19.01506234 | 22.15869110 | 17.37248563 |
| C | 19.23263237 | 21.48769763 | 16.12805835 |
| C | 19.14124247 | 20.02795931 | 16.06781236 |
| C | 18.51551357 | 19.35429874 | 17.15216364 |
| C | 18.07168075 | 18.01171551 | 16.98040599 |
| C | 17.19945439 | 17.43978870 | 18.00938101 |
| C | 17.21783992 | 18.02330200 | 19.30886134 |
| C | 16.51783401 | 17.38728147 | 20.37289214 |
| C | 16.74340334 | 17.86872260 | 21.73836396 |
| C | 17.35274146 | 19.14359298 | 21.94010140 |
| C | 18.14954797 | 21.88055589 | 22.26558122 |
| C | 17.86625777 | 21.08089901 | 23.41804828 |
| C | 17.47637320 | 19.67361978 | 23.25723870 |
| C | 18.36054809 | 23.28710241 | 22.40043213 |
| C | 18.56860804 | 24.10798728 | 21.19687054 |
| C | 18.69550583 | 23.46533155 | 19.92250383 |
| C | 19.03453714 | 23.58558993 | 17.43151137 |
| C | 18.85717485 | 24.24467449 | 18.73099937 |
| C | 19.57664447 | 19.27327324 | 14.96108664 |
| C | 19.31981035 | 17.89435886 | 14.86587071 |
| C | 18.49036069 | 17.30150394 | 15.84052649 |
| C | 19.35999449 | 22.24975762 | 14.95806505 |
| C | 19.29977278 | 23.66179107 | 14.98583562 |
| C | 19.17921724 | 24.31176225 | 16.23540214 |
| C | 18.83392935 | 25.64181990 | 18.83567513 |
| C | 18.74857960 | 26.29908190 | 20.08319336 |
| C | 18.61888586 | 25.51611090 | 21.25273192 |
| C | 17.84771348 | 21.70573873 | 24.67923454 |
| C | 18.04108374 | 23.08981331 | 24.83719084 |
| C | 18.29769948 | 23.85867612 | 23.68975926 |
| C | 16.38338861 | 17.10041026 | 22.85907664 |
| C | 16.60074502 | 17.55495951 | 24.17300500 |
| C | 17.12486366 | 18.84759642 | 24.34893746 |
| C | 16.30123959 | 16.38688213 | 17.74828249 |
| C | 15.44272352 | 15.88246891 | 18.74604732 |
| C | 15.61170773 | 16.35254474 | 20.06219690 |
| C | 19.91911108 | 17.02265618 | 13.74025016 |
| C | 14.29759615 | 14.90182028 | 18.39656484 |
| C | 16.16560580 | 16.65641614 | 25.35574585 |
| C | 17.87786280 | 23.71191612 | 26.24521893 |
| C | 18.78566190 | 16.33712865 | 12.94378192 |
| C | 20.82570662 | 15.95651715 | 14.39853355 |
| C | 20.77294824 | 17.84411985 | 12.75175359 |
| C | 13.04420320 | 15.75925424 | 18.09588291 |
| C | 13.98693684 | 13.94115553 | 19.56549545 |
| C | 14.62886216 | 14.04100586 | 17.15804850 |
| C | 16.63368907 | 17.20053208 | 26.72062078 |
| C | 16.74917227 | 15.23399556 | 25.18341831 |
| C | 14.61922582 | 16.58772676 | 25.36404487 |
| C | 16.42899175 | 23.45255012 | 26.72714368 |
| C | 18.11441270 | 25.23502612 | 26.25482303 |
| C | 18.87649237 | 23.05608813 | 27.22682720 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 20.15575801 | 19.78141071 | 14.17678649 |
| H | 18.20623327 | 16.24154325 | 15.74524780 |
| H | 19.45916604 | 21.74670990 | 13.98382430 |
| H | 19.14847695 | 25.41170911 | 16.23274119 |
| H | 18.92995524 | 26.26861953 | 17.93676133 |
| H | 18.49834474 | 26.02879936 | 22.21781145 |
| H | 17.63739163 | 21.09545698 | 25.57020585 |
| H | 18.46110164 | 24.93938866 | 23.79858127 |
| H | 15.93736836 | 16.10741251 | 22.69676360 |
| H | 17.25235635 | 19.23473991 | 25.36937415 |
| H | 16.23570458 | 15.99687101 | 16.72200770 |
| H | 14.99199852 | 15.93423664 | 20.86849456 |
| H | 18.18632316 | 15.65635816 | 13.56629482 |
| H | 19.18845084 | 15.73777649 | 12.11320080 |
| H | 18.09733868 | 17.07872077 | 12.51190502 |
| H | 21.34196806 | 15.34381332 | 13.64365644 |
| H | 20.25702454 | 15.26424360 | 15.03500926 |
| H | 21.59289044 | 16.42717819 | 15.03107306 |
| H | 20.18172651 | 18.60594698 | 12.22085018 |
| H | 21.20935578 | 17.19142486 | 11.98007307 |
| H | 21.61409776 | 18.35308295 | 13.24680625 |
| H | 12.75810278 | 16.37168244 | 18.96391996 |
| H | 12.17939723 | 15.13001211 | 17.83519624 |
| H | 13.22027110 | 16.44560650 | 17.25431251 |
| H | 14.88631939 | 13.39561683 | 19.89158397 |
| H | 13.24223590 | 13.18834645 | 19.26667217 |
| H | 13.57214559 | 14.45615606 | 20.44447300 |
| H | 13.84232630 | 13.29200385 | 16.98182695 |
| H | 15.57386205 | 13.49246811 | 17.28222233 |
| H | 14.70452821 | 14.63348497 | 16.23436432 |
| H | 16.33803816 | 16.51863200 | 27.53231533 |
| H | 16.19155646 | 18.17952269 | 26.95957703 |
| H | 17.72661003 | 17.30029605 | 26.77454575 |
| H | 16.37008864 | 14.72331293 | 24.28596054 |
| H | 16.49517279 | 14.59343346 | 26.04129688 |
| H | 17.84486809 | 15.25526375 | 25.10550421 |
| H | 14.24945574 | 15.98099133 | 26.20476193 |
| H | 14.21824749 | 16.14074592 | 24.44219714 |
| H | 14.17698479 | 17.59035552 | 25.46076596 |
| H | 16.21124167 | 22.38098672 | 26.84905354 |
| H | 15.69479608 | 23.85693543 | 26.01482276 |
| H | 16.24080647 | 23.92993748 | 27.70092284 |
| H | 17.38589744 | 25.77430805 | 25.63070644 |
| H | 19.12239234 | 25.50429129 | 25.90913332 |
| H | 18.01308750 | 25.63701326 | 27.27438002 |
| H | 18.77462672 | 23.47551234 | 28.23915913 |
| H | 19.91591490 | 23.21843415 | 26.91024434 |
| H | 18.73035159 | 21.96898544 | 27.31534708 |
| C | 22.73356891 | 20.27727507 | 21.19763120 |
| C | 23.27171558 | 19.45447270 | 20.17262792 |
| C | 23.27877855 | 19.91283033 | 18.82742728 |
| C | 22.83227278 | 21.22898817 | 18.52197178 |
| C | 22.44419872 | 22.10835979 | 19.57489308 |
| C | 22.34119912 | 21.61306259 | 20.90802417 |
| C | 22.24511890 | 23.50787521 | 19.31086299 |
| C | 22.34795117 | 24.00779411 | 17.97198240 |
| C | 22.59364386 | 23.06629376 | 16.86796589 |
| C | 22.86316487 | 21.69396657 | 17.15971165 |
| C | 23.18289241 | 20.78244858 | 16.10386857 |
| C | 23.63131499 | 19.41989097 | 16.42109240 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| C | 23.77374737 | 19.04709176 | 17.78921360  |
| C | 24.43614772 | 17.83006263 | 18.13176042  |
| C | 24.67868903 | 17.51549847 | 19.54220464  |
| C | 23.94937357 | 18.23667487 | 20.52949974  |
| C | 22.59182831 | 19.74600346 | 22.52586298  |
| C | 23.09152611 | 18.45120815 | 22.84659125  |
| C | 23.98944917 | 17.80446404 | 21.88632251  |
| C | 21.93630747 | 20.51067785 | 23.52922328  |
| C | 21.78379837 | 21.94920986 | 23.30525524  |
| C | 21.97526295 | 22.48430912 | 21.99255625  |
| C | 22.04781887 | 24.40888537 | 20.40742221  |
| C | 21.89575857 | 23.89338881 | 21.77329760  |
| C | 22.63609590 | 23.49147129 | 15.52244497  |
| C | 22.92806361 | 22.61000355 | 14.46823479  |
| C | 23.17871537 | 21.26177773 | 14.78040260  |
| C | 22.23821680 | 25.39725575 | 17.75804869  |
| C | 22.07226031 | 26.30073067 | 18.83222935  |
| C | 22.01183592 | 25.78509236 | 20.14601551  |
| C | 21.71823084 | 24.74288921 | 22.88042968  |
| C | 21.62284438 | 24.23332971 | 24.19558750  |
| C | 21.62237712 | 22.83214810 | 24.38239311  |
| C | 22.70104846 | 17.85709122 | 24.06049659  |
| C | 21.84529835 | 18.52050284 | 24.96437909  |
| C | 21.53080625 | 19.86786385 | 24.71510015  |
| C | 25.62818507 | 16.56273427 | 19.96527586  |
| C | 25.81364917 | 16.25131357 | 21.32555402  |
| C | 24.93097376 | 16.82667362 | 22.26199813  |
| C | 24.02052123 | 18.49201547 | 15.42849502  |
| C | 24.59857298 | 17.25081198 | 15.74760540  |
| C | 24.83147235 | 16.95654577 | 17.10386546  |
| C | 23.06948181 | 23.07627785 | 12.99896232  |
| C | 25.07473166 | 16.24440303 | 14.67244319  |
| C | 26.99967827 | 15.36731776 | 21.78054387  |
| C | 21.28130383 | 17.75688199 | 26.18291421  |
| C | 24.52944557 | 22.82525234 | 12.54699864  |
| C | 22.76958627 | 24.57744270 | 12.81866840  |
| C | 22.10215988 | 22.27311770 | 12.098889137 |
| C | 24.55278103 | 14.82659218 | 15.00547565  |
| C | 26.62264406 | 16.24200394 | 14.66770451  |
| C | 24.58657639 | 16.61062467 | 13.25623765  |
| C | 28.21476291 | 16.30667822 | 21.97510431  |
| C | 27.35225438 | 14.29263100 | 20.72860543  |
| C | 26.70503754 | 14.64149687 | 23.11130735  |
| C | 20.38958922 | 18.64722269 | 27.07348796  |
| C | 22.44139908 | 17.21653567 | 27.04964594  |
| C | 20.42395465 | 16.58426519 | 25.65201451  |
| H | 22.42777842 | 24.54527133 | 15.29313258  |
| H | 23.41691176 | 20.56458845 | 13.96327573  |
| H | 22.33956374 | 25.80264836 | 16.74112937  |
| H | 21.88701720 | 26.50448216 | 20.96884303  |
| H | 21.70257205 | 25.83645340 | 22.75915231  |
| H | 21.54294365 | 22.43831571 | 25.40739662  |
| H | 23.02976650 | 16.82770224 | 24.27408165  |
| H | 20.92931438 | 20.43638220 | 25.43876027  |
| H | 26.26778265 | 16.08384663 | 19.20978865  |
| H | 25.01033499 | 16.55767788 | 23.32545953  |
| H | 23.87946348 | 18.75614625 | 14.37125309  |
| H | 25.31889560 | 16.00800706 | 17.37593547  |
| H | 25.24385249 | 23.33728925 | 13.20837248  |
| H | 24.70072320 | 23.19786501 | 11.52554489  |

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| H | 24.79205595 | 21.75680721 | 12.54575104 |
| H | 22.85733232 | 24.86628281 | 11.76025925 |
| H | 23.47295687 | 25.21339688 | 13.37718255 |
| H | 21.75014315 | 24.84140280 | 13.13344431 |
| H | 22.18933737 | 22.58023016 | 11.04571531 |
| H | 21.05592171 | 22.42613896 | 12.39710596 |
| H | 22.29399717 | 21.19005416 | 12.13265758 |
| H | 24.95262461 | 14.43661141 | 15.95308888 |
| H | 24.83499663 | 14.10529181 | 14.22389470 |
| H | 23.45710895 | 14.80943180 | 15.08476479 |
| H | 27.02141460 | 17.24546086 | 14.45732491 |
| H | 27.02001012 | 15.56084433 | 13.89972584 |
| H | 27.04055763 | 15.91953973 | 15.63296571 |
| H | 24.91314075 | 15.85503734 | 12.52570239 |
| H | 24.98653848 | 17.57462219 | 12.90731855 |
| H | 23.49050436 | 16.65645506 | 13.19438600 |
| H | 29.10541274 | 15.74957617 | 22.30400865 |
| H | 28.00823055 | 17.07800723 | 22.73188618 |
| H | 28.47560352 | 16.82577507 | 21.04080107 |
| H | 26.47796394 | 13.67383493 | 20.47267585 |
| H | 28.12985559 | 13.61304149 | 21.10820318 |
| H | 27.74328285 | 14.72035639 | 19.79372575 |
| H | 27.52273350 | 13.95176893 | 23.36889050 |
| H | 25.78429750 | 14.04272712 | 23.05528861 |
| H | 26.60389694 | 15.33264988 | 23.96103828 |
| H | 19.52875453 | 19.05980458 | 26.52542042 |
| H | 20.94556480 | 19.48925173 | 27.51355670 |
| H | 19.97947081 | 18.06785908 | 27.91497770 |
| H | 23.09538106 | 18.03181873 | 27.39299749 |
| H | 23.07174724 | 16.49642344 | 26.50716479 |
| H | 22.06289400 | 16.69832532 | 27.94380351 |
| H | 19.63895760 | 16.94602842 | 24.97148932 |
| H | 19.93246003 | 16.03957408 | 26.47268789 |
| H | 21.02409960 | 15.84938453 | 25.09743257 |
| C | 18.76920733 | 27.75552057 | 20.04321473 |
| C | 19.21448884 | 28.66972080 | 20.98204991 |
| C | 20.10222481 | 29.61847472 | 22.85149357 |
| C | 20.66202133 | 29.70425135 | 24.12512153 |
| C | 21.02948059 | 28.55284302 | 24.88964261 |
| N | 21.05458848 | 27.29834424 | 24.40494773 |
| C | 21.43887853 | 26.45288673 | 25.44354343 |
| C | 21.62692729 | 25.08439565 | 25.37095356 |
| C | 21.62971301 | 27.25940399 | 26.65635823 |
| C | 21.41036249 | 28.55714164 | 26.30841555 |
| C | 19.70346995 | 30.68745882 | 21.95445722 |
| C | 19.18346674 | 30.11714331 | 20.82533828 |
| C | 19.26299193 | 24.37391599 | 13.72199084 |
| C | 19.39329204 | 25.73213725 | 13.49473699 |
| N | 19.73835318 | 26.70527938 | 14.43020841 |
| C | 19.71205200 | 27.89672799 | 13.80641559 |
| C | 20.02824822 | 29.14190877 | 14.43477131 |
| C | 20.58722923 | 29.22491263 | 15.70893187 |
| N | 20.94506175 | 28.13593325 | 16.47054736 |
| C | 21.50852878 | 28.53255920 | 17.67231901 |
| C | 21.98950902 | 27.75016356 | 18.70768476 |
| C | 21.47801107 | 29.98841900 | 17.66384013 |
| C | 20.93790435 | 30.40458142 | 16.47822947 |
| C | 19.33575285 | 27.72416820 | 12.39694797 |
| C | 19.17232220 | 26.38728265 | 12.19868926 |
| H | 18.46149952 | 28.20059770 | 19.08235037 |

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| H | 20.79819952 | 30.70103053 | 24.56736791 |
| H | 21.84940908 | 24.57606691 | 26.32567909 |
| H | 21.93075715 | 26.88189751 | 27.64215561 |
| H | 21.47504279 | 29.43747752 | 26.96051807 |
| H | 19.81589620 | 31.75853968 | 22.15661798 |
| H | 18.78945293 | 30.64467119 | 19.94864764 |
| H | 19.06492167 | 23.75208272 | 12.83120875 |
| H | 19.85153948 | 30.07541431 | 13.88245433 |
| H | 20.76003074 | 27.16711508 | 16.14529916 |
| H | 22.27539056 | 28.31363372 | 19.61145795 |
| H | 21.84674951 | 30.62812601 | 18.47434399 |
| H | 20.78120076 | 31.44013075 | 16.15603494 |
| H | 19.23609975 | 28.52141393 | 11.64937573 |
| H | 18.89064304 | 25.88815749 | 11.26249977 |
| N | 19.79197839 | 28.43604745 | 22.21936328 |
| H | 20.01682991 | 27.51899207 | 22.65187894 |
| C | 22.90162256 | 9.72012896  | 21.54145605 |
| C | 21.86309647 | 9.75639133  | 22.56082507 |
| C | 22.02898238 | 10.98020162 | 23.33040398 |
| C | 23.17023630 | 11.69974589 | 22.78562556 |
| C | 23.70980560 | 10.92187089 | 21.67998674 |
| C | 24.20531387 | 11.57381881 | 20.52966059 |
| C | 22.61468514 | 9.20791242  | 20.25766323 |
| C | 20.56791282 | 9.28004937  | 22.26521492 |
| C | 20.89570499 | 11.69219103 | 23.78091371 |
| C | 23.13833034 | 13.10802900 | 22.70609813 |
| C | 19.39964228 | 10.01296879 | 22.72978524 |
| C | 19.56059869 | 11.20109631 | 23.47553236 |
| C | 20.86756179 | 13.14557495 | 23.70365019 |
| C | 21.97328942 | 13.84376756 | 23.17357456 |
| C | 23.64050721 | 13.77494604 | 21.51702806 |
| C | 24.17481909 | 13.02555629 | 20.44844246 |
| C | 23.91109441 | 11.04613347 | 19.20596285 |
| C | 23.12669538 | 9.88044998  | 19.07270909 |
| C | 21.27942447 | 8.71611537  | 19.95352695 |
| C | 20.27199398 | 8.75173984  | 20.94181998 |
| C | 20.96681133 | 9.08475612  | 18.58078378 |
| C | 22.10803001 | 9.80515583  | 18.03625963 |
| C | 18.92003054 | 9.15732495  | 20.58831357 |
| C | 18.38100349 | 9.93628716  | 21.69341825 |
| C | 18.70822335 | 12.35074586 | 23.20947577 |
| C | 19.51616184 | 13.55335856 | 23.34897138 |
| C | 21.76128548 | 14.96845949 | 22.27439811 |
| C | 22.79075085 | 14.92190525 | 21.25057706 |
| C | 23.86400380 | 13.39645483 | 19.07557068 |
| C | 23.70146873 | 12.17248527 | 18.30726637 |
| C | 19.65544569 | 9.47739545  | 18.23734498 |
| C | 18.61690723 | 9.51462948  | 19.25666658 |
| C | 17.55417701 | 11.05041944 | 21.43474161 |
| C | 17.71998051 | 12.27556686 | 22.20403948 |
| C | 19.31347604 | 14.64723458 | 22.47866171 |
| C | 20.45329469 | 15.37076998 | 21.93400888 |
| C | 23.03488555 | 14.50814649 | 18.81722111 |
| C | 22.49293267 | 15.28459803 | 19.92103072 |
| C | 21.90459447 | 10.89752912 | 17.16503720 |
| C | 22.71317591 | 12.10024204 | 17.30165015 |
| C | 17.76498205 | 10.66310873 | 18.98883059 |
| C | 17.24337233 | 11.41843437 | 20.06176066 |
| C | 20.55281312 | 11.30227551 | 16.81034107 |
| C | 19.44581948 | 10.60242562 | 17.33853113 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 21.86146308 | 13.24948574 | 17.03268434 |
| C | 22.02162546 | 14.43897531 | 17.77733560 |
| C | 21.14762216 | 15.70273021 | 19.56688731 |
| C | 20.14358768 | 15.73878314 | 20.55959089 |
| C | 17.51366889 | 13.40103735 | 21.30647054 |
| C | 18.30039805 | 14.56441882 | 21.43959744 |
| C | 18.27756974 | 11.33454166 | 17.80346323 |
| C | 20.52684277 | 12.75539138 | 16.72765954 |
| C | 20.85465876 | 15.17513474 | 18.24166846 |
| C | 18.81534198 | 15.23488310 | 20.25619830 |
| C | 17.21979553 | 12.87044126 | 19.98323401 |
| C | 19.56319817 | 14.68968416 | 17.95015669 |
| C | 18.53428833 | 14.71738194 | 18.97517449 |
| C | 17.72824275 | 13.51741761 | 18.83791988 |
| C | 18.25706164 | 12.74326917 | 17.72802848 |
| C | 19.39491242 | 13.46601191 | 17.18025032 |

## Optimized Cartesian coordinates of the BP-NCT@C60.

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 16.60515345 | 20.93976387 | 20.08700926 |
| C | 15.86106581 | 19.75195770 | 19.84191856 |
| C | 15.66688718 | 19.30234816 | 18.50457276 |
| C | 16.21707284 | 20.04442581 | 17.42145912 |
| C | 16.83748324 | 21.30166391 | 17.66230993 |
| C | 17.03163423 | 21.75113481 | 18.99768455 |
| C | 17.27354611 | 22.11416085 | 16.55992330 |
| C | 17.24849672 | 21.59666727 | 15.22650972 |
| C | 16.90078204 | 20.18315170 | 15.03754035 |
| C | 16.27144043 | 19.47227683 | 16.10289741 |
| C | 15.81370172 | 18.13803352 | 15.89245339 |
| C | 15.05288095 | 17.46698935 | 16.95122477 |
| C | 15.00568234 | 18.04718552 | 18.25404270 |
| C | 14.39404324 | 17.33237927 | 19.32937421 |
| C | 14.59612178 | 17.79568854 | 20.70866311 |
| C | 15.40175375 | 18.95059762 | 20.94791841 |
| C | 17.05547484 | 21.24766907 | 21.41834067 |
| C | 16.79153546 | 20.34239920 | 22.48698909 |
| C | 15.83443541 | 19.25217696 | 22.27432278 |
| C | 17.88707635 | 22.38344078 | 21.64404314 |
| C | 18.01912179 | 23.38577860 | 20.58134226 |
| C | 17.65753740 | 23.01975904 | 19.24949710 |
| C | 17.66977108 | 23.46606760 | 16.80016158 |
| C | 17.86496889 | 23.93988109 | 18.17561361 |
| C | 17.23025121 | 19.48548950 | 13.85890069 |
| C | 16.95108459 | 18.11624182 | 13.70726748 |
| C | 16.18953592 | 17.47998474 | 14.70525789 |
| C | 17.58274067 | 22.44341228 | 14.15229186 |
| C | 17.93147851 | 23.79815874 | 14.36660841 |
| C | 17.91775877 | 24.29109751 | 15.69542583 |
| C | 18.29280603 | 25.24335593 | 18.47963424 |
| C | 18.54505413 | 25.66808996 | 19.81132643 |
| C | 18.44745958 | 24.69685479 | 20.84233458 |
| C | 17.53319650 | 20.47555699 | 23.67851952 |
| C | 18.48290342 | 21.49810867 | 23.85877669 |
| C | 18.59944459 | 22.47701749 | 22.85453299 |
| C | 14.16459688 | 17.03635169 | 21.81496287 |
| C | 14.54059797 | 17.34537756 | 23.13451360 |
| C | 15.38588089 | 18.44758502 | 23.34077307 |
| C | 14.41453894 | 16.23018156 | 16.72979999 |
| C | 13.74516589 | 15.54506030 | 17.75664818 |
| C | 13.75395656 | 16.10934977 | 19.04497708 |
| C | 17.51454262 | 17.28237920 | 12.53368957 |
| C | 13.11598027 | 14.14979851 | 17.53522333 |
| C | 14.13203645 | 16.40082006 | 24.28849887 |
| C | 19.42761310 | 21.47486937 | 25.08276120 |
| C | 18.55610217 | 16.29691524 | 13.12013452 |
| C | 18.21677428 | 18.15259526 | 11.47078054 |
| C | 16.37727551 | 16.50235008 | 11.83605928 |
| C | 11.73276354 | 14.06775512 | 18.22036334 |
| C | 14.07130973 | 13.09710212 | 18.14815454 |
| C | 12.91817684 | 13.82602442 | 16.03932114 |
| C | 14.36010755 | 17.03649867 | 25.67611346 |
| C | 15.00092745 | 15.12404042 | 24.17880279 |
| C | 12.63512483 | 16.03126998 | 24.18111895 |
| C | 20.54505203 | 20.44527346 | 24.78612444 |
| C | 18.67089399 | 21.06302791 | 26.36538920 |
| C | 20.07261682 | 22.85192620 | 25.33991956 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 17.77673651 | 20.02022720 | 13.06933092 |
| H | 15.93216774 | 16.41716240 | 14.58327411 |
| H | 17.57896850 | 22.06314394 | 13.11911898 |
| H | 18.06495963 | 25.36850583 | 15.85928370 |
| H | 18.41108087 | 25.98979080 | 17.67775335 |
| H | 18.60483369 | 24.99475843 | 21.88899757 |
| H | 17.41601273 | 19.71453844 | 24.46375788 |
| H | 19.31392719 | 23.30483936 | 22.97776439 |
| H | 13.54998223 | 16.14166537 | 21.64063786 |
| H | 15.72123874 | 18.68874124 | 24.35878484 |
| H | 14.45085785 | 15.79159931 | 15.72322709 |
| H | 13.28197387 | 15.55061141 | 19.86574455 |
| H | 19.35515011 | 16.83510132 | 13.65224309 |
| H | 19.03145078 | 15.69601358 | 12.32990222 |
| H | 18.10660692 | 15.59239235 | 13.83575887 |
| H | 18.58811478 | 17.52883017 | 10.64340481 |
| H | 19.09051835 | 18.68707328 | 11.87418444 |
| H | 17.53757197 | 18.89598824 | 11.02624219 |
| H | 15.89510491 | 15.77098429 | 12.50136408 |
| H | 16.75412937 | 15.93995084 | 10.96838518 |
| H | 15.59326857 | 17.18281729 | 11.47216186 |
| H | 11.23553531 | 13.11187989 | 17.99650648 |
| H | 11.06766165 | 14.87284564 | 17.87475615 |
| H | 11.79520666 | 14.13835738 | 19.31631014 |
| H | 15.06172508 | 13.13209349 | 17.67017572 |
| H | 13.67947179 | 12.07635113 | 18.02173267 |
| H | 14.22407096 | 13.25720315 | 19.22605867 |
| H | 12.40881032 | 12.85819773 | 15.91588760 |
| H | 13.87009661 | 13.74629217 | 15.49281838 |
| H | 12.29783731 | 14.58089004 | 15.53276529 |
| H | 13.99839580 | 16.36894199 | 26.47293018 |
| H | 13.81991267 | 17.98894509 | 25.78688891 |
| H | 15.42389438 | 17.22266671 | 25.88792153 |
| H | 14.84751524 | 14.60193089 | 23.22244485 |
| H | 14.76895409 | 14.40873965 | 24.98252891 |
| H | 16.07207726 | 15.36493375 | 24.24959339 |
| H | 12.31286451 | 15.42830903 | 25.04345427 |
| H | 12.40545143 | 15.43947818 | 23.28277981 |
| H | 12.00277688 | 16.93094888 | 24.15457990 |
| H | 21.10851529 | 20.71145440 | 23.87958733 |
| H | 20.13670407 | 19.43510390 | 24.63457242 |
| H | 21.26368994 | 20.38556683 | 25.61654524 |
| H | 18.31888720 | 20.02120402 | 26.33743383 |
| H | 17.79492471 | 21.70531447 | 26.54014317 |
| H | 19.32114646 | 21.14708971 | 27.24938990 |
| H | 20.69167171 | 22.83109514 | 26.24917798 |
| H | 19.31945296 | 23.64268529 | 25.48163023 |
| H | 20.73765756 | 23.15999675 | 24.51981868 |
| C | 24.87567743 | 20.25094830 | 22.47567903 |
| C | 25.41251241 | 19.39925917 | 21.46926203 |
| C | 25.24131808 | 19.73085795 | 20.09451301 |
| C | 24.51694115 | 20.90145566 | 19.73440158 |
| C | 24.09067498 | 21.81367212 | 20.74100711 |
| C | 24.28014752 | 21.49231058 | 22.11453633 |
| C | 23.48595161 | 23.06233547 | 20.36508513 |
| C | 23.14150477 | 23.30891331 | 19.00125826 |
| C | 23.28863063 | 22.22053147 | 18.02980767 |
| C | 24.10353812 | 21.10197022 | 18.37060164 |
| C | 24.39918125 | 20.11904326 | 17.38171182 |
| C | 25.34542485 | 19.04795772 | 17.70775832 |

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|---|-------------|-------------|-------------|
| C | 25.72714121 | 18.84410563 | 19.06779577 |
| C | 26.51332650 | 17.70502892 | 19.42017203 |
| C | 26.65474768 | 17.34139525 | 20.83615317 |
| C | 26.04524410 | 18.15860995 | 21.83746551 |
| C | 24.84688760 | 19.82388931 | 23.84947829 |
| C | 25.28962632 | 18.51286610 | 24.19415689 |
| C | 25.98582377 | 17.70350340 | 23.18890568 |
| C | 24.28592512 | 20.67123084 | 24.85299652 |
| C | 23.93558410 | 22.05587270 | 24.51441647 |
| C | 23.87695127 | 22.42350905 | 23.13289473 |
| C | 23.28591948 | 24.08318699 | 21.34489242 |
| C | 23.49024058 | 23.74779375 | 22.75875504 |
| C | 22.61994071 | 22.22591903 | 16.79061890 |
| C | 22.76830685 | 21.17717119 | 15.86502628 |
| C | 23.70442268 | 20.16714019 | 16.15607408 |
| C | 22.72615920 | 24.59366389 | 18.61711813 |
| C | 22.62289997 | 25.65587660 | 19.55291617 |
| C | 22.86696432 | 25.35521098 | 20.91893490 |
| C | 23.26735852 | 24.68789565 | 23.77295815 |
| C | 23.27314085 | 24.34017392 | 25.14654806 |
| C | 23.62838799 | 23.01642157 | 25.49739495 |
| C | 24.99803809 | 18.01864091 | 25.48310895 |
| C | 24.33107228 | 18.79365917 | 26.44516685 |
| C | 24.04042953 | 20.13478369 | 26.13040458 |
| C | 27.24093130 | 16.12122529 | 21.22733145 |
| C | 27.20704141 | 15.66144793 | 22.55591308 |
| C | 26.57021088 | 16.46269135 | 23.51647912 |
| C | 25.83944618 | 18.17420191 | 16.71878148 |
| C | 26.68329930 | 17.09697660 | 17.03447692 |
| C | 26.99733348 | 16.87636045 | 18.38764998 |
| C | 21.89570314 | 21.07749851 | 14.59163716 |
| C | 27.15987189 | 16.09030474 | 15.96178744 |
| C | 27.76850322 | 14.26085810 | 22.89517292 |
| C | 23.88786346 | 18.22093814 | 27.81162300 |
| C | 20.83889353 | 19.97042276 | 14.82421132 |
| C | 22.76391612 | 20.72270123 | 13.36326042 |
| C | 21.16203475 | 22.39831168 | 14.28469257 |
| C | 26.29723226 | 14.81208146 | 16.09755110 |
| C | 28.65153784 | 15.74374219 | 16.17147156 |
| C | 27.00363969 | 16.64274902 | 14.52924173 |
| C | 27.88732184 | 14.02624866 | 24.41575402 |
| C | 29.17589323 | 14.08525338 | 22.28029789 |
| C | 26.79969524 | 13.20571731 | 22.30823521 |
| C | 22.34842707 | 18.34926758 | 27.91952191 |
| C | 24.56904833 | 19.01461817 | 28.95008995 |
| C | 24.25376587 | 16.73124302 | 27.97658493 |
| H | 21.92007035 | 23.04805108 | 16.57879396 |
| H | 23.84986659 | 19.35190412 | 15.43175390 |
| H | 22.58543687 | 24.79695851 | 17.54579440 |
| H | 22.75141956 | 26.17454428 | 21.64642354 |
| H | 23.12476692 | 25.74305824 | 23.49843281 |
| H | 23.65453388 | 22.75204665 | 26.56563103 |
| H | 25.27093010 | 16.98268785 | 25.72517970 |
| H | 23.55748818 | 20.77067206 | 26.88806627 |
| H | 27.69952168 | 15.47989985 | 20.46111643 |
| H | 26.51693430 | 16.11193664 | 24.55576582 |
| H | 25.54571635 | 18.34297987 | 15.67366874 |
| H | 27.60821890 | 16.00028343 | 18.64829349 |
| H | 21.30474997 | 18.99149022 | 15.01162504 |
| H | 20.18221396 | 19.85408379 | 13.94900471 |

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| H | 20.19846864 | 20.20089832 | 15.68844636 |
| H | 22.16655861 | 20.73950619 | 12.43906147 |
| H | 23.20697814 | 19.71815261 | 13.43111910 |
| H | 23.58821991 | 21.43982003 | 13.23477092 |
| H | 20.57419102 | 22.31317352 | 13.35851313 |
| H | 21.85872567 | 23.23972184 | 14.14410586 |
| H | 20.45201301 | 22.67273441 | 15.07875672 |
| H | 26.58375191 | 14.05243226 | 15.35439360 |
| H | 25.23006916 | 15.03430770 | 15.94819465 |
| H | 26.39789720 | 14.35107156 | 17.09161240 |
| H | 29.27426204 | 16.65040493 | 16.18362799 |
| H | 29.02609181 | 15.09863655 | 15.36240863 |
| H | 28.83554339 | 15.20378932 | 17.11199326 |
| H | 27.41415076 | 15.93474068 | 13.79332377 |
| H | 27.54136253 | 17.59333249 | 14.39341234 |
| H | 25.95175870 | 16.80457198 | 14.24902634 |
| H | 28.34153567 | 13.04518213 | 24.62222154 |
| H | 26.91025255 | 14.02783525 | 24.92232011 |
| H | 28.52405822 | 14.78088313 | 24.90205106 |
| H | 29.16447632 | 14.09884438 | 21.18044982 |
| H | 29.62180834 | 13.12400955 | 22.57738013 |
| H | 29.85850189 | 14.88110425 | 22.61294863 |
| H | 27.13879522 | 12.18194520 | 22.52802613 |
| H | 26.70856010 | 13.29059079 | 21.21500221 |
| H | 25.78914471 | 13.31618432 | 22.72895490 |
| H | 21.84828476 | 17.84742693 | 27.07769481 |
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| H | 21.97223626 | 17.89214380 | 28.84735467 |
| H | 24.28735421 | 20.07800540 | 28.94771516 |
| H | 25.66489653 | 18.96572465 | 28.86770537 |
| H | 24.29411802 | 18.61322641 | 29.93736664 |
| H | 23.77879312 | 16.09717310 | 27.21242526 |
| H | 23.91297254 | 16.35492684 | 28.95324704 |
| H | 25.34017856 | 16.55902392 | 27.93623985 |
| C | 18.77645314 | 27.07894362 | 20.04742355 |
| C | 19.20019240 | 27.71444646 | 21.21995230 |
| C | 20.04341114 | 28.03899747 | 23.31995895 |
| C | 20.72224495 | 27.70145256 | 24.51273526 |
| N | 21.28402376 | 26.45243009 | 24.69908447 |
| C | 22.06835639 | 26.41128351 | 25.84037927 |
| C | 22.91798092 | 25.34229186 | 26.14268783 |
| C | 21.89204883 | 27.69631998 | 26.47698164 |
| C | 21.10967595 | 28.48440142 | 25.65310591 |
| C | 19.55864397 | 29.29925549 | 22.83786857 |
| C | 19.08182115 | 29.11414024 | 21.55455601 |
| H | 22.36865198 | 28.01033022 | 27.41179013 |
| H | 20.82967426 | 29.52939845 | 25.82491603 |
| H | 19.58988193 | 30.24194841 | 23.39459718 |
| H | 18.64143213 | 29.88270975 | 20.91002191 |
| N | 19.79670266 | 27.11475217 | 22.31503712 |
| H | 20.15723115 | 26.15182656 | 22.31119836 |
| H | 18.48751620 | 27.75656562 | 19.22821661 |
| H | 21.08468988 | 25.63003217 | 24.11382495 |
| H | 23.36706447 | 25.29154248 | 27.14554539 |
| C | 18.30156451 | 24.68847798 | 13.27400329 |
| C | 19.14792356 | 25.78416679 | 13.47086976 |
| C | 20.48138439 | 27.20790980 | 14.66836286 |
| C | 21.15130957 | 27.66720000 | 15.82487104 |
| N | 21.38578636 | 26.85098799 | 16.92198014 |
| C | 21.98201829 | 27.55692533 | 17.95186792 |

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| C | 22.11105188 | 28.91375462 | 17.47498032 |
| C | 21.64196943 | 28.96764021 | 16.17654561 |
| C | 20.10906426 | 27.86456790 | 13.44622291 |
| C | 19.33461734 | 26.99342993 | 12.70235392 |
| H | 22.55417971 | 29.74207274 | 18.03850281 |
| H | 21.62051500 | 29.84746859 | 15.52460337 |
| H | 20.39392013 | 28.88466599 | 13.16661762 |
| H | 18.87002374 | 27.20574862 | 11.73349107 |
| N | 19.91803046 | 25.94714427 | 14.61088637 |
| H | 20.10851508 | 25.19206107 | 15.28330097 |
| H | 17.86534909 | 24.53052944 | 12.27662953 |
| H | 21.01513910 | 25.89747048 | 17.02537807 |
| H | 22.68872464 | 27.79161663 | 19.93380245 |
| C | 23.79566346 | 14.31917044 | 18.75562617 |
| C | 23.91676142 | 13.96448663 | 20.16267603 |
| C | 23.96227260 | 15.19572840 | 20.93472625 |
| C | 23.86336456 | 16.30619276 | 20.00528684 |
| C | 23.76534995 | 15.76899004 | 18.66013951 |
| C | 22.94513628 | 16.40645616 | 17.70632653 |
| C | 22.98728158 | 13.54509766 | 17.89642136 |
| C | 23.22555595 | 12.84479953 | 20.67114850 |
| C | 23.33240055 | 15.27653880 | 22.19424710 |
| C | 23.14179999 | 17.46280261 | 20.35949879 |
| C | 22.56602810 | 12.92606156 | 21.96652746 |
| C | 22.61929862 | 14.12158967 | 22.71731293 |
| C | 22.58794221 | 16.47268058 | 22.56143404 |
| C | 22.49655314 | 17.55278279 | 21.65734164 |
| C | 22.29914790 | 18.12353699 | 19.37931400 |
| C | 22.19987606 | 17.60101036 | 18.07230318 |
| C | 22.11316169 | 15.60863984 | 16.81930372 |
| C | 22.13302031 | 14.19950388 | 16.91545478 |
| C | 22.27156174 | 12.39177248 | 18.42154268 |
| C | 22.38897164 | 12.04741969 | 19.78613520 |
| C | 20.97484373 | 12.33239162 | 17.76399102 |
| C | 20.88927443 | 13.44855442 | 16.83345404 |
| C | 21.21267082 | 11.63342430 | 20.53557304 |
| C | 21.32210264 | 12.17589255 | 21.88185710 |
| C | 21.43151124 | 14.60395146 | 23.40705895 |
| C | 21.41362702 | 16.05716406 | 23.31293241 |
| C | 21.24063938 | 18.26371497 | 21.47851900 |
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| C | 20.90764605 | 17.54479675 | 17.40917136 |
| C | 20.85120370 | 16.31123543 | 16.63659899 |
| C | 19.83393271 | 11.92949170 | 18.49101081 |
| C | 19.95486551 | 11.57450255 | 19.89742504 |
| C | 20.16999004 | 12.64281487 | 22.55052212 |
| C | 20.22525008 | 13.87496638 | 23.32366072 |
| C | 20.18938604 | 16.73870977 | 23.13687226 |
| C | 20.10244804 | 17.85684155 | 22.20713866 |
| C | 19.75817743 | 18.01579345 | 18.07877405 |
| C | 19.86646906 | 18.55951226 | 19.42679545 |
| C | 19.66456890 | 14.12811046 | 16.65555567 |
| C | 19.64545954 | 15.58059020 | 16.55605705 |
| C | 18.76696579 | 12.05436656 | 20.58689662 |
| C | 18.87325471 | 12.58049628 | 21.89315323 |
| C | 18.48815024 | 13.71180362 | 17.40549749 |
| C | 18.57111097 | 12.62919293 | 18.30917117 |
| C | 18.45952805 | 16.06198706 | 17.24699456 |
| C | 18.52196489 | 17.25460653 | 17.99896276 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 18.70005987 | 18.12950095 | 20.17917936 |
| C | 18.81110163 | 17.78877862 | 21.54364122 |
| C | 18.96264020 | 14.57574013 | 23.14423993 |
| C | 18.94655116 | 15.98508549 | 23.05127768 |
| C | 17.91140545 | 12.70461677 | 19.60485676 |
| C | 17.74406500 | 14.90737493 | 17.77086615 |
| C | 17.87644344 | 17.32192964 | 19.29751693 |
| C | 18.09671976 | 16.63444984 | 22.06637030 |
| C | 18.12705114 | 13.77459851 | 22.26089839 |
| C | 17.18278096 | 16.20565657 | 19.80394955 |
| C | 17.29292858 | 15.85527699 | 21.20874552 |
| C | 17.29965919 | 14.40558398 | 21.30768334 |
| C | 17.18993931 | 13.86354907 | 19.96046421 |
| C | 17.11277326 | 14.97942919 | 19.03074368 |