

Designing Thermally Activated Delayed Fluorescence Emitters with Through-Space Charge Transfer: A Theoretical Study

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Table S1. The emission wavelengths (nm) are calculated using different functionals for AC-BO and QAC-BO in toluene. The corresponding experimental values in toluene are also listed for comparison.¹ The wavelengths are also given in eV in parentheses.

| | B3LYP | PBE0 | BMK | M062X | CAM-B3LYP | wB97XD | LC-PBE | Exp. |
|--------|---------------|---------------|-----------------------------|---------------|---------------|---------------|---------------|---------------|
| HF% | 20 | 25 | 42 | 54 | - | - | - | |
| AC-BO | 503 (2.47) | 466 (2.66) | 405 (3.06) | 370 (3.35) | 341 (3.64) | 339 (3.66) | 302 (4.11) | 432 (2.87) |
| QAC-BO | 494 (2.51) | 464 (2.67) | 407 (3.05) | 368 (3.37) | 340 (3.65) | 339 (3.66) | 303 (4.09) | 415 (2.99) |

We studied the thin film configurations of AC-BO and QAC-BO by using the Materials Studio software with the Forcite module and the Universal force field.² To generate the initial configuration, a TADF molecule is placed within a box measuring approximately $29.7 \times 29.7 \times 29.7$ Å and surrounded by 25 methyl methacrylate molecules. Subsequently, we conducted molecular dynamics simulations at 298K, with a total duration of 500 ps, and a time step of 0.1 fs. The chosen ensemble of dynamics is NVT, and the initial velocity is selected randomly.³

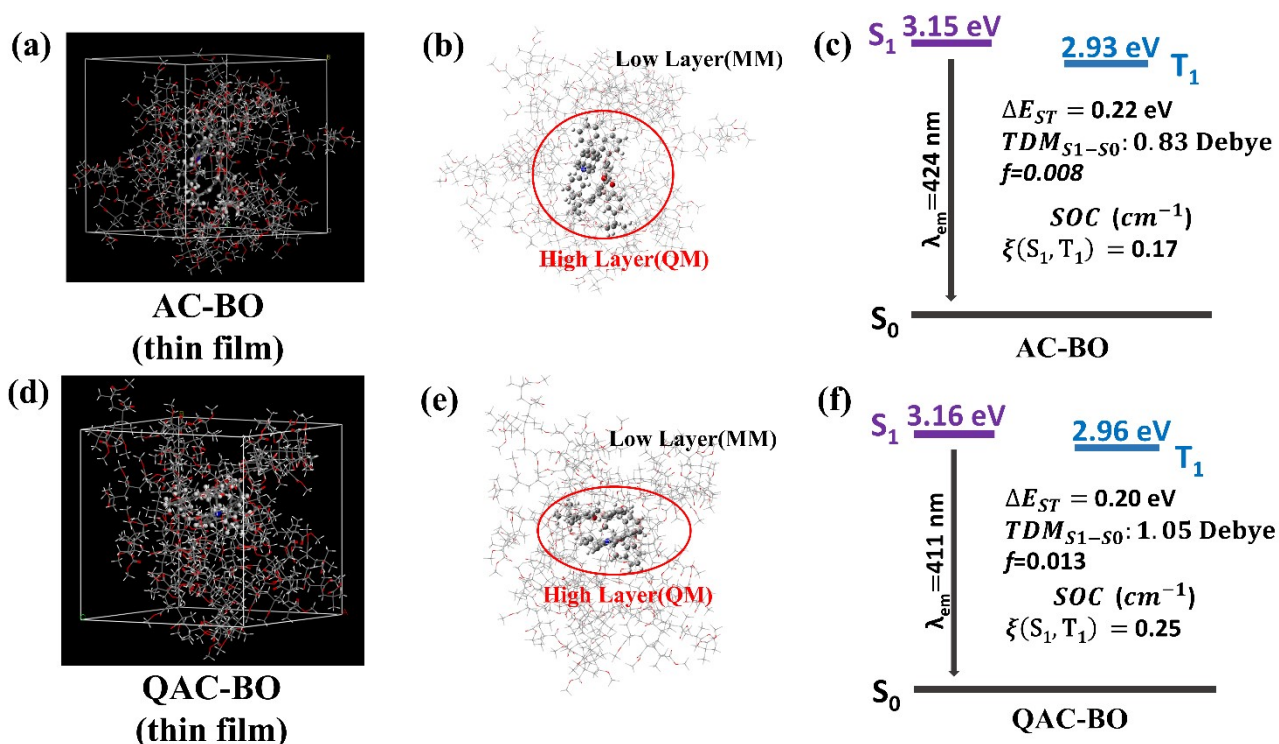


Figure S1. The thin film configuration of AC-BO (a) and QAC-BO (d). In the ONIOM model of (b) and (e), the AC-BO and QAC-BO as the high layer respectively, and surrounding methyl methacrylate molecules are

regarded as the low layer. Calculated oscillator strengths (f), TDMs between S_0 and S_1 , SOC between S_1 and T_1 at the BMK/6-311g** level for (c) and (f).

Table S2. The dihedral angles of the optimized structures and experimental structures in crystal phase.¹

| | $\theta_{ph}(\text{°})$ | $\theta_D(\text{°})$ | $\theta_A(\text{°})$ | $\Delta\theta_{D-A}(\text{°})$ |
|---------------|-------------------------|----------------------|----------------------|--------------------------------|
| AC-BO(QM/MM) | 89.72 | 55.54 | 85.90 | 30.36 |
| AC-BO(Cry.) | 88.53 | 54.97 | 86.05 | 31.08 |
| QAC-BO(QM/MM) | 59.93 | 86.94 | 86.29 | 0.65 |
| QAC-BO(Cry.) | 60.72 | 82.50 | 82.93 | 0.43 |

The root mean square displacements (RMSD) can be calculated based on the following formula⁴:

$$RMSD = \sqrt{\frac{1}{N} \sum_i^{natom} [(x_i - x_i')^2 + (y_i - y_i')^2 + (z_i - z_i')^2]} \quad S(1)$$

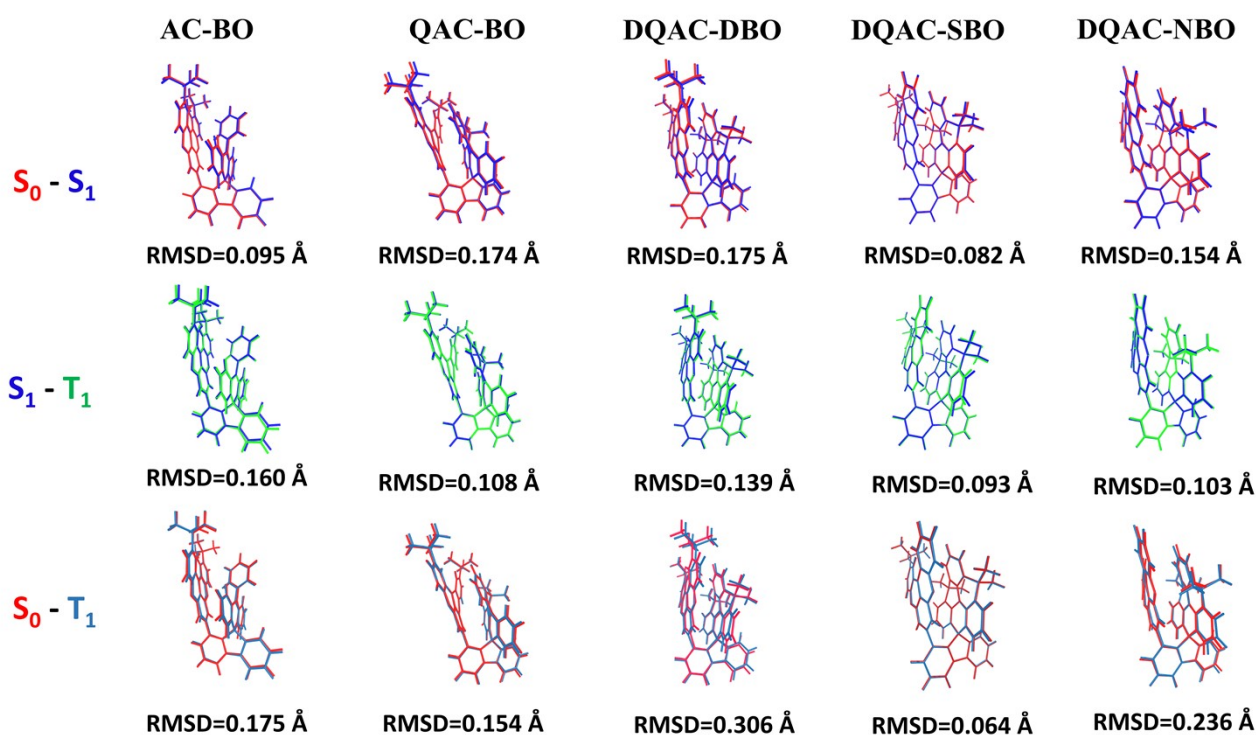


Figure S2. Molecular geometries and RMSD values in the gas state.

The independent gradient model (IGM) based on Hirshfeld partition of molecular density (IGMH) can clearly and intuitive demonstrate the intramolecular and intermolecular interactions, while the density gradient can be calculated as^{5,6}:

$$\delta g(r) = g^{\text{IGM}}(r) - g(r). \quad \text{S (2)}$$

$$g^{\text{IGM}}(r) = \sum_i \text{abs}[\nabla \rho_i^{\text{free}}(r)]. \quad \text{S (3)}$$

$$G(r) = |\sum_i \nabla \rho_i(r)|. \quad \text{S (4)}$$

Here, $\delta g(r)$ function equals the $g^{\text{IGM}}(r)$ minus the initial molecular density gradient $g(r)$, $\rho_i^{\text{free}}(r)$ means the spherically averaged density of atom i in the free state, $\nabla \rho_i^{\text{free}}(r)$ means the gradient vector.

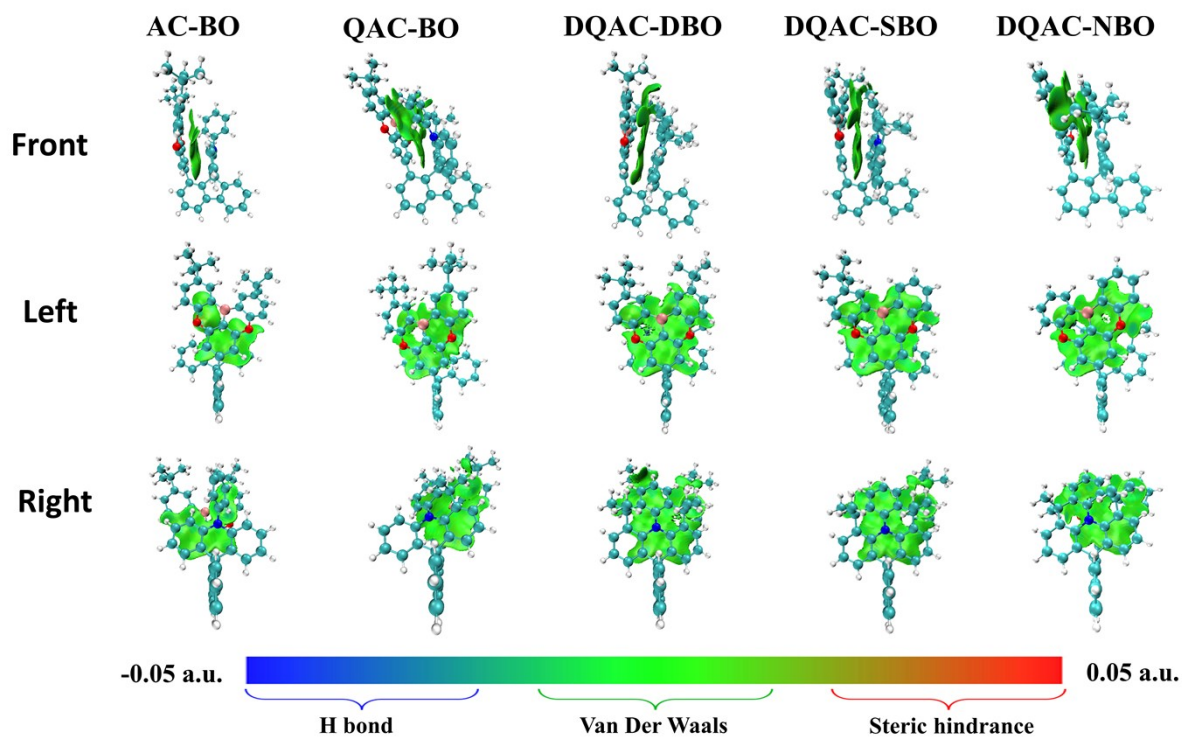


Figure S3. The inter-fragment intramolecular interaction for studied molecules measured by the IGMH method. (The iso-surface values are set as 0.004).

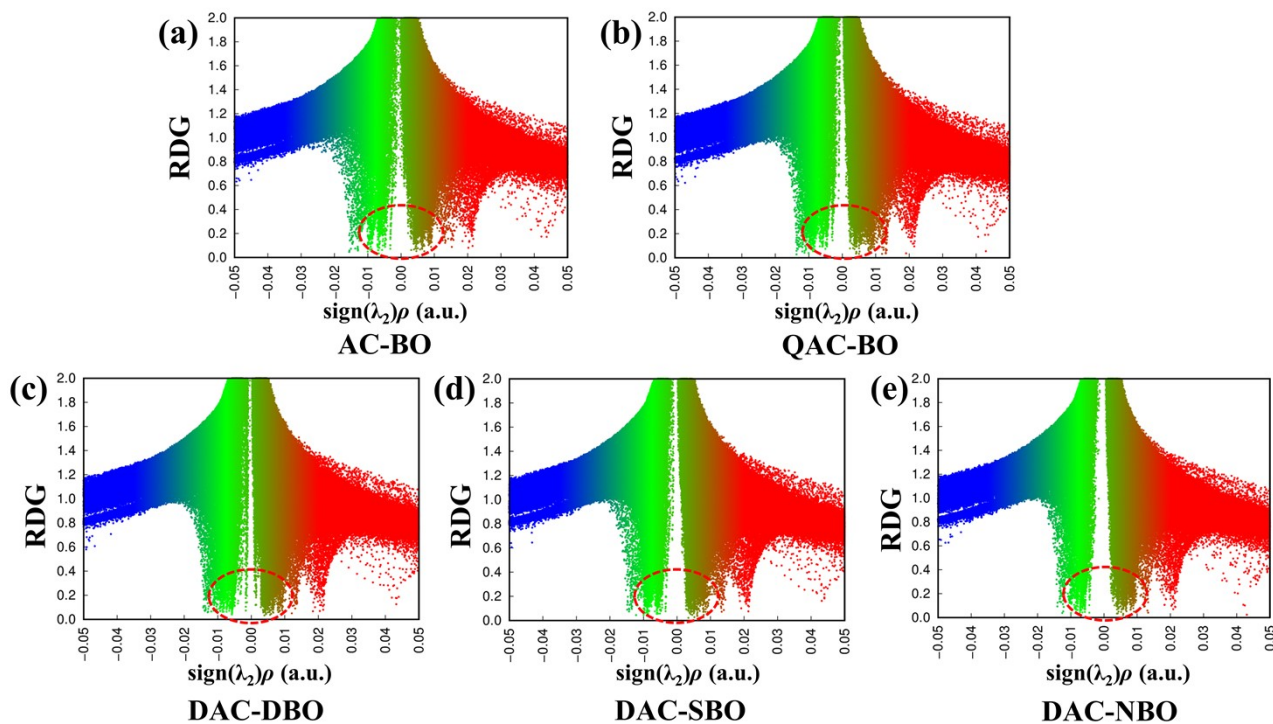


Figure S4. The scatter plot of RDG versus $\text{sign}(\lambda_2)\rho$ for the investigated molecules in the gas state with the optimized S_1 states.

The $S(r)$ can be calculated by the following formula^{7,8}:

$$S_r = \int \sqrt{\rho^{hole}(r)\rho^{ele}(r)} dr \quad S(5)$$

where ρ^{hole} and ρ^{ele} are the hole and electron density distributions, respectively.

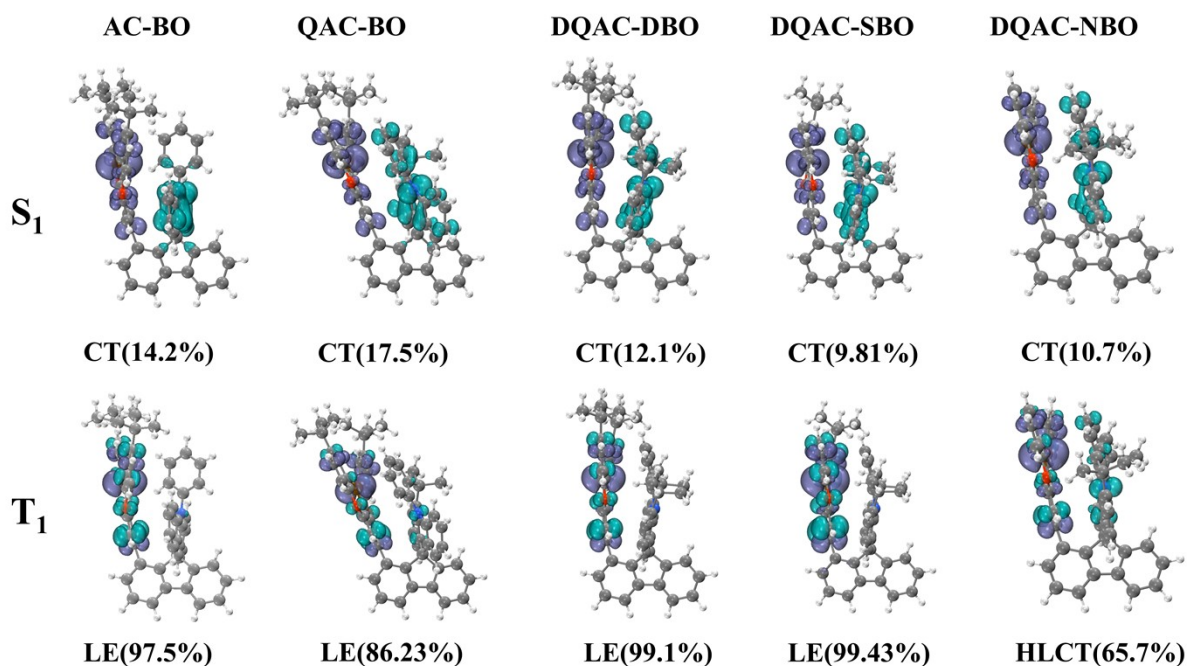


Figure S5. The hole–electron distribution and transition properties for the S₁ and T₁ states at the BMK/6-311g** level. Blue represents holes, and purple represents electrons. The values in parentheses are the LE proportions in the excitation.

Table S3. The calculated radiative and nonradiative rates of S₁ (*K_r*, *K_{nr}*) and T₁ (*K_r*, *K_{nr}*), and the intersystem crossing rates and reverse intersystem crossing rates (*K_{ISC}*, *K_{RISC}*) obtained with the MOMAP for the thin film environment. The experimental values corresponding to the film made of 10 wt% emitters doped in polymethyl methacrylate are also listed for comparison.

| Molecule | | <i>K_r^S</i> (×10 ⁶ s ⁻¹) | <i>K_{nr}^S</i> (×10 ² s ⁻¹) | <i>K_r^T</i> (s ⁻¹) | <i>K_{nr}^T</i> (×10 ⁻³ s ⁻¹) | <i>K_{ISC}</i> (×10 ⁶ s ⁻¹) | <i>K_{RISC}</i> (×10 ⁶ s ⁻¹) |
|---------------|-------------|---|--|--|---|---|--|
| AC-BO | Exp. | 5.10 | | | | 11.12 | 0.23 |
| (thin film) | Cal. | 3.05 | 0.39 | 3.64 | 0.75 | 1.94 | 0.85 |
| QAC-BO | Exp. | 12.80 | | | | 10.90 | 16.10 |
| (thin film) | Cal. | 5.01 | 0.28 | 3.63 | 0.69 | 27.88 | 17.98 |

In MOMAP software, the emission spectrum can be integrated to calculate the radiation rate ^{2,9}

$$k_r(T) = \int \sigma_{em}(\omega, T) d\omega \quad \text{S(6)}$$

The emission spectrum $\sigma_{em}(\omega, T)$ can be expressed based on the following formula:

$$\sigma_{em}(\omega, T) = \frac{4\omega^3}{3\hbar c^3} |\mu_{fi}|^2 \sum_{u,v} P_{iv} |\langle \Theta_{fu} | \Theta_{iv} \rangle|^2 \delta(\omega_{iv, fu} - \omega) \quad \text{S(7)}$$

where \hbar is Planck's constant, c is the speed of light, and ω is frequency. $\mu_{fi} = \langle \Phi_f | \hat{\mu} | \Phi_i \rangle$ represents the transition dipole moment between two electronic states P_{iv} represents the Boltzmann distribution function and Θ represents the nuclear vibrational wave function.

According to Fermi's Golden Rule, the non-radiative rate can be expressed as^{9,10}:

$$k_{nr} = \frac{2\pi}{\hbar} \sum_{v,u} P_{iv} \left| H_{fu,iu} + \sum_{n,\mu} \frac{H_{fu,n\mu} H_{n\mu,iv}}{E_{iv} - E_{n\mu}} \right|^2 \delta(E_{iv} - E_{fu}) \quad \text{S(8)}$$

Here, H' represents the interaction between two different states, and it can be expressed as:

$$\hat{H}' \psi_{iv} = \hat{H}^{BO} \Phi_i(r; Q) \Theta_v(Q) + \hat{H}^{SO} \Phi_i(r; Q) \Theta_v(Q) \quad \text{S(9)}$$

where \hat{H}^{BO} is the nonadiabatic coupling, and \hat{H}^{SO} is the spin–orbit coupling. The intersystem crossing rates K_{ISC} between S₁ and T₁ can be expressed as¹¹⁻¹³:

$$K_{ISC} = \frac{1}{\hbar^2} \langle \Phi_f | H^{SO} | \Phi_i \rangle \int_{-\infty}^{+\infty} dt [e^{i\omega_{if}t} Z_i^{-1} \rho_{ISC}(t, T)] \quad S(10)$$

where $\rho_{ISC}(t, T)$ is the Franck-Condon overlap between singlet and triplet excited states, and Z_i is the distribution function.

Coordinates of optimized molecular structures at the BMK/6-311G** level (unit: Å)

AC-BO (gas), S₀

| | | | |
|---|-------------|-------------|-------------|
| C | -3.61595300 | 0.04917600 | -2.32244200 |
| C | -4.26528800 | 0.12567600 | -3.56432900 |
| C | -5.65706900 | 0.25060500 | -3.64429800 |
| C | -6.43322400 | 0.33221800 | -2.48540600 |
| C | -5.79106000 | 0.26410200 | -1.24846500 |
| C | -4.39812900 | 0.09832100 | -1.16715400 |
| C | -6.33152900 | 0.37949800 | 0.11762700 |
| C | -5.26994600 | 0.27557700 | 1.02900400 |
| C | -3.94125400 | 0.02518600 | 0.30351100 |
| C | -7.63762900 | 0.57840400 | 0.56905400 |
| C | -7.86099700 | 0.67373700 | 1.94540300 |
| C | -6.79672300 | 0.57181900 | 2.85194800 |
| C | -5.48923200 | 0.36853300 | 2.39618200 |
| C | -3.43517400 | -1.38042400 | 0.64683400 |
| C | -2.21068300 | -1.59187000 | 1.30634900 |
| N | -1.34503100 | -0.52368200 | 1.57138600 |
| C | -1.63354600 | 0.77481500 | 1.13156700 |
| C | -2.89891500 | 1.09649300 | 0.61190200 |
| C | -0.64138800 | 1.77981400 | 1.17102200 |
| C | -0.93327400 | 3.08030400 | 0.78258300 |
| C | -2.21770000 | 3.42133300 | 0.34926300 |
| C | -3.17915100 | 2.42099200 | 0.25967200 |
| C | -4.24655000 | -2.47789200 | 0.33592800 |
| C | -3.88953800 | -3.77666200 | 0.67867200 |
| C | -2.69797100 | -3.97943700 | 1.37953300 |
| C | -1.87309300 | -2.90737200 | 1.69542800 |
| C | -0.08678300 | -0.76347300 | 2.20417000 |
| C | 0.89249000 | -1.48669400 | 1.52646800 |
| C | 2.14837100 | -1.69000700 | 2.09609200 |
| C | 2.42232300 | -1.16456800 | 3.36174200 |
| C | 1.43538500 | -0.45016700 | 4.04954600 |
| C | 0.17768300 | -0.25105300 | 3.47644100 |
| C | -2.12227600 | 0.02439900 | -2.22490000 |
| C | -1.43300300 | -1.17674600 | -2.01077000 |
| C | -0.05336700 | -1.11909000 | -1.81854500 |
| C | 0.63727100 | 0.10305800 | -1.73531400 |
| C | -0.09665700 | 1.28102700 | -1.96605900 |
| C | -1.45230900 | 1.25446700 | -2.26463500 |
| B | 2.08037000 | 0.15742900 | -1.31241800 |

| | | | |
|---|-------------|-------------|-------------|
| C | 2.57392500 | 1.56960800 | -0.97612100 |
| C | 1.72045100 | 2.64176500 | -1.30659400 |
| O | 0.49742900 | 2.49050300 | -1.87193600 |
| O | 0.60640000 | -2.29133200 | -1.64931200 |
| C | 1.94370200 | -2.34691900 | -1.39866700 |
| C | 2.76308800 | -1.21373500 | -1.23329900 |
| C | 3.78700000 | 1.90139800 | -0.32202200 |
| C | 4.17711700 | 3.20389000 | -0.04073100 |
| C | 3.29787500 | 4.23973500 | -0.43622300 |
| C | 2.08776600 | 3.97220100 | -1.05173800 |
| C | 2.45118600 | -3.64411100 | -1.23335000 |
| C | 3.78847700 | -3.81791400 | -0.92015300 |
| C | 4.66949500 | -2.71975700 | -0.77999100 |
| C | 4.13089800 | -1.45170500 | -0.95507200 |
| C | 5.49606200 | 3.54810500 | 0.66963900 |
| C | 6.35855100 | 4.44165500 | -0.25428000 |
| C | 6.31385000 | 2.28782600 | 1.02252800 |
| C | 5.19051900 | 4.30969600 | 1.98213100 |
| C | 6.14666300 | -2.96225700 | -0.43154400 |
| C | 6.23299000 | -3.70189900 | 0.92563200 |
| C | 6.94227300 | -1.64524100 | -0.31395100 |
| C | 6.80354600 | -3.82919300 | -1.53242100 |
| H | -3.66852400 | 0.09577400 | -4.47091800 |
| H | -6.13276200 | 0.30234600 | -4.61857100 |
| H | -7.51023300 | 0.45720000 | -2.54442600 |
| H | -8.46121500 | 0.66026400 | -0.13414100 |
| H | -8.86855000 | 0.82996300 | 2.31769600 |
| H | -6.99063800 | 0.65071700 | 3.91698300 |
| H | -4.65815000 | 0.28344100 | 3.09025300 |
| H | 0.36655200 | 1.52993300 | 1.47889000 |
| H | -0.14072600 | 3.82186800 | 0.80102900 |
| H | -2.45464300 | 4.43958800 | 0.06089400 |
| H | -4.16968500 | 2.64674100 | -0.12681300 |
| H | -5.18452400 | -2.29327800 | -0.17938700 |
| H | -4.53423600 | -4.61020200 | 0.42273700 |
| H | -2.40478400 | -4.97833000 | 1.68691100 |
| H | -0.96007800 | -3.08816700 | 2.24617900 |
| H | 0.63431100 | -1.91270500 | 0.57122100 |
| H | 2.90077600 | -2.24295200 | 1.53941600 |
| H | 3.39762100 | -1.31144400 | 3.81439600 |
| H | 1.64547600 | -0.04629600 | 5.03487100 |
| H | -0.59068400 | 0.31834700 | 3.98921700 |
| H | -1.95449700 | -2.12603600 | -1.96421800 |
| H | -1.99461400 | 2.18239700 | -2.39382000 |
| H | 4.41724600 | 1.08344600 | -0.00585700 |
| H | 3.56121400 | 5.27488200 | -0.24231000 |
| H | 1.40319900 | 4.76454000 | -1.33523900 |
| H | 1.77787800 | -4.48705100 | -1.34607600 |
| H | 4.16013400 | -4.82897500 | -0.78591200 |

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|---|------------|-------------|-------------|
| H | 4.77619700 | -0.58874600 | -0.88234800 |
| H | 6.58385100 | 3.92033900 | -1.19041500 |
| H | 5.84727300 | 5.37705100 | -0.50051000 |
| H | 7.30332300 | 4.69380400 | 0.24038200 |
| H | 5.76348400 | 1.63335600 | 1.70659200 |
| H | 6.57669300 | 1.71435900 | 0.12658600 |
| H | 7.24456100 | 2.58462600 | 1.51647700 |
| H | 4.57610900 | 3.69461800 | 2.64775400 |
| H | 6.12361500 | 4.55894000 | 2.49990400 |
| H | 4.65285800 | 5.24270600 | 1.78835000 |
| H | 5.72131900 | -4.66826100 | 0.89042700 |
| H | 7.28058800 | -3.88352900 | 1.19060600 |
| H | 5.77380400 | -3.10191700 | 1.71834200 |
| H | 6.94343200 | -1.09311400 | -1.25963000 |
| H | 6.53490600 | -0.99528700 | 0.46878500 |
| H | 7.98178200 | -1.87045400 | -0.05524000 |
| H | 6.74562500 | -3.32506200 | -2.50257400 |
| H | 7.85843100 | -4.00553300 | -1.29393100 |
| H | 6.31175300 | -4.80212800 | -1.62454900 |

AC-BO (gas), S₁

| | | | |
|---|-------------|-------------|-------------|
| C | -3.64697600 | -0.07421200 | -2.31404900 |
| C | -4.32702300 | -0.06036400 | -3.54350100 |
| C | -5.72145000 | 0.05165500 | -3.60721300 |
| C | -6.48539700 | 0.17732900 | -2.44414500 |
| C | -5.82345900 | 0.16873100 | -1.21590200 |
| C | -4.42838600 | 0.02284200 | -1.16074700 |
| C | -6.34145600 | 0.33299500 | 0.15309400 |
| C | -5.26654300 | 0.27916700 | 1.05340200 |
| C | -3.94534000 | 0.01942400 | 0.30704300 |
| C | -7.64051700 | 0.53309800 | 0.62315500 |
| C | -7.84046000 | 0.67926400 | 1.99908800 |
| C | -6.76172700 | 0.62648700 | 2.89115000 |
| C | -5.45937500 | 0.42181600 | 2.41967700 |
| C | -3.41798100 | -1.35319300 | 0.69927400 |
| C | -2.15316100 | -1.51836800 | 1.30640000 |
| N | -1.29188400 | -0.43221700 | 1.43716100 |
| C | -1.61320200 | 0.82985400 | 0.99359100 |
| C | -2.93061900 | 1.11915300 | 0.54585000 |
| C | -0.62086200 | 1.85016000 | 0.97252700 |
| C | -0.97291500 | 3.14087100 | 0.63895900 |
| C | -2.30450900 | 3.44990800 | 0.32024400 |
| C | -3.26252800 | 2.43752700 | 0.25760800 |
| C | -4.22168700 | -2.47491900 | 0.50261200 |
| C | -3.81196400 | -3.73986500 | 0.91508200 |
| C | -2.58318100 | -3.89202100 | 1.57178600 |
| C | -1.76348200 | -2.79738600 | 1.77762100 |
| C | -0.02174900 | -0.62304600 | 2.09045500 |

| | | | |
|---|-------------|-------------|-------------|
| C | 0.94557700 | -1.39778200 | 1.46040700 |
| C | 2.19040000 | -1.56767200 | 2.06437800 |
| C | 2.44406300 | -0.96630500 | 3.29850600 |
| C | 1.45896000 | -0.19615700 | 3.92969800 |
| C | 0.21599100 | -0.01465500 | 3.32473100 |
| C | -2.15563900 | -0.08554000 | -2.22688700 |
| C | -1.43175000 | -1.27326600 | -2.02177400 |
| C | -0.05264500 | -1.19604000 | -1.83420800 |
| C | 0.63641500 | 0.03084300 | -1.76086400 |
| C | -0.12058100 | 1.19368800 | -2.00375800 |
| C | -1.48568200 | 1.15279800 | -2.25822700 |
| B | 2.08865200 | 0.10571000 | -1.35820900 |
| C | 2.55790700 | 1.52487000 | -1.02841200 |
| C | 1.69455600 | 2.59958400 | -1.36325900 |
| O | 0.46764300 | 2.42029200 | -1.95836900 |
| O | 0.61913400 | -2.36881900 | -1.64904600 |
| C | 1.97425400 | -2.41262400 | -1.37894500 |
| C | 2.77436200 | -1.25120900 | -1.22985100 |
| C | 3.76204000 | 1.89326500 | -0.37089500 |
| C | 4.13054800 | 3.21149500 | -0.09469000 |
| C | 3.24657600 | 4.23372500 | -0.48547300 |
| C | 2.03129800 | 3.92603000 | -1.10704000 |
| C | 2.47825700 | -3.68970200 | -1.16332600 |
| C | 3.82351900 | -3.86196000 | -0.80898800 |
| C | 4.68091900 | -2.75357100 | -0.68786800 |
| C | 4.13942300 | -1.48605100 | -0.91422200 |
| C | 5.45660600 | 3.57037900 | 0.59991200 |
| C | 6.30647400 | 4.45720700 | -0.34207700 |
| C | 6.28938500 | 2.32194000 | 0.96139700 |
| C | 5.16498600 | 4.34737400 | 1.90632500 |
| C | 6.15689300 | -2.96539800 | -0.30440000 |
| C | 6.23237400 | -3.66012900 | 1.07677800 |
| C | 6.94074900 | -1.63857400 | -0.21477600 |
| C | 6.84574000 | -3.85941600 | -1.36328600 |
| H | -3.74408200 | -0.12825700 | -4.45661000 |
| H | -6.21134400 | 0.05692600 | -4.57586800 |
| H | -7.56410100 | 0.28974000 | -2.49321400 |
| H | -8.47722900 | 0.57754600 | -0.06732200 |
| H | -8.84347100 | 0.83765600 | 2.38215400 |
| H | -6.93764000 | 0.74500500 | 3.95532100 |
| H | -4.61808800 | 0.37561200 | 3.10520100 |
| H | 0.41626100 | 1.60002900 | 1.15794600 |
| H | -0.19958800 | 3.89808300 | 0.58643900 |
| H | -2.58097300 | 4.46906700 | 0.07234200 |
| H | -4.27706700 | 2.65673100 | -0.06083200 |
| H | -5.18652900 | -2.34235700 | 0.02403800 |
| H | -4.45167800 | -4.59894200 | 0.74461600 |
| H | -2.26624500 | -4.86753900 | 1.92309900 |
| H | -0.82040400 | -2.91783100 | 2.29088900 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.70797900 | -1.86933100 | 0.52206900 |
| H | 2.94813500 | -2.14964800 | 1.54749700 |
| H | 3.41267200 | -1.08992500 | 3.77130100 |
| H | 1.66068700 | 0.26894500 | 4.88866900 |
| H | -0.55425000 | 0.59475600 | 3.78578700 |
| H | -1.92722300 | -2.23794900 | -1.99368900 |
| H | -2.03052500 | 2.07781700 | -2.40613900 |
| H | 4.41306600 | 1.09039400 | -0.05817400 |
| H | 3.49440600 | 5.27482900 | -0.30745200 |
| H | 1.34044400 | 4.70605100 | -1.41187700 |
| H | 1.81109300 | -4.53896200 | -1.26895800 |
| H | 4.19354600 | -4.86730600 | -0.63888600 |
| H | 4.78013100 | -0.61902600 | -0.85673600 |
| H | 6.51845500 | 3.92573900 | -1.27554700 |
| H | 5.78611800 | 5.38637500 | -0.59217800 |
| H | 7.25815000 | 4.71726100 | 0.13641600 |
| H | 5.74812700 | 1.66910000 | 1.65412000 |
| H | 6.54820200 | 1.74012900 | 0.07029300 |
| H | 7.22137100 | 2.63212600 | 1.44572300 |
| H | 4.56139100 | 3.73625600 | 2.58581800 |
| H | 6.10242400 | 4.60852300 | 2.41150100 |
| H | 4.61784000 | 5.27324500 | 1.70574800 |
| H | 5.72729600 | -4.63033400 | 1.06403100 |
| H | 7.27749100 | -3.82260200 | 1.36555000 |
| H | 5.75496300 | -3.03773600 | 1.84155200 |
| H | 6.95263800 | -1.11802000 | -1.17777400 |
| H | 6.51006600 | -0.96547700 | 0.53507600 |
| H | 7.97739400 | -1.84540600 | 0.07144500 |
| H | 6.79237600 | -3.38860600 | -2.35027800 |
| H | 7.90041600 | -4.01120900 | -1.10484200 |
| H | 6.36685900 | -4.84061900 | -1.42980500 |

AC-BO (gas), T₁

| | | | |
|---|-------------|-------------|-------------|
| C | -3.59399600 | -0.22491600 | -2.29321200 |
| C | -4.21253300 | -0.34749100 | -3.54849200 |
| C | -5.60195700 | -0.24662900 | -3.68494300 |
| C | -6.41175700 | 0.00258100 | -2.57374200 |
| C | -5.80553400 | 0.11864200 | -1.32260600 |
| C | -4.41443500 | -0.01816300 | -1.18322500 |
| C | -6.38697500 | 0.38980700 | 0.00394500 |
| C | -5.35497400 | 0.38820600 | 0.95457500 |
| C | -4.00432800 | 0.06069500 | 0.30120600 |
| C | -7.70630200 | 0.63290900 | 0.39006600 |
| C | -7.97269500 | 0.87793300 | 1.73995500 |
| C | -6.93796700 | 0.87808000 | 2.68520600 |
| C | -5.61678000 | 0.62890600 | 2.29590100 |
| C | -3.52076200 | -1.31242500 | 0.77941800 |
| C | -2.24606800 | -1.50126500 | 1.34056500 |
| N | -1.33232200 | -0.43712700 | 1.42009300 |

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|---|-------------|-------------|-------------|
| C | -1.66561200 | 0.84600700 | 1.01469000 |
| C | -2.96621500 | 1.14796200 | 0.54596600 |
| C | -0.69251100 | 1.87632600 | 1.03918200 |
| C | -1.03448600 | 3.17469100 | 0.70043100 |
| C | -2.34663700 | 3.49281000 | 0.32675900 |
| C | -3.28977200 | 2.47458400 | 0.24027900 |
| C | -4.38363800 | -2.40791300 | 0.66238400 |
| C | -4.02136100 | -3.67566100 | 1.10309400 |
| C | -2.76877700 | -3.85086300 | 1.69728400 |
| C | -1.89240000 | -2.78094600 | 1.82105200 |
| C | -0.08062500 | -0.64277400 | 2.09297200 |
| C | 0.91784000 | -1.38227900 | 1.46761700 |
| C | 2.14791500 | -1.57818700 | 2.09485400 |
| C | 2.36966700 | -1.02762500 | 3.35890300 |
| C | 1.35975000 | -0.29460600 | 3.99278000 |
| C | 0.12863400 | -0.10270400 | 3.36424600 |
| C | -2.10704900 | -0.20982600 | -2.15654000 |
| C | -1.33743000 | -1.36252100 | -2.01461500 |
| C | 0.06049200 | -1.24832700 | -1.82743100 |
| C | 0.72714600 | -0.01341300 | -1.71250100 |
| C | -0.07263700 | 1.12381800 | -1.89509700 |
| C | -1.45926800 | 1.04997600 | -2.11249400 |
| B | 2.17954600 | 0.08943300 | -1.34188900 |
| C | 2.62006000 | 1.51941800 | -1.02481900 |
| C | 1.70655300 | 2.57359100 | -1.30896100 |
| O | 0.45790400 | 2.35400000 | -1.83401600 |
| O | 0.74557200 | -2.39723600 | -1.69512400 |
| C | 2.09000400 | -2.43350800 | -1.37170200 |
| C | 2.87795100 | -1.26472500 | -1.20343800 |
| C | 3.83922200 | 1.92969000 | -0.42833400 |
| C | 4.16826300 | 3.26068000 | -0.16332300 |
| C | 3.23076200 | 4.25886900 | -0.50582400 |
| C | 2.00376900 | 3.91430600 | -1.06948000 |
| C | 2.58875600 | -3.71339000 | -1.15338300 |
| C | 3.92284600 | -3.87952000 | -0.77383100 |
| C | 4.77158300 | -2.76555600 | -0.62897600 |
| C | 4.23095300 | -1.49611800 | -0.85719500 |
| C | 5.50587100 | 3.66538300 | 0.47763100 |
| C | 6.28012200 | 4.58701700 | -0.49618600 |
| C | 6.39815000 | 2.44853100 | 0.80150400 |
| C | 5.23330700 | 4.42695200 | 1.79791000 |
| C | 6.23877500 | -2.97329400 | -0.21668200 |
| C | 6.28475100 | -3.66297600 | 1.16856400 |
| C | 7.01878600 | -1.64505100 | -0.11904500 |
| C | 6.94673500 | -3.87109400 | -1.26030400 |
| H | -3.59041000 | -0.50662400 | -4.42398600 |
| H | -6.04996600 | -0.34568000 | -4.66861000 |
| H | -7.48744100 | 0.10513200 | -2.68027600 |
| H | -8.50703600 | 0.63448400 | -0.34346800 |

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|---|-------------|-------------|-------------|
| H | -8.99120500 | 1.07175600 | 2.06109600 |
| H | -7.16486100 | 1.07255300 | 3.72857800 |
| H | -4.80961800 | 0.62281100 | 3.02250100 |
| H | 0.33516900 | 1.63969500 | 1.28850700 |
| H | -0.25958500 | 3.93420200 | 0.70285300 |
| H | -2.61845400 | 4.51318700 | 0.07940800 |
| H | -4.30103400 | 2.68828400 | -0.09485800 |
| H | -5.36161600 | -2.24790400 | 0.21901300 |
| H | -4.70716400 | -4.50907000 | 0.99747300 |
| H | -2.46839900 | -4.82504300 | 2.06923400 |
| H | -0.92953100 | -2.93451900 | 2.28793900 |
| H | 0.70341700 | -1.82629700 | 0.51116400 |
| H | 2.92048900 | -2.14212700 | 1.57873800 |
| H | 3.32582700 | -1.16696200 | 3.85276200 |
| H | 1.53120300 | 0.12934500 | 4.97694800 |
| H | -0.65954000 | 0.47606300 | 3.83491800 |
| H | -1.79277500 | -2.34775800 | -2.00859500 |
| H | -2.02505300 | 1.97025800 | -2.20352500 |
| H | 4.53825200 | 1.15476800 | -0.15241400 |
| H | 3.45138700 | 5.30521200 | -0.32606600 |
| H | 1.26433000 | 4.66553800 | -1.32745800 |
| H | 1.92410400 | -4.56233100 | -1.27490900 |
| H | 4.29552600 | -4.88268100 | -0.59847600 |
| H | 4.86983800 | -0.63048100 | -0.76932100 |
| H | 6.47816000 | 4.06621800 | -1.43871700 |
| H | 5.71478000 | 5.49574300 | -0.72225000 |
| H | 7.23789100 | 4.88314800 | -0.05305600 |
| H | 5.91138400 | 1.77565100 | 1.51515600 |
| H | 6.64520100 | 1.87914500 | -0.10079300 |
| H | 7.33566200 | 2.79429500 | 1.24899700 |
| H | 4.67667100 | 3.79334700 | 2.49632000 |
| H | 6.18033900 | 4.71601600 | 2.26788200 |
| H | 4.65013500 | 5.33579000 | 1.62391700 |
| H | 5.78421300 | -4.63534500 | 1.14864700 |
| H | 7.32433900 | -3.82080900 | 1.47791100 |
| H | 5.78974100 | -3.04028700 | 1.92133100 |
| H | 7.04619800 | -1.12751900 | -1.08346900 |
| H | 6.57830200 | -0.97107000 | 0.62395800 |
| H | 8.05076700 | -1.85093100 | 0.18319300 |
| H | 6.91234700 | -3.40526000 | -2.25051300 |
| H | 7.99616100 | -4.01837500 | -0.98036000 |
| H | 6.47346800 | -4.85458400 | -1.33074200 |

QAC-BO (gas), S₀

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|---|-------------|-------------|-------------|
| C | -0.84737500 | -0.77948800 | -1.45403300 |
| C | -0.30886200 | -2.04569300 | -1.16729200 |

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|---|-------------|-------------|-------------|
| C | 1.05620200 | -2.31077100 | -1.28891300 |
| C | 1.88756600 | -1.29561200 | -1.77943800 |
| C | 1.36894000 | -0.05199600 | -2.16467700 |
| C | 0.02183100 | 0.20137100 | -1.96185500 |
| B | -2.28404900 | -0.45796300 | -1.15754400 |
| C | -3.13228100 | -1.67590800 | -0.78577700 |
| C | -2.44904000 | -2.89031100 | -0.58434400 |
| O | -1.10509600 | -3.04256400 | -0.72205400 |
| O | -0.43271100 | 1.43317400 | -2.28165700 |
| C | -1.64750200 | 1.87077800 | -1.86741500 |
| C | -2.61386800 | 1.03817100 | -1.26119300 |
| C | -4.53299400 | -1.68523200 | -0.58284200 |
| C | -5.23692700 | -2.80461500 | -0.15700700 |
| C | -4.49312400 | -3.99016200 | 0.05419000 |
| C | -3.12711800 | -4.04337400 | -0.16236300 |
| C | -1.88471100 | 3.23564900 | -2.06425700 |
| C | -3.05576900 | 3.80675900 | -1.58038500 |
| C | -4.00486000 | 3.04389300 | -0.87025500 |
| C | -3.75978100 | 1.67672100 | -0.74817900 |
| C | -6.75509100 | -2.80277900 | 0.08380700 |
| C | -7.38337600 | -1.41690300 | -0.17081200 |
| C | -5.23304400 | 3.65615300 | -0.17663100 |
| C | -5.40400600 | 5.15378100 | -0.50058200 |
| C | 5.67360200 | -0.88558100 | -1.59317100 |
| C | 6.45285500 | 0.00227700 | -0.71554600 |
| C | 5.58486100 | 0.57046600 | 0.22497800 |
| C | 4.31445100 | -0.81275400 | -1.22855800 |
| C | 3.35436600 | -1.50590300 | -1.97164000 |
| C | 3.79490100 | -2.33469900 | -3.01823500 |
| C | 5.14995400 | -2.44032400 | -3.34276900 |
| C | 6.10216200 | -1.69544000 | -2.64399400 |
| C | 7.81231500 | 0.32098300 | -0.71320700 |
| C | 8.28337500 | 1.22387300 | 0.24346100 |
| C | 7.40974700 | 1.79450200 | 1.17972300 |
| C | 6.04946900 | 1.46642400 | 1.17786800 |
| C | -7.42836600 | -3.82289700 | -0.86587300 |
| C | -7.04392800 | -3.20080800 | 1.55163600 |
| C | -6.52086400 | 2.91781300 | -0.61480500 |
| C | -5.04670800 | 3.50474900 | 1.35399700 |
| C | 1.95678700 | 1.13492000 | 0.74183800 |
| C | 3.14279900 | 1.16179000 | -0.00245300 |
| C | 4.15851700 | 0.02405200 | 0.06413800 |
| C | 3.86391800 | -0.91015200 | 1.25363400 |
| C | 2.65450600 | -0.83876800 | 1.96036100 |
| N | 1.63141900 | 0.03157100 | 1.54358200 |
| C | 1.04777400 | 2.21834700 | 0.69631700 |
| C | 1.26828100 | 3.23330200 | -0.22976100 |
| C | 2.42646500 | 3.24636000 | -1.01623900 |
| C | 3.37536200 | 2.24323600 | -0.86017500 |

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|---|-------------|-------------|-------------|
| C | 4.84408900 | -1.81967800 | 1.67957800 |
| C | 4.66145500 | -2.61991200 | 2.79954700 |
| C | 3.48613100 | -2.48522600 | 3.54719800 |
| C | 2.50090900 | -1.59867100 | 3.13923600 |
| C | 0.26447500 | -0.23464500 | 1.79427400 |
| C | -0.21948500 | -1.54856300 | 1.90570200 |
| C | -1.56675700 | -1.77937500 | 2.15336600 |
| C | -2.46311200 | -0.71093200 | 2.22876900 |
| C | -1.99218500 | 0.58869000 | 2.06288400 |
| C | -0.63003500 | 0.84673000 | 1.86756700 |
| C | -0.04116700 | 2.25167900 | 1.77400400 |
| C | 0.65832500 | 2.57282400 | 3.13055300 |
| C | -1.11569100 | 3.32092100 | 1.52303700 |
| H | 1.45427100 | -3.27988500 | -1.01069300 |
| H | 2.01046000 | 0.72763200 | -2.55229700 |
| H | -5.06440300 | -0.76545000 | -0.78571000 |
| H | -4.99908700 | -4.89133000 | 0.38649400 |
| H | -2.56109300 | -4.95571900 | -0.00673600 |
| H | -1.12742500 | 3.82843800 | -2.56601500 |
| H | -3.20371500 | 4.86956700 | -1.72929300 |
| H | -4.45895300 | 1.06680500 | -0.18751200 |
| H | -6.95132800 | -0.65458400 | 0.48730100 |
| H | -7.24702000 | -1.09880500 | -1.20948100 |
| H | -8.45879400 | -1.46177900 | 0.02850200 |
| H | -5.51675400 | 5.31726700 | -1.57765600 |
| H | -4.55206600 | 5.74174700 | -0.14417000 |
| H | -6.30230300 | 5.53481700 | -0.00441500 |
| H | 3.05285900 | -2.87422300 | -3.59903200 |
| H | 5.45654100 | -3.08514600 | -4.16020700 |
| H | 7.15361100 | -1.74295800 | -2.91070100 |
| H | 8.48693900 | -0.11859200 | -1.44187400 |
| H | 9.33562900 | 1.48967900 | 0.26114800 |
| H | 7.79369500 | 2.49731200 | 1.91233200 |
| H | 5.36433700 | 1.90062800 | 1.89987800 |
| H | -7.05600800 | -4.83710400 | -0.69297800 |
| H | -7.23145800 | -3.56142500 | -1.91065100 |
| H | -8.51254500 | -3.82874700 | -0.70624400 |
| H | -6.66074700 | -4.19930900 | 1.78168100 |
| H | -6.57710400 | -2.48990800 | 2.24131100 |
| H | -8.12422400 | -3.20417800 | 1.73516400 |
| H | -6.48896100 | 1.85390400 | -0.35932400 |
| H | -6.66180100 | 3.00292300 | -1.69725100 |
| H | -7.39245000 | 3.35494900 | -0.11489000 |
| H | -4.97684000 | 2.45033200 | 1.64065100 |
| H | -4.12755300 | 4.00576900 | 1.67674500 |
| H | -5.89454100 | 3.94858500 | 1.88833100 |
| H | 0.54692700 | 4.03547200 | -0.33201500 |
| H | 2.59502300 | 4.05232500 | -1.72243600 |
| H | 4.29544200 | 2.25842500 | -1.43755000 |

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|---|-------------|-------------|------------|
| H | 5.76982000 | -1.88648600 | 1.11767900 |
| H | 5.43279600 | -3.31982800 | 3.10199700 |
| H | 3.34114700 | -3.06368200 | 4.45398300 |
| H | 1.59543300 | -1.48669400 | 3.72340100 |
| H | 0.45711000 | -2.38378900 | 1.77383500 |
| H | -1.92792900 | -2.79921700 | 2.22943500 |
| H | -3.52222100 | -0.89742400 | 2.37119300 |
| H | -2.69559900 | 1.41365400 | 2.07571700 |
| H | 1.42801500 | 1.83024300 | 3.35923700 |
| H | 1.12749700 | 3.56107900 | 3.08006800 |
| H | -0.08338100 | 2.56719800 | 3.93616300 |
| H | -1.67756800 | 3.12036900 | 0.61041000 |
| H | -0.65764600 | 4.31126800 | 1.45205800 |
| H | -1.81342800 | 3.34954100 | 2.36481400 |

QAC-BO (gas), S₁

| | | | |
|---|-------------|-------------|-------------|
| C | -0.80403000 | -0.66668200 | -1.56131000 |
| C | -0.24370200 | -1.94700100 | -1.37646500 |
| C | 1.11816100 | -2.19928300 | -1.51527100 |
| C | 1.96864300 | -1.14360700 | -1.90034700 |
| C | 1.42927100 | 0.12535300 | -2.17998200 |
| C | 0.07541000 | 0.34926100 | -1.98896200 |
| B | -2.24548000 | -0.37427100 | -1.25755500 |
| C | -3.06756800 | -1.60505300 | -0.88809300 |
| C | -2.38714600 | -2.84610400 | -0.79152400 |
| O | -1.03408500 | -2.98358100 | -0.97765400 |
| O | -0.38936700 | 1.60200500 | -2.24660600 |
| C | -1.62085200 | 2.01269700 | -1.80713900 |
| C | -2.58662300 | 1.11762700 | -1.26662100 |
| C | -4.45799700 | -1.64007700 | -0.59959500 |
| C | -5.14296700 | -2.79017700 | -0.20160400 |
| C | -4.40781700 | -3.98700400 | -0.10944600 |
| C | -3.04214200 | -4.01518600 | -0.41396100 |
| C | -1.86403200 | 3.37518500 | -1.92490700 |
| C | -3.06482300 | 3.92549000 | -1.44094400 |
| C | -4.01183500 | 3.10915100 | -0.81011800 |
| C | -3.74933500 | 1.73142900 | -0.74720500 |
| C | -6.64825900 | -2.78984500 | 0.12097900 |
| C | -7.28289500 | -1.39016000 | -0.02311600 |
| C | -5.27477800 | 3.65854800 | -0.12493900 |
| C | -5.48513600 | 5.16188500 | -0.39506800 |
| C | 5.73435300 | -0.65913600 | -1.57754100 |
| C | 6.45470100 | 0.17179500 | -0.59851700 |
| C | 5.54008700 | 0.63382700 | 0.35717200 |
| C | 4.36117300 | -0.64698700 | -1.27111400 |
| C | 3.43484500 | -1.31847600 | -2.07758600 |
| C | 3.94729900 | -2.08451700 | -3.14108100 |
| C | 5.31623000 | -2.13378200 | -3.41917900 |
| C | 6.22505400 | -1.39793300 | -2.65339900 |

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|---|-------------|-------------|-------------|
| C | 7.80290600 | 0.52335200 | -0.51152900 |
| C | 8.21333600 | 1.34668200 | 0.54103100 |
| C | 7.29285300 | 1.80829600 | 1.49108800 |
| C | 5.94253200 | 1.44890600 | 1.40563500 |
| C | -7.38260600 | -3.75169800 | -0.84407500 |
| C | -6.86619500 | -3.26559000 | 1.57775100 |
| C | -6.53128900 | 2.90089700 | -0.61791100 |
| C | -5.12376100 | 3.45689200 | 1.40407800 |
| C | 1.88382200 | 1.06194100 | 0.80490500 |
| C | 3.09845200 | 1.17960600 | 0.10224200 |
| C | 4.13478800 | 0.06802300 | 0.08509900 |
| C | 3.83348600 | -0.97980400 | 1.16116300 |
| C | 2.60525300 | -1.00445600 | 1.84151900 |
| N | 1.56531900 | -0.13477700 | 1.45628000 |
| C | 0.93921200 | 2.11877000 | 0.83770200 |
| C | 1.17215100 | 3.23045000 | 0.04301300 |
| C | 2.35403900 | 3.33743800 | -0.70188100 |
| C | 3.32317800 | 2.34288800 | -0.63406500 |
| C | 4.81137400 | -1.91278300 | 1.52471200 |
| C | 4.61434900 | -2.79997300 | 2.57679200 |
| C | 3.43208400 | -2.73820800 | 3.32469700 |
| C | 2.43750800 | -1.84486200 | 2.96618300 |
| C | 0.22757100 | -0.45547800 | 1.68955500 |
| C | -0.19536300 | -1.80740000 | 1.73000000 |
| C | -1.51568000 | -2.10515200 | 1.98574400 |
| C | -2.45531000 | -1.07127900 | 2.11799200 |
| C | -2.05169900 | 0.26215900 | 2.03006000 |
| C | -0.71458800 | 0.59413100 | 1.83734800 |
| C | -0.19270500 | 2.02115900 | 1.85611100 |
| C | 0.44018800 | 2.27119900 | 3.26773100 |
| C | -1.30150400 | 3.06395200 | 1.64901700 |
| H | 1.50826700 | -3.19316900 | -1.32173600 |
| H | 2.05891700 | 0.93440200 | -2.52566700 |
| H | -5.00061100 | -0.71430100 | -0.72277000 |
| H | -4.89471100 | -4.90985100 | 0.18780000 |
| H | -2.46993000 | -4.93537800 | -0.35011400 |
| H | -1.10560600 | 3.99980600 | -2.38598100 |
| H | -3.22243900 | 4.99141600 | -1.54651600 |
| H | -4.46607200 | 1.09202000 | -0.24646900 |
| H | -6.81179600 | -0.66547100 | 0.65050200 |
| H | -7.19645700 | -1.01544300 | -1.04796300 |
| H | -8.34716400 | -1.44323300 | 0.22925500 |
| H | -5.57309800 | 5.36074300 | -1.46825300 |
| H | -4.65893300 | 5.75971000 | 0.00316700 |
| H | -6.40692900 | 5.49817100 | 0.09121600 |
| H | 3.24312700 | -2.61439600 | -3.77533400 |
| H | 5.67053000 | -2.72660200 | -4.25665400 |
| H | 7.28604700 | -1.40475900 | -2.88311600 |
| H | 8.51541600 | 0.16915100 | -1.25028500 |

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|---|-------------|-------------|-------------|
| H | 9.25642700 | 1.63539600 | 0.62248700 |
| H | 7.62987000 | 2.45036500 | 2.29842200 |
| H | 5.22199700 | 1.80214800 | 2.13744500 |
| H | -7.00937400 | -4.77528400 | -0.74581600 |
| H | -7.23425200 | -3.43502900 | -1.88153800 |
| H | -8.45798500 | -3.75777100 | -0.63035800 |
| H | -6.47618300 | -4.27576100 | 1.73218900 |
| H | -6.35862300 | -2.59395800 | 2.27877900 |
| H | -7.93555000 | -3.27328800 | 1.81941200 |
| H | -6.47469400 | 1.83076900 | -0.39561600 |
| H | -6.64355100 | 3.01519800 | -1.70092500 |
| H | -7.42812000 | 3.29936700 | -0.12949000 |
| H | -5.01624200 | 2.39490000 | 1.64897500 |
| H | -4.23491100 | 3.98395000 | 1.76870200 |
| H | -6.00244600 | 3.84426900 | 1.93344800 |
| H | 0.43230300 | 4.01905400 | -0.00678900 |
| H | 2.51770300 | 4.20926700 | -1.32608900 |
| H | 4.24909600 | 2.43226800 | -1.19322000 |
| H | 5.74736000 | -1.92390000 | 0.97736400 |
| H | 5.39085600 | -3.51128000 | 2.83668500 |
| H | 3.29214800 | -3.37747900 | 4.18946300 |
| H | 1.53418800 | -1.77461100 | 3.55751600 |
| H | 0.50316300 | -2.59663100 | 1.48579300 |
| H | -1.84724700 | -3.13562200 | 1.98024300 |
| H | -3.50680300 | -1.31581300 | 2.21845900 |
| H | -2.79824800 | 1.04572100 | 2.07085500 |
| H | 1.23861900 | 1.55808900 | 3.49132800 |
| H | 0.85615400 | 3.28268900 | 3.30351800 |
| H | -0.33649300 | 2.17521600 | 4.03240400 |
| H | -1.81540300 | 2.91636200 | 0.70206300 |
| H | -0.88289500 | 4.07275000 | 1.68247300 |
| H | -2.03167800 | 2.99542700 | 2.45969000 |

QAC-BO (gas), T₁

| | | | |
|---|-------------|-------------|-------------|
| C | -0.81266800 | -0.69987100 | -1.52595100 |
| C | -0.25087400 | -1.97140900 | -1.32822800 |
| C | 1.12646300 | -2.23407400 | -1.46872600 |
| C | 1.98677200 | -1.21035200 | -1.89309800 |
| C | 1.44067000 | 0.05359800 | -2.18703100 |
| C | 0.07147600 | 0.29343000 | -1.97634900 |
| B | -2.25009800 | -0.40273600 | -1.23063800 |
| C | -3.06881200 | -1.63475700 | -0.85739700 |
| C | -2.37736400 | -2.87189900 | -0.73776200 |
| O | -1.02466100 | -2.99649200 | -0.93335000 |
| O | -0.36681300 | 1.53378900 | -2.24031600 |
| C | -1.59883500 | 1.96725400 | -1.82567600 |
| C | -2.57777400 | 1.08972500 | -1.27335100 |
| C | -4.45761900 | -1.68483400 | -0.58476300 |
| C | -5.12741900 | -2.84267200 | -0.18238800 |

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|---|-------------|-------------|-------------|
| C | -4.37836300 | -4.03369500 | -0.06505300 |
| C | -3.01394100 | -4.04929800 | -0.35119900 |
| C | -1.81485800 | 3.33273300 | -1.97537900 |
| C | -3.00416000 | 3.90488600 | -1.50652300 |
| C | -3.96366200 | 3.11006600 | -0.85715500 |
| C | -3.72890200 | 1.72903500 | -0.76826600 |
| C | -6.63319500 | -2.86221800 | 0.12964500 |
| C | -7.29049500 | -1.47635700 | -0.03885900 |
| C | -5.21276900 | 3.69692100 | -0.18058800 |
| C | -5.37259900 | 5.20765000 | -0.44414300 |
| C | 5.74068600 | -0.74492100 | -1.54101800 |
| C | 6.44541600 | 0.10358100 | -0.56499500 |
| C | 5.51123800 | 0.58701200 | 0.36110700 |
| C | 4.36499100 | -0.72668500 | -1.24820800 |
| C | 3.45259100 | -1.39544300 | -2.06843200 |
| C | 3.96430900 | -2.16238200 | -3.13014300 |
| C | 5.33712100 | -2.22083300 | -3.38894200 |
| C | 6.23846900 | -1.49042100 | -2.60944200 |
| C | 7.79297600 | 0.45394500 | -0.46258900 |
| C | 8.18513500 | 1.30073800 | 0.57781000 |
| C | 7.24612800 | 1.78499600 | 1.49890800 |
| C | 5.89736800 | 1.42565600 | 1.39727600 |
| C | -7.34274700 | -3.85108400 | -0.82750300 |
| C | -6.84890200 | -3.32133400 | 1.59252500 |
| C | -6.48723100 | 2.98116500 | -0.68996300 |
| C | -5.07680700 | 3.48104500 | 1.34840200 |
| C | 1.86033900 | 1.05751800 | 0.73473700 |
| C | 3.07316500 | 1.13343500 | 0.02388200 |
| C | 4.11061400 | 0.01816700 | 0.08090100 |
| C | 3.77248500 | -0.99387700 | 1.19028000 |
| C | 2.53724300 | -0.97520700 | 1.85596400 |
| N | 1.51604700 | -0.09244300 | 1.44490900 |
| C | 0.96284300 | 2.15637700 | 0.74901800 |
| C | 1.21473400 | 3.23150400 | -0.09173500 |
| C | 2.39072400 | 3.28895900 | -0.85408900 |
| C | 3.33037800 | 2.27339700 | -0.74940600 |
| C | 4.74326700 | -1.92178700 | 1.59404700 |
| C | 4.53045100 | -2.78473900 | 2.66136400 |
| C | 3.33451700 | -2.69399200 | 3.38100200 |
| C | 2.35423000 | -1.79397500 | 2.98991200 |
| C | 0.14600400 | -0.34499800 | 1.70970700 |
| C | -0.35253200 | -1.65752500 | 1.77458800 |
| C | -1.69355700 | -1.88059800 | 2.04975400 |
| C | -2.57268900 | -0.80164400 | 2.19041100 |
| C | -2.09132700 | 0.49655600 | 2.06772800 |
| C | -0.73065400 | 0.74502500 | 1.85082600 |
| C | -0.12831400 | 2.14477300 | 1.82117400 |
| C | 0.57555000 | 2.39065600 | 3.19355800 |
| C | -1.18557800 | 3.24123400 | 1.62334900 |

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|---|-------------|-------------|-------------|
| H | 1.50483100 | -3.22498900 | -1.23794200 |
| H | 2.05929800 | 0.85582600 | -2.56822500 |
| H | -5.01059200 | -0.76486900 | -0.70985100 |
| H | -4.85894500 | -4.95607400 | 0.24159200 |
| H | -2.42689800 | -4.95808300 | -0.26721200 |
| H | -1.03681000 | 3.93540100 | -2.43234500 |
| H | -3.14614600 | 4.97125100 | -1.62368500 |
| H | -4.45273800 | 1.10917400 | -0.25258500 |
| H | -6.83977700 | -0.73539700 | 0.63050100 |
| H | -7.20299000 | -1.11431600 | -1.06818300 |
| H | -8.35551800 | -1.54643900 | 0.20496400 |
| H | -5.45462900 | 5.41657900 | -1.51594700 |
| H | -4.52866400 | 5.77620100 | -0.04048800 |
| H | -6.28369800 | 5.56973100 | 0.04307500 |
| H | 3.26599600 | -2.68772800 | -3.77490800 |
| H | 5.69970600 | -2.81657300 | -4.22064100 |
| H | 7.30220200 | -1.50427300 | -2.82648000 |
| H | 8.51883400 | 0.08043900 | -1.17872200 |
| H | 9.22707800 | 1.58937000 | 0.67336700 |
| H | 7.56936500 | 2.44446100 | 2.29800000 |
| H | 5.16289500 | 1.79292400 | 2.10793800 |
| H | -6.95776900 | -4.86811300 | -0.71045900 |
| H | -7.19281700 | -3.54816500 | -1.86886200 |
| H | -8.41897400 | -3.86856900 | -0.62054600 |
| H | -6.44918800 | -4.32499500 | 1.76261100 |
| H | -6.35214700 | -2.63493900 | 2.28635800 |
| H | -7.91925200 | -3.33778100 | 1.82775500 |
| H | -6.46739400 | 1.90913600 | -0.47273900 |
| H | -6.58860600 | 3.10630700 | -1.77291600 |
| H | -7.37371800 | 3.40600900 | -0.20555700 |
| H | -5.01649400 | 2.41566800 | 1.59226900 |
| H | -4.16918000 | 3.96828700 | 1.72135800 |
| H | -5.94214200 | 3.90459200 | 1.87125600 |
| H | 0.50338600 | 4.04709200 | -0.14280300 |
| H | 2.57947700 | 4.14309600 | -1.49558100 |
| H | 4.26778000 | 2.32628500 | -1.29538700 |
| H | 5.68749600 | -1.95025300 | 1.06049000 |
| H | 5.29640500 | -3.49703400 | 2.94808600 |
| H | 3.16743700 | -3.31781200 | 4.25304100 |
| H | 1.43742700 | -1.71584900 | 3.55962000 |
| H | 0.31068000 | -2.49318800 | 1.58700500 |
| H | -2.07154700 | -2.89571400 | 2.09012500 |
| H | -3.63172300 | -0.98266900 | 2.33827600 |
| H | -2.78407500 | 1.32822700 | 2.12333300 |
| H | 1.33711800 | 1.63069700 | 3.39130800 |
| H | 1.05422600 | 3.37552500 | 3.19191200 |
| H | -0.16870700 | 2.35394600 | 3.99558500 |
| H | -1.74785300 | 3.09354700 | 0.70188700 |
| H | -0.71156300 | 4.22622700 | 1.60223800 |

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|--------------------------------|-------------|-------------|-------------|
| H | -1.88337900 | 3.24129100 | 2.46511700 |
| DQAC-DBO (gas), S ₀ | | | |
| C | 5.86615000 | 0.51317200 | -1.18833700 |
| C | 6.27249400 | 0.41023600 | 0.22478500 |
| C | 5.12647300 | 0.19873100 | 1.00749800 |
| C | 3.86900800 | 0.10350000 | 0.13174100 |
| C | 4.47407900 | 0.35641800 | -1.26419800 |
| C | 3.80120300 | 0.48456000 | -2.48070500 |
| C | 4.55704400 | 0.74769000 | -3.63138300 |
| C | 5.95041800 | 0.87213600 | -3.56100200 |
| C | 6.61796500 | 0.76280200 | -2.33811000 |
| C | 7.53055800 | 0.50499900 | 0.82204500 |
| C | 7.62124300 | 0.38630600 | 2.21182500 |
| C | 6.47371700 | 0.17734800 | 2.98894700 |
| C | 5.21370000 | 0.08005600 | 2.38730900 |
| C | 2.84381400 | 1.16727300 | 0.48912800 |
| C | 1.58917200 | 0.85779400 | 1.03628100 |
| N | 1.18198100 | -0.48410200 | 1.26973100 |
| C | 2.00459400 | -1.53959500 | 0.79369500 |
| C | 3.26916100 | -1.29370300 | 0.23158700 |
| C | 3.18233300 | 2.49824100 | 0.21576400 |
| C | 2.27291600 | 3.52398200 | 0.40186800 |
| C | 1.03607600 | 3.22572300 | 0.97457600 |
| C | 0.71142000 | 1.92805000 | 1.35831200 |
| C | 1.54135700 | -2.87982400 | 0.85186400 |
| C | 2.29103300 | -3.89329700 | 0.25973600 |
| C | 3.53523700 | -3.64071800 | -0.31761000 |
| C | 4.02696100 | -2.34793300 | -0.29117800 |
| C | -0.19436700 | -0.74297200 | 1.51484800 |
| C | -1.07752200 | 0.31451700 | 1.82544600 |
| C | -2.44825200 | 0.06514000 | 1.90953900 |
| C | -2.95549400 | -1.21791000 | 1.74892300 |
| C | -2.06915900 | -2.27925300 | 1.60175200 |
| C | -0.69020900 | -2.06525400 | 1.52998500 |
| C | -0.47567200 | 1.63869500 | 2.26276600 |
| C | 0.31110200 | -3.19945600 | 1.68903800 |
| C | 0.76187100 | -3.19604200 | 3.18365400 |
| C | 0.08760200 | 1.43176200 | 3.70517400 |
| C | 2.30853000 | 0.42253600 | -2.47135100 |
| C | 1.59890900 | 1.63022500 | -2.42445800 |
| C | 0.25087300 | 1.59266200 | -2.09190500 |
| C | -0.43087000 | 0.37785500 | -1.89035100 |
| C | 0.30056700 | -0.81230600 | -2.04674000 |
| C | 1.66513700 | -0.80980200 | -2.31815200 |
| B | -1.87563400 | 0.34994400 | -1.47262900 |
| C | -2.44861600 | 1.73627000 | -1.13882300 |
| C | -2.49227600 | -1.05196800 | -1.45787200 |
| C | -1.63114000 | 2.85713500 | -1.40781200 |

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|---|-------------|-------------|-------------|
| C | -2.06654100 | 4.15805100 | -1.12845400 |
| C | -3.31211500 | 4.36033000 | -0.54656300 |
| C | -4.14844100 | 3.27698400 | -0.21093900 |
| C | -3.68894100 | 1.99945700 | -0.52313300 |
| C | -3.84938000 | -1.36732400 | -1.21054900 |
| C | -4.33008200 | -2.66353700 | -1.09867200 |
| C | -3.41105700 | -3.71418100 | -1.32535200 |
| C | -2.08269100 | -3.46390900 | -1.61486100 |
| C | -1.62171400 | -2.13952100 | -1.65613700 |
| C | -0.29177000 | -4.58138800 | 1.38288700 |
| C | -1.49871300 | 2.78563500 | 2.32878400 |
| O | -0.38306500 | 2.77619600 | -1.93489800 |
| O | -0.29010100 | -2.01541500 | -1.88068800 |
| C | -5.77746100 | -2.98559000 | -0.69722100 |
| C | -5.49906400 | 3.43917300 | 0.50709000 |
| C | -6.47403500 | -3.78089500 | -1.82607800 |
| C | -6.59975400 | -1.70986600 | -0.41839600 |
| C | -5.75956100 | -3.83722800 | 0.59689200 |
| C | -6.62326400 | 2.79970100 | -0.34332300 |
| C | -5.85535000 | 4.91867100 | 0.75193800 |
| C | -5.42938700 | 2.72033100 | 1.87712600 |
| H | 4.04652800 | 0.85752500 | -4.58327100 |
| H | 6.51426700 | 1.06930600 | -4.46732900 |
| H | 7.69571600 | 0.88178400 | -2.28063400 |
| H | 8.41912800 | 0.66939200 | 0.21969000 |
| H | 8.59005300 | 0.45792500 | 2.69599400 |
| H | 6.56493800 | 0.09016100 | 4.06698500 |
| H | 4.31823500 | -0.08399700 | 2.97979400 |
| H | 4.16342000 | 2.70217900 | -0.20175000 |
| H | 2.52410000 | 4.54428000 | 0.13287600 |
| H | 0.32740000 | 4.02439800 | 1.15271800 |
| H | 1.91640800 | -4.90790100 | 0.27118900 |
| H | 4.11436700 | -4.44665500 | -0.75535300 |
| H | 5.00240200 | -2.12399200 | -0.71024200 |
| H | -3.12342900 | 0.88788400 | 2.10196100 |
| H | -4.02586300 | -1.39442900 | 1.76592700 |
| H | -2.46187800 | -3.28517100 | 1.52640300 |
| H | 1.19833100 | -2.23000500 | 3.45402400 |
| H | 1.51337700 | -3.97607600 | 3.34633000 |
| H | -0.10159400 | -3.38099900 | 3.83134300 |
| H | 0.57130700 | 2.35258100 | 4.04806300 |
| H | 0.82329900 | 0.62305500 | 3.72827600 |
| H | -0.73108600 | 1.17631900 | 4.38622100 |
| H | 2.10911700 | 2.58156900 | -2.50635500 |
| H | 2.21474500 | -1.74380900 | -2.32872300 |
| H | -1.40917100 | 4.98823500 | -1.36356500 |
| H | -3.61812800 | 5.37765700 | -0.33320000 |
| H | -4.29490000 | 1.14956500 | -0.23648400 |
| H | -4.53124500 | -0.54003800 | -1.08403000 |

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|---|-------------|-------------|-------------|
| H | -3.74508200 | -4.74603100 | -1.27539800 |
| H | -1.37771200 | -4.26562300 | -1.80525800 |
| H | 0.43903600 | -5.36919400 | 1.57889900 |
| H | -1.14419600 | -4.77329300 | 2.03823900 |
| H | -0.62291000 | -4.64773700 | 0.34407000 |
| H | -1.02308400 | 3.69225500 | 2.71096600 |
| H | -1.94282600 | 2.99948700 | 1.35657400 |
| H | -2.29515200 | 2.53221800 | 3.03285300 |
| H | -5.94797900 | -4.71693200 | -2.03719400 |
| H | -7.50243800 | -4.02745500 | -1.53834700 |
| H | -6.50163800 | -3.19104600 | -2.74803500 |
| H | -6.67725800 | -1.07877800 | -1.30992100 |
| H | -7.61404800 | -1.98714100 | -0.11417100 |
| H | -6.15563000 | -1.11712000 | 0.39019000 |
| H | -5.25450900 | -4.79489600 | 0.44076400 |
| H | -5.23848300 | -3.30695700 | 1.40157200 |
| H | -6.78341000 | -4.04708400 | 0.92621700 |
| H | -6.44794400 | 1.73020000 | -0.50055700 |
| H | -6.68544900 | 3.28233300 | -1.32409000 |
| H | -7.58883400 | 2.91184300 | 0.16280800 |
| H | -5.92397900 | 5.47303200 | -0.18994700 |
| H | -5.11436800 | 5.40765000 | 1.39303400 |
| H | -6.82669300 | 4.98340600 | 1.25249300 |
| H | -5.27131400 | 1.64444200 | 1.75114600 |
| H | -4.60664700 | 3.12023500 | 2.47948400 |
| H | -6.36656400 | 2.86014500 | 2.42763100 |

DQAC-DBO (gas), S₁

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|---|-------------|-------------|-------------|
| C | -5.86581700 | -0.65259700 | -1.03516400 |
| C | -6.19386300 | -0.35274000 | 0.36995600 |
| C | -5.00804700 | -0.05471600 | 1.05747200 |
| C | -3.79945000 | -0.08749200 | 0.10145200 |
| C | -4.48271600 | -0.50922600 | -1.22024300 |
| C | -3.86494600 | -0.85904200 | -2.42761100 |
| C | -4.69035500 | -1.33338900 | -3.45916200 |
| C | -6.07656400 | -1.44107800 | -3.29049100 |
| C | -6.68000800 | -1.10541100 | -2.07567300 |
| C | -7.41485000 | -0.35564200 | 1.04639400 |
| C | -7.42610700 | -0.05723500 | 2.41233500 |
| C | -6.23721800 | 0.23751100 | 3.09214600 |
| C | -5.01338800 | 0.24273600 | 2.41223000 |
| C | -2.78588800 | -1.11691000 | 0.54788900 |
| C | -1.50779800 | -0.77389300 | 1.03542500 |
| N | -1.08274000 | 0.57779000 | 1.10793900 |
| C | -1.93336100 | 1.60160200 | 0.61286400 |
| C | -3.19514000 | 1.30002200 | 0.05773200 |
| C | -3.14810900 | -2.45951300 | 0.43346600 |
| C | -2.24082800 | -3.46853200 | 0.70497700 |
| C | -0.98226000 | -3.13847600 | 1.21005000 |

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|---|-------------|-------------|-------------|
| C | -0.62942200 | -1.81844400 | 1.44591100 |
| C | -1.49865700 | 2.95685300 | 0.63250400 |
| C | -2.26330800 | 3.92454100 | -0.00342700 |
| C | -3.48905000 | 3.61031000 | -0.59547400 |
| C | -3.96203400 | 2.31270800 | -0.52218200 |
| C | 0.24983400 | 0.87417100 | 1.42463200 |
| C | 1.15251100 | -0.16428500 | 1.80428400 |
| C | 2.50587700 | 0.11523900 | 1.89169200 |
| C | 2.98075300 | 1.41249700 | 1.69996300 |
| C | 2.08236600 | 2.46348400 | 1.52973900 |
| C | 0.72093800 | 2.22066900 | 1.40811700 |
| C | 0.57807700 | -1.47432200 | 2.28943200 |
| C | -0.29854200 | 3.33730500 | 1.47698700 |
| C | -0.80114700 | 3.38136000 | 2.96219800 |
| C | 0.03031600 | -1.19253900 | 3.73480900 |
| C | -2.38025200 | -0.78870000 | -2.51087000 |
| C | -1.62133600 | -1.96141800 | -2.35653200 |
| C | -0.27081700 | -1.85313600 | -2.04243200 |
| C | 0.38108700 | -0.61030300 | -1.91793700 |
| C | -0.40082000 | 0.53341200 | -2.16458100 |
| C | -1.75513400 | 0.46820800 | -2.45268000 |
| B | 1.82694500 | -0.50112300 | -1.50121700 |
| C | 2.44690200 | -1.83401400 | -1.07835200 |
| C | 2.37163400 | 0.92578800 | -1.51083800 |
| C | 1.66607300 | -3.01241300 | -1.25582500 |
| C | 2.13762300 | -4.26675200 | -0.88805100 |
| C | 3.40970300 | -4.40652000 | -0.30441400 |
| C | 4.20931500 | -3.28134500 | -0.07202000 |
| C | 3.70682400 | -2.03208800 | -0.46604400 |
| C | 3.70737900 | 1.33634500 | -1.25134700 |
| C | 4.11657700 | 2.67053400 | -1.17730300 |
| C | 3.16020700 | 3.66770100 | -1.44685300 |
| C | 1.84776600 | 3.31717000 | -1.77882400 |
| C | 1.46168200 | 1.97913200 | -1.78348100 |
| C | 0.28593000 | 4.72003400 | 1.14144500 |
| C | 1.60848700 | -2.60969800 | 2.39807500 |
| O | 0.40631300 | -3.00940100 | -1.79759400 |
| O | 0.13609800 | 1.77834700 | -2.05311900 |
| C | 5.55531500 | 3.07638200 | -0.81246300 |
| C | 5.58575400 | -3.34954600 | 0.61278700 |
| C | 6.20223900 | 3.81608300 | -2.00839000 |
| C | 6.44160300 | 1.86254000 | -0.46205300 |
| C | 5.53248100 | 4.02338600 | 0.41335200 |
| C | 6.67181400 | -2.79554700 | -0.34045800 |
| C | 5.97514400 | -4.78815800 | 1.00672300 |
| C | 5.55902000 | -2.48842100 | 1.90025400 |
| H | -4.23121000 | -1.61799200 | -4.40083000 |
| H | -6.68672300 | -1.80415400 | -4.11170300 |
| H | -7.75056600 | -1.21722500 | -1.93422300 |

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|---|-------------|-------------|-------------|
| H | -8.33656900 | -0.58767200 | 0.52142300 |
| H | -8.36646000 | -0.05552300 | 2.95428400 |
| H | -6.26634600 | 0.46316100 | 4.15322500 |
| H | -4.08597900 | 0.47282500 | 2.92934700 |
| H | -4.13676000 | -2.69453900 | 0.05522900 |
| H | -2.50580300 | -4.50662100 | 0.53618400 |
| H | -0.27438300 | -3.92544200 | 1.43038800 |
| H | -1.91428300 | 4.94730200 | -0.02929000 |
| H | -4.07119000 | 4.38174200 | -1.08817400 |
| H | -4.92604500 | 2.05010300 | -0.94385300 |
| H | 3.20640600 | -0.68282300 | 2.09287800 |
| H | 4.04635400 | 1.60804800 | 1.71960400 |
| H | 2.46469500 | 3.47024200 | 1.44097800 |
| H | -1.23186500 | 2.42074500 | 3.26030700 |
| H | -1.56785800 | 4.15563700 | 3.06479100 |
| H | 0.03884900 | 3.60906000 | 3.62545800 |
| H | -0.43759200 | -2.10068500 | 4.12683100 |
| H | -0.71310000 | -0.38956100 | 3.73059800 |
| H | 0.85982200 | -0.89939000 | 4.38549200 |
| H | -2.09469100 | -2.93671900 | -2.35558800 |
| H | -2.31722800 | 1.38530100 | -2.57777900 |
| H | 1.50573600 | -5.13083400 | -1.06614000 |
| H | 3.74472000 | -5.39995100 | -0.03391300 |
| H | 4.30518600 | -1.15291300 | -0.26257800 |
| H | 4.43494100 | 0.55499700 | -1.09272300 |
| H | 3.43538300 | 4.71702100 | -1.42900800 |
| H | 1.10612200 | 4.06772700 | -2.03302000 |
| H | -0.47156000 | 5.49562400 | 1.27042500 |
| H | 1.09493300 | 4.96259900 | 1.83325800 |
| H | 0.67245700 | 4.74802800 | 0.12128600 |
| H | 1.14743100 | -3.49149000 | 2.84824000 |
| H | 2.01949300 | -2.87321400 | 1.42548700 |
| H | 2.42183200 | -2.31560900 | 3.06465300 |
| H | 5.63730400 | 4.71609200 | -2.26862100 |
| H | 7.22922400 | 4.11322300 | -1.76469100 |
| H | 6.22564100 | 3.16484700 | -2.88797900 |
| H | 6.54301100 | 1.18368000 | -1.31446000 |
| H | 7.44308500 | 2.20670700 | -0.18342900 |
| H | 6.03253600 | 1.29334400 | 0.38078700 |
| H | 4.96849700 | 4.93652700 | 0.20346300 |
| H | 5.07128400 | 3.53250200 | 1.27739100 |
| H | 6.55320200 | 4.31226100 | 0.68955200 |
| H | 6.46818300 | -1.75535900 | -0.61305800 |
| H | 6.70597100 | -3.38571700 | -1.26191600 |
| H | 7.65699300 | -2.83711600 | 0.13920000 |
| H | 6.03119600 | -5.43744200 | 0.12711300 |
| H | 5.25372700 | -5.21708000 | 1.71022000 |
| H | 6.95872900 | -4.78542900 | 1.48818100 |
| H | 5.38546300 | -1.43327400 | 1.66540000 |

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|---|------------|-------------|------------|
| H | 4.76281300 | -2.83043300 | 2.57100900 |
| H | 6.51618500 | -2.56073600 | 2.42981300 |

DQAC-DBO (gas), T₁

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|---|-------------|-------------|-------------|
| C | -5.85619300 | -0.72962100 | -0.90855900 |
| C | -6.13088900 | -0.31177000 | 0.47798000 |
| C | -4.91683800 | 0.02333800 | 1.09550500 |
| C | -3.74425500 | -0.09898400 | 0.10712400 |
| C | -4.47986800 | -0.61304400 | -1.15263500 |
| C | -3.91295300 | -1.08146100 | -2.34670000 |
| C | -4.77317300 | -1.64337700 | -3.30148800 |
| C | -6.15313400 | -1.72142000 | -3.07428900 |
| C | -6.70894300 | -1.26859700 | -1.87502600 |
| C | -7.32714100 | -0.24573400 | 1.19412200 |
| C | -7.28551200 | 0.15988200 | 2.53152100 |
| C | -6.06896800 | 0.49221500 | 3.14251500 |
| C | -4.87073700 | 0.42809200 | 2.42174700 |
| C | -2.71512100 | -1.10743100 | 0.58399400 |
| C | -1.44304700 | -0.73635400 | 1.05406300 |
| N | -1.03633300 | 0.62536500 | 1.10317800 |
| C | -1.87243800 | 1.60843800 | 0.52024800 |
| C | -3.11602000 | 1.27429500 | -0.05458300 |
| C | -3.05881200 | -2.45958600 | 0.50252600 |
| C | -2.13423700 | -3.45095400 | 0.77967200 |
| C | -0.87745200 | -3.08894800 | 1.26604900 |
| C | -0.54864800 | -1.75731600 | 1.48071700 |
| C | -1.44206200 | 2.96517900 | 0.47836700 |
| C | -2.16957500 | 3.88728000 | -0.25958100 |
| C | -3.37331800 | 3.53634400 | -0.88245300 |
| C | -3.85872100 | 2.25241200 | -0.72937300 |
| C | 0.30615900 | 0.94409500 | 1.39468500 |
| C | 1.22112400 | -0.07108800 | 1.78830500 |
| C | 2.57181400 | 0.23465200 | 1.89367600 |
| C | 3.02722900 | 1.54009500 | 1.71513800 |
| C | 2.11070200 | 2.56647800 | 1.51188700 |
| C | 0.75339900 | 2.29147800 | 1.35913300 |
| C | 0.65684600 | -1.37469600 | 2.31484400 |
| C | -0.29573300 | 3.38806600 | 1.38144700 |
| C | -0.86545900 | 3.44062100 | 2.83833000 |
| C | 0.11201600 | -1.05826500 | 3.75123200 |
| C | -2.43202100 | -1.01878300 | -2.48065700 |
| C | -1.64241100 | -2.16165400 | -2.28929700 |
| C | -0.28374800 | -2.01028000 | -1.98634300 |
| C | 0.33981400 | -0.75292200 | -1.90846200 |
| C | -0.46997500 | 0.35349100 | -2.20817300 |
| C | -1.82608500 | 0.25097400 | -2.49059900 |
| B | 1.77878000 | -0.58617200 | -1.48872600 |
| C | 2.44298200 | -1.89412100 | -1.05085800 |
| C | 2.26695900 | 0.85735100 | -1.51799900 |

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|---|-------------|-------------|-------------|
| C | 1.68457800 | -3.09267100 | -1.17747300 |
| C | 2.18363000 | -4.32449400 | -0.77225200 |
| C | 3.46341700 | -4.41675100 | -0.20414600 |
| C | 4.24869600 | -3.26989000 | -0.03016800 |
| C | 3.71732700 | -2.04522700 | -0.46242400 |
| C | 3.57192200 | 1.33631900 | -1.25259600 |
| C | 3.92003500 | 2.69711900 | -1.22331500 |
| C | 2.92587800 | 3.65197200 | -1.52051800 |
| C | 1.63526000 | 3.23688200 | -1.84686300 |
| C | 1.31650500 | 1.87534300 | -1.83706500 |
| C | 0.26824500 | 4.78205700 | 1.05799600 |
| C | 1.69488900 | -2.50050200 | 2.45595800 |
| O | 0.41217800 | -3.13413200 | -1.69201100 |
| O | 0.03143800 | 1.61077300 | -2.16623400 |
| C | 5.34335400 | 3.17059700 | -0.89098300 |
| C | 5.63638100 | -3.29125300 | 0.63375900 |
| C | 5.93893800 | 3.87969800 | -2.13337800 |
| C | 6.28173000 | 2.00824300 | -0.50457700 |
| C | 5.30370500 | 4.17315400 | 0.28985900 |
| C | 6.69804000 | -2.76665500 | -0.36252400 |
| C | 6.05064900 | -4.70667500 | 1.08271600 |
| C | 5.61868200 | -2.37574000 | 1.88348700 |
| H | -4.35012300 | -2.01743800 | -4.22880800 |
| H | -6.79503100 | -2.15350300 | -3.83569200 |
| H | -7.77419000 | -1.35883200 | -1.68571000 |
| H | -8.26987700 | -0.50651200 | 0.72250400 |
| H | -8.20526200 | 0.21691400 | 3.10495600 |
| H | -6.05755400 | 0.80186000 | 4.18263900 |
| H | -3.92166100 | 0.68739700 | 2.88318000 |
| H | -4.04791100 | -2.71878700 | 0.14146600 |
| H | -2.38626800 | -4.49633500 | 0.63727300 |
| H | -0.15661400 | -3.86070100 | 1.49950200 |
| H | -1.81932400 | 4.90834700 | -0.33189400 |
| H | -3.93320000 | 4.27521700 | -1.44581500 |
| H | -4.81366600 | 1.96589200 | -1.15735200 |
| H | 3.28004100 | -0.55038100 | 2.12140700 |
| H | 4.08643400 | 1.75880700 | 1.78526300 |
| H | 2.46756200 | 3.58385500 | 1.43516000 |
| H | -1.28286000 | 2.47355100 | 3.13342100 |
| H | -1.65713500 | 4.19464800 | 2.89692700 |
| H | -0.06303900 | 3.70003500 | 3.53616900 |
| H | -0.35339500 | -1.95597200 | 4.17039900 |
| H | -0.63369800 | -0.25796200 | 3.72586800 |
| H | 0.94080500 | -0.74344700 | 4.39329800 |
| H | -2.08870300 | -3.14850000 | -2.24588500 |
| H | -2.39981700 | 1.15041800 | -2.67130000 |
| H | 1.56301900 | -5.20504500 | -0.90293700 |
| H | 3.81974100 | -5.39187200 | 0.10344200 |
| H | 4.30285300 | -1.14851600 | -0.30490600 |

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|---|-------------|-------------|-------------|
| H | 4.33717100 | 0.60227800 | -1.05362000 |
| H | 3.15790800 | 4.71099700 | -1.52051500 |
| H | 0.85316100 | 3.94107000 | -2.11203000 |
| H | -0.51442300 | 5.53898500 | 1.14481600 |
| H | 1.03976800 | 5.04938800 | 1.78338900 |
| H | 0.70102500 | 4.81686600 | 0.05633600 |
| H | 1.24257100 | -3.36355900 | 2.95048600 |
| H | 2.09212000 | -2.80916100 | 1.49115900 |
| H | 2.51791300 | -2.17271800 | 3.09445800 |
| H | 5.34055600 | 4.74993100 | -2.41820200 |
| H | 6.95974500 | 4.21812500 | -1.92119800 |
| H | 5.96827500 | 3.19306500 | -2.98541300 |
| H | 6.40548400 | 1.30352900 | -1.33259800 |
| H | 7.26980700 | 2.40553400 | -0.25080600 |
| H | 5.90504900 | 1.45659100 | 0.36364300 |
| H | 4.69401800 | 5.04991600 | 0.05559600 |
| H | 4.89337300 | 3.70424100 | 1.18945600 |
| H | 6.31787200 | 4.51989300 | 0.51820500 |
| H | 6.47426600 | -1.74353500 | -0.67928300 |
| H | 6.72764400 | -3.39873500 | -1.25597300 |
| H | 7.69081500 | -2.77146000 | 0.10273000 |
| H | 6.10220500 | -5.39356800 | 0.23180800 |
| H | 5.34723700 | -5.11317300 | 1.81700000 |
| H | 7.04169800 | -4.66986300 | 1.54695300 |
| H | 5.42381800 | -1.33404100 | 1.60942400 |
| H | 4.84024400 | -2.70023900 | 2.58276100 |
| H | 6.58657400 | -2.41268500 | 2.39671200 |

DQAC-SBO (gas), S₀

| | | | |
|---|-------------|-------------|-------------|
| C | 5.25620200 | -1.41776200 | 1.03517400 |
| C | 5.65968700 | -1.32048500 | -0.37928600 |
| C | 4.57341400 | -0.83463800 | -1.12420900 |
| C | 3.37190400 | -0.53459900 | -0.21680000 |
| C | 3.92621300 | -0.98694800 | 1.14961600 |
| C | 3.25378100 | -1.04322100 | 2.37164800 |
| C | 3.95316200 | -1.51604200 | 3.49071700 |
| C | 5.29160000 | -1.91477200 | 3.38399500 |
| C | 5.95406800 | -1.87670800 | 2.15400100 |
| C | 6.86514000 | -1.63644200 | -1.00826900 |
| C | 6.96390500 | -1.45989600 | -2.39135300 |
| C | 5.87567800 | -0.97678300 | -3.13072400 |
| C | 4.66888500 | -0.65813600 | -2.49728300 |
| C | 3.07361800 | 0.95957200 | -0.21886100 |
| C | 1.87054300 | 1.49473900 | -0.71059300 |
| N | 0.83466300 | 0.66282600 | -1.21313200 |
| C | 0.96617400 | -0.74650300 | -1.08377300 |
| C | 2.14461100 | -1.34092400 | -0.60780700 |
| C | -0.46667200 | 1.21083900 | -1.37937000 |

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|---|-------------|-------------|-------------|
| C | 4.04716300 | 1.79944700 | 0.33424500 |
| C | 3.83357400 | 3.16026600 | 0.46003700 |
| C | 2.65024300 | 3.69839600 | -0.04453200 |
| C | 1.68995600 | 2.90149300 | -0.66323400 |
| C | -0.11983000 | -1.59156000 | -1.43956800 |
| C | -0.05794300 | -2.95154700 | -1.15145200 |
| C | 1.10583500 | -3.53307600 | -0.64648900 |
| C | 2.21041500 | -2.72856000 | -0.43161900 |
| C | -0.68194100 | 2.60258800 | -1.28648500 |
| C | -1.98994000 | 3.09398900 | -1.28722900 |
| C | -3.07946800 | 2.24795300 | -1.46102800 |
| C | -2.85019900 | 0.90212600 | -1.72165800 |
| C | -1.55638300 | 0.37757500 | -1.71829300 |
| C | -1.24469700 | -1.00119300 | -2.27459500 |
| C | 0.52236900 | 3.52299300 | -1.41561800 |
| C | 0.22245900 | 4.96873100 | -0.98256600 |
| C | 1.80175000 | -0.69133700 | 2.39900600 |
| C | 0.87403000 | -1.73758000 | 2.31036600 |
| C | -0.44939000 | -1.42641300 | 2.02652700 |
| C | -0.89276200 | -0.09560700 | 1.91679100 |
| C | 0.05747100 | 0.92319700 | 2.10113100 |
| C | 1.40300600 | 0.64784700 | 2.32375700 |
| B | -2.32323100 | 0.22814700 | 1.58148500 |
| C | -3.15429200 | -1.00007000 | 1.17999800 |
| C | -2.67123700 | 1.71584800 | 1.71348700 |
| C | -2.55174100 | -2.26852600 | 1.34054200 |
| C | -3.22242600 | -3.44260000 | 0.98095800 |
| C | -4.49118200 | -3.36864000 | 0.42043100 |
| C | -5.12009500 | -2.12927500 | 0.18771500 |
| C | -4.43187100 | -0.98299600 | 0.58379100 |
| C | -3.96197000 | 2.29222200 | 1.65734700 |
| C | -4.16904400 | 3.66009400 | 1.74191800 |
| C | -3.06704700 | 4.51696500 | 1.90725000 |
| C | -1.78673300 | 3.99715000 | 2.00318600 |
| C | -1.59617100 | 2.61027800 | 1.91078800 |
| O | -0.29999200 | 2.22320500 | 2.01544600 |
| O | -1.30027200 | -2.45722900 | 1.82970800 |
| C | -6.48555400 | -1.99666500 | -0.50833200 |
| C | -7.08298700 | -3.36519900 | -0.89218300 |
| C | -7.48204800 | -1.27897700 | 0.43314000 |
| C | -6.31250300 | -1.16417800 | -1.80275900 |
| C | -2.47830900 | -1.91256100 | -2.38818400 |
| C | 0.91241300 | 3.54640800 | -2.92668200 |
| C | -0.68368700 | -0.79586800 | -3.71840900 |
| H | 3.44100400 | -1.57357700 | 4.44631500 |
| H | 5.81355600 | -2.27072100 | 4.26664300 |
| H | 6.98454000 | -2.20776900 | 2.06722900 |
| H | 7.70718200 | -2.01326700 | -0.43523500 |
| H | 7.89215800 | -1.70054300 | -2.89984300 |

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|---|-------------|-------------|-------------|
| H | 5.97148600 | -0.84888400 | -4.20429500 |
| H | 3.82027300 | -0.28100800 | -3.06065200 |
| H | 4.96745300 | 1.35394200 | 0.69723200 |
| H | 4.57900500 | 3.79985000 | 0.92021300 |
| H | 2.49015500 | 4.76594800 | 0.02345100 |
| H | -0.91766300 | -3.57801800 | -1.35152300 |
| H | 1.14922500 | -4.59928200 | -0.45210600 |
| H | 3.13920600 | -3.15507100 | -0.06545900 |
| H | -2.16535000 | 4.15174800 | -1.14558600 |
| H | -4.08908800 | 2.64199600 | -1.42528800 |
| H | -3.68586300 | 0.24858000 | -1.93468000 |
| H | -0.05578900 | 5.01548700 | 0.07310800 |
| H | 1.09036000 | 5.60876400 | -1.15479000 |
| H | -0.59199500 | 5.38158500 | -1.58150100 |
| H | 1.19478800 | -2.77151500 | 2.32633900 |
| H | 2.12101200 | 1.45851200 | 2.36802800 |
| H | -2.72455500 | -4.39403100 | 1.13428300 |
| H | -4.97873700 | -4.29450700 | 0.14037400 |
| H | -4.86973500 | -0.01380700 | 0.37664800 |
| H | -4.81902600 | 1.63594000 | 1.55683400 |
| H | -5.17299700 | 4.06872200 | 1.69396100 |
| H | -3.21730100 | 5.58972700 | 1.98078200 |
| H | -0.92049200 | 4.62884900 | 2.16447400 |
| H | -6.43465400 | -3.90307900 | -1.59185400 |
| H | -7.24316700 | -3.99297000 | -0.00937600 |
| H | -8.05210400 | -3.21635600 | -1.37891500 |
| H | -7.61870100 | -1.85236400 | 1.35581100 |
| H | -7.12719500 | -0.28016100 | 0.70390000 |
| H | -8.45581200 | -1.17169400 | -0.05816200 |
| H | -5.57972400 | -1.63630700 | -2.46587700 |
| H | -5.96979200 | -0.14873700 | -1.58152400 |
| H | -7.26740300 | -1.08853100 | -2.33498900 |
| H | -2.93843900 | -2.10875000 | -1.42006500 |
| H | -2.20139900 | -2.86355400 | -2.85010600 |
| H | -3.22039000 | -1.45262100 | -3.04544600 |
| H | 1.13657600 | 2.53653500 | -3.28283000 |
| H | 1.79953600 | 4.17230600 | -3.07143400 |
| H | 0.08249700 | 3.94781200 | -3.51775400 |
| H | 0.19906400 | -0.15065000 | -3.70984900 |
| H | -0.40354100 | -1.76433200 | -4.14622000 |
| H | -1.44940900 | -0.32910300 | -4.34692400 |

DQAC-SBO (gas), S₁

| | | | |
|---|-------------|-------------|-------------|
| C | -5.27361100 | -1.34982700 | -1.08734000 |
| C | -5.66709300 | -1.31953800 | 0.33228100 |
| C | -4.57820400 | -0.86946000 | 1.09554400 |
| C | -3.38061300 | -0.53027400 | 0.18782800 |
| C | -3.94501000 | -0.91483100 | -1.19665200 |
| C | -3.26679600 | -0.91095200 | -2.41753400 |

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|---|-------------|-------------|-------------|
| C | -3.98135000 | -1.33756000 | -3.54790200 |
| C | -5.31821600 | -1.74512700 | -3.45190500 |
| C | -5.97809400 | -1.76203500 | -2.21996000 |
| C | -6.86701200 | -1.66400500 | 0.95652800 |
| C | -6.95615900 | -1.55235300 | 2.34733700 |
| C | -5.86449600 | -1.10470000 | 3.10241700 |
| C | -4.66178700 | -0.75685900 | 2.47551300 |
| C | -3.08666500 | 0.95254600 | 0.27009300 |
| C | -1.86300800 | 1.47123000 | 0.74274500 |
| N | -0.80673200 | 0.60642700 | 1.14206600 |
| C | -0.97255800 | -0.79718800 | 1.03036300 |
| C | -2.17221600 | -1.36013500 | 0.54925500 |
| C | 0.46262900 | 1.13248300 | 1.40481200 |
| C | -4.08788900 | 1.81514100 | -0.17566000 |
| C | -3.89006200 | 3.18431700 | -0.20133700 |
| C | -2.68850800 | 3.70411400 | 0.27619500 |
| C | -1.68293400 | 2.88090000 | 0.77049200 |
| C | 0.09667300 | -1.66881500 | 1.38987800 |
| C | 0.00236300 | -3.01953100 | 1.09356100 |
| C | -1.17518200 | -3.56344300 | 0.57504000 |
| C | -2.26702900 | -2.74006400 | 0.36343600 |
| C | 0.69914700 | 2.53727800 | 1.33409500 |
| C | 2.00754700 | 2.99607000 | 1.33183900 |
| C | 3.07762300 | 2.11669900 | 1.48803000 |
| C | 2.83515600 | 0.77202800 | 1.76852700 |
| C | 1.54609700 | 0.27003300 | 1.75312300 |
| C | 1.22535300 | -1.12311600 | 2.23857700 |
| C | -0.47379800 | 3.48443200 | 1.45612000 |
| C | -0.14881700 | 4.90986700 | 0.97426200 |
| C | -1.81649400 | -0.56409100 | -2.43708600 |
| C | -0.88970100 | -1.61639400 | -2.34186600 |
| C | 0.43687700 | -1.32410900 | -2.05849700 |
| C | 0.90881700 | -0.00353500 | -1.92489100 |
| C | -0.04020400 | 1.02261900 | -2.09078000 |
| C | -1.38726300 | 0.76901100 | -2.32520900 |
| B | 2.35356700 | 0.29379700 | -1.60781500 |
| C | 3.15746500 | -0.94650800 | -1.21043300 |
| C | 2.71200400 | 1.77599000 | -1.66556900 |
| C | 2.54025400 | -2.21908700 | -1.38011000 |
| C | 3.18432400 | -3.40292700 | -1.04187400 |
| C | 4.47120600 | -3.37520500 | -0.47847100 |
| C | 5.10913900 | -2.15227300 | -0.23456800 |
| C | 4.44018900 | -0.97832600 | -0.61386300 |
| C | 4.00353800 | 2.35844800 | -1.54382200 |
| C | 4.21678200 | 3.73701700 | -1.55748900 |
| C | 3.14185200 | 4.61065500 | -1.74380700 |
| C | 1.85458100 | 4.07943100 | -1.92637900 |
| C | 1.65174900 | 2.70563300 | -1.86703500 |
| O | 0.33166400 | 2.32858300 | -1.96156000 |

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|---|-------------|-------------|-------------|
| O | 1.28064100 | -2.37938100 | -1.89447200 |
| C | 6.48008600 | -2.04694300 | 0.45658300 |
| C | 7.05937100 | -3.42686100 | 0.82757400 |
| C | 7.48799600 | -1.33581300 | -0.47741800 |
| C | 6.32562400 | -1.22558500 | 1.76104700 |
| C | 2.45341200 | -2.04275900 | 2.32438600 |
| C | -0.81755500 | 3.55274800 | 2.98403900 |
| C | 0.64831400 | -0.96777000 | 3.69023200 |
| H | -3.47383900 | -1.35267100 | -4.50739400 |
| H | -5.84292800 | -2.06489900 | -4.34681200 |
| H | -7.00698500 | -2.09976000 | -2.14227900 |
| H | -7.71276000 | -2.01398700 | 0.37240500 |
| H | -7.88110400 | -1.81723200 | 2.84959800 |
| H | -5.95248400 | -1.02788500 | 4.18131100 |
| H | -3.81045300 | -0.40808500 | 3.05305500 |
| H | -5.01682100 | 1.38638200 | -0.53443500 |
| H | -4.66039500 | 3.84622600 | -0.58224400 |
| H | -2.54467600 | 4.77478800 | 0.26867600 |
| H | 0.84986100 | -3.66497200 | 1.27882300 |
| H | -1.23482600 | -4.62380600 | 0.35514900 |
| H | -3.20034700 | -3.14329900 | -0.01486300 |
| H | 2.21502200 | 4.04270700 | 1.16313500 |
| H | 4.09279500 | 2.48753800 | 1.41481000 |
| H | 3.66859800 | 0.10820000 | 1.95080800 |
| H | 0.08837300 | 4.91213900 | -0.09054000 |
| H | -0.98618400 | 5.58233900 | 1.16743500 |
| H | 0.69998700 | 5.31302700 | 1.52883800 |
| H | -1.21166200 | -2.64991700 | -2.39205500 |
| H | -2.08616400 | 1.59623600 | -2.38365500 |
| H | 2.67120100 | -4.34184200 | -1.22335500 |
| H | 4.94314300 | -4.31570100 | -0.22417400 |
| H | 4.91437100 | -0.02430300 | -0.41597600 |
| H | 4.85861300 | 1.69885400 | -1.44615800 |
| H | 5.22361000 | 4.13066200 | -1.45030200 |
| H | 3.29676900 | 5.68373500 | -1.78297200 |
| H | 1.00138800 | 4.72009100 | -2.12227700 |
| H | 6.40242300 | -3.96152900 | 1.52169700 |
| H | 7.20324000 | -4.04752500 | -0.06268500 |
| H | 8.03312200 | -3.29930200 | 1.31212600 |
| H | 7.61173800 | -1.90448500 | -1.40471900 |
| H | 7.14674900 | -0.33106900 | -0.74203900 |
| H | 8.46516300 | -1.24848000 | 0.01236100 |
| H | 5.58546600 | -1.69566300 | 2.41882100 |
| H | 5.99846800 | -0.20310000 | 1.54802600 |
| H | 7.28112400 | -1.16995200 | 2.29567200 |
| H | 2.91810200 | -2.18857000 | 1.35053300 |
| H | 2.17031700 | -3.01222200 | 2.74029800 |
| H | 3.18925500 | -1.61561400 | 3.00984600 |
| H | -1.05991000 | 2.56015600 | 3.37596000 |

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|---|-------------|-------------|------------|
| H | -1.68075600 | 4.20873000 | 3.13384400 |
| H | 0.04147400 | 3.94745600 | 3.53516700 |
| H | -0.23376500 | -0.32083400 | 3.70481300 |
| H | 0.36575400 | -1.95294900 | 4.07370500 |
| H | 1.41373800 | -0.53136400 | 4.33910800 |

DQAC-SBO (gas), T₁

| | | | |
|---|-------------|-------------|-------------|
| C | -5.28253100 | -1.36845100 | -1.05571000 |
| C | -5.66055200 | -1.31596900 | 0.36840600 |
| C | -4.55947800 | -0.85604300 | 1.10869000 |
| C | -3.37032600 | -0.54146800 | 0.19029800 |
| C | -3.95329900 | -0.93989300 | -1.17823200 |
| C | -3.30303200 | -0.93042500 | -2.41338500 |
| C | -4.02565900 | -1.34997300 | -3.53987200 |
| C | -5.36069700 | -1.75895500 | -3.42430300 |
| C | -6.00064100 | -1.77679900 | -2.18166300 |
| C | -6.85656900 | -1.64442800 | 1.00861800 |
| C | -6.93087300 | -1.50638400 | 2.39774400 |
| C | -5.82827200 | -1.04871100 | 3.13185500 |
| C | -4.63035100 | -0.71813500 | 2.48751500 |
| C | -3.04829800 | 0.94696500 | 0.22538600 |
| C | -1.84249800 | 1.45026800 | 0.74434200 |
| N | -0.82593600 | 0.58945200 | 1.23807200 |
| C | -0.96912600 | -0.81106600 | 1.05740800 |
| C | -2.14814300 | -1.37540200 | 0.54125900 |
| C | 0.48348100 | 1.11750000 | 1.43252200 |
| C | -4.00163600 | 1.81621200 | -0.32001600 |
| C | -3.76387500 | 3.17581900 | -0.41134800 |
| C | -2.57941700 | 3.68243400 | 0.12368000 |
| C | -1.64200000 | 2.85592800 | 0.73830100 |
| C | 0.10203300 | -1.68078100 | 1.39924200 |
| C | 0.02464600 | -3.03123900 | 1.07061000 |
| C | -1.13548200 | -3.58147700 | 0.52409900 |
| C | -2.22566800 | -2.75551300 | 0.31137900 |
| C | 0.71494900 | 2.50747100 | 1.37106700 |
| C | 2.02867000 | 2.98085000 | 1.37245300 |
| C | 3.10481100 | 2.11284500 | 1.52013100 |
| C | 2.85922200 | 0.76713000 | 1.76137400 |
| C | 1.55829500 | 0.26181000 | 1.75306800 |
| C | 1.22939200 | -1.13171000 | 2.25948400 |
| C | -0.47852900 | 3.43707900 | 1.52654100 |
| C | -0.15894400 | 4.89546500 | 1.15632800 |
| C | -1.85459800 | -0.57232600 | -2.44445500 |
| C | -0.90618500 | -1.60163400 | -2.32397200 |
| C | 0.44330900 | -1.29351900 | -2.03147700 |
| C | 0.92140100 | 0.02146200 | -1.90996200 |
| C | -0.04140400 | 1.02596500 | -2.08632700 |
| C | -1.41192700 | 0.75554500 | -2.32773100 |

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|---|-------------|-------------|-------------|
| B | 2.35156200 | 0.32806200 | -1.59092000 |
| C | 3.16398500 | -0.91535300 | -1.22223300 |
| C | 2.68367700 | 1.81987800 | -1.65376200 |
| C | 2.54082900 | -2.18789900 | -1.38356400 |
| C | 3.17168100 | -3.38505800 | -1.06736700 |
| C | 4.46085500 | -3.36592700 | -0.52218400 |
| C | 5.10988100 | -2.14401300 | -0.28332300 |
| C | 4.45134300 | -0.95830500 | -0.65023700 |
| C | 3.95559400 | 2.42902100 | -1.54179400 |
| C | 4.13029100 | 3.81185700 | -1.56516100 |
| C | 3.03116200 | 4.66365400 | -1.72853400 |
| C | 1.75857700 | 4.11017600 | -1.88973900 |
| C | 1.60390200 | 2.72733300 | -1.84840600 |
| O | 0.29881000 | 2.31331600 | -1.99626200 |
| O | 1.25796300 | -2.33356700 | -1.85275300 |
| C | 6.48257300 | -2.05503200 | 0.40266200 |
| C | 7.05681600 | -3.44186300 | 0.75520200 |
| C | 7.48814800 | -1.33658000 | -0.52892900 |
| C | 6.32937700 | -1.24744000 | 1.71641200 |
| C | 2.45672000 | -2.05487000 | 2.33583400 |
| C | -0.88612600 | 3.40605900 | 3.03317200 |
| C | 0.66225000 | -0.97468100 | 3.70625500 |
| H | -3.53541500 | -1.35706600 | -4.50865600 |
| H | -5.89972000 | -2.07442800 | -4.31204900 |
| H | -7.03053000 | -2.10900600 | -2.09243400 |
| H | -7.71026500 | -2.00079700 | 0.43979400 |
| H | -7.85160400 | -1.75704900 | 2.91491100 |
| H | -5.90566500 | -0.95022700 | 4.20996400 |
| H | -3.77027500 | -0.36156500 | 3.04693100 |
| H | -4.92514500 | 1.39515300 | -0.70315700 |
| H | -4.49293800 | 3.83841700 | -0.86512700 |
| H | -2.40094700 | 4.74854300 | 0.08466700 |
| H | 0.87314400 | -3.67383600 | 1.26690000 |
| H | -1.18960800 | -4.64109100 | 0.29858500 |
| H | -3.15426000 | -3.15798900 | -0.08166200 |
| H | 2.22037600 | 4.03712600 | 1.23829600 |
| H | 4.11998100 | 2.49067200 | 1.47345300 |
| H | 3.68950900 | 0.09812900 | 1.94464900 |
| H | 0.13726400 | 4.98323900 | 0.10854200 |
| H | -1.02325700 | 5.53681700 | 1.34310600 |
| H | 0.65174100 | 5.27251000 | 1.78349400 |
| H | -1.20439300 | -2.64337000 | -2.36431700 |
| H | -2.10562400 | 1.58986800 | -2.36721700 |
| H | 2.63854300 | -4.31557400 | -1.23144600 |
| H | 4.92953700 | -4.30767200 | -0.26915700 |
| H | 4.93242000 | -0.00966700 | -0.44548200 |
| H | 4.82572800 | 1.79185000 | -1.43182700 |
| H | 5.12663600 | 4.23166200 | -1.46277000 |
| H | 3.16260100 | 5.73996400 | -1.75332000 |

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|---|-------------|-------------|-------------|
| H | 0.88146600 | 4.72663000 | -2.05348100 |
| H | 6.40424000 | -3.97949400 | 1.45087300 |
| H | 7.19476700 | -4.05543700 | -0.14105100 |
| H | 8.03356000 | -3.32123900 | 1.23459100 |
| H | 7.60902100 | -1.89417100 | -1.46340800 |
| H | 7.15334000 | -0.32589000 | -0.77797900 |
| H | 8.46567000 | -1.26110300 | -0.03908300 |
| H | 5.58328900 | -1.71690000 | 2.36711200 |
| H | 6.01288000 | -0.21901000 | 1.51907700 |
| H | 7.28539100 | -1.21098200 | 2.25088000 |
| H | 2.91495400 | -2.20517300 | 1.35798900 |
| H | 2.17699700 | -3.02475300 | 2.75480500 |
| H | 3.20055400 | -1.62610800 | 3.01212600 |
| H | -1.12619900 | 2.38674600 | 3.34957000 |
| H | -1.76633000 | 4.03803300 | 3.19343600 |
| H | -0.05725200 | 3.77387100 | 3.64688500 |
| H | -0.21532400 | -0.32166300 | 3.71366400 |
| H | 0.37247700 | -1.95512900 | 4.09917200 |
| H | 1.42780300 | -0.53569900 | 4.35446600 |

DQAC-NBO (gas), S₀

| | | | |
|---|-------------|-------------|-------------|
| C | -4.82232300 | -0.49726100 | -1.36925600 |
| C | -5.36602400 | -0.43100300 | -0.00102100 |
| C | -4.30517600 | -0.21774400 | 0.89245800 |
| C | -2.97291100 | -0.06797900 | 0.14348800 |
| C | -3.42817900 | -0.33871700 | -1.30531900 |
| C | -2.63930700 | -0.47264400 | -2.44862900 |
| C | -3.28277500 | -0.70950800 | -3.67256900 |
| C | -4.67683200 | -0.81633500 | -3.74369400 |
| C | -5.45945800 | -0.72628700 | -2.58942100 |
| C | -6.67409400 | -0.56145100 | 0.46912000 |
| C | -6.90017600 | -0.47880400 | 1.84591300 |
| C | -5.83653700 | -0.26984500 | 2.73448100 |
| C | -4.52688300 | -0.13496900 | 2.25959200 |
| C | -2.45680600 | 1.36252600 | 0.27886100 |
| C | -1.15369300 | 1.66763200 | 0.72603000 |
| N | -0.28013500 | 0.65054900 | 1.17673000 |
| C | -0.69514100 | -0.70118700 | 1.12737600 |
| C | -1.94552300 | -1.07732400 | 0.61640000 |
| C | -3.33238100 | 2.38194800 | -0.10314100 |
| C | -2.94921300 | 3.71224000 | -0.06636300 |
| C | -1.64899800 | 4.00968500 | 0.32310500 |
| C | -0.73605100 | 3.01846900 | 0.69390600 |
| C | 0.16614200 | -1.72102400 | 1.61409900 |
| C | -0.14978400 | -3.05622200 | 1.38422800 |
| C | -1.36611800 | -3.42467200 | 0.80539100 |
| C | -2.27425800 | -2.43160700 | 0.48394900 |
| C | 1.08316900 | 0.95235900 | 1.42391700 |
| C | 1.59768300 | 2.24863700 | 1.22450100 |

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|---|-------------|-------------|-------------|
| C | 2.97411100 | 2.46219200 | 1.37858400 |
| C | 3.84175100 | 1.44058700 | 1.73161100 |
| C | 3.31352800 | 0.18758100 | 2.02649100 |
| C | 1.94497200 | -0.05618100 | 1.92689300 |
| C | 0.68577100 | 3.45833600 | 1.03283700 |
| C | 1.31150900 | -1.30451600 | 2.52194100 |
| C | 0.67197500 | 4.24517700 | 2.37447000 |
| C | 0.68420600 | -0.89339600 | 3.89260200 |
| C | -1.14958700 | -0.49863500 | -2.31355000 |
| C | -0.55315800 | -1.75455700 | -2.13442700 |
| C | 0.77942700 | -1.80623000 | -1.75276600 |
| C | 1.57112800 | -0.64830300 | -1.66096900 |
| C | 0.96131800 | 0.58171900 | -1.96264000 |
| C | -0.40219600 | 0.68222200 | -2.23973500 |
| B | 3.00753100 | -0.71996000 | -1.21625600 |
| C | 3.42988900 | -2.10521900 | -0.70057200 |
| C | 3.77641500 | 0.59430400 | -1.38772500 |
| C | 2.50537500 | -3.16229400 | -0.86444600 |
| C | 2.77611000 | -4.46610800 | -0.41868000 |
| C | 3.97906500 | -4.73360100 | 0.21555900 |
| C | 4.91361600 | -3.70480800 | 0.42637900 |
| C | 4.63104400 | -2.42370200 | -0.02370300 |
| C | 5.16964900 | 0.78004000 | -1.22757500 |
| C | 5.77857500 | 2.01342800 | -1.39324100 |
| C | 4.99848200 | 3.12268300 | -1.76090100 |
| C | 3.63468200 | 2.98441300 | -1.96005400 |
| C | 3.03109800 | 1.73228400 | -1.76593000 |
| O | 1.29128700 | -3.01969800 | -1.44908800 |
| O | 1.68530700 | 1.72390500 | -1.96079200 |
| C | 2.31525700 | -2.43552700 | 2.80086800 |
| C | 1.20450600 | 4.38555100 | -0.09811200 |
| H | -2.68088800 | -0.82409200 | -4.56890900 |
| H | -5.14961400 | -0.99485300 | -4.70429100 |
| H | -6.53758900 | -0.84604100 | -2.63767600 |
| H | -7.49697300 | -0.72738500 | -0.21990100 |
| H | -7.90927400 | -0.58001200 | 2.23274500 |
| H | -6.03213900 | -0.21274800 | 3.80058000 |
| H | -3.69614200 | 0.02852300 | 2.93977700 |
| H | -4.32866300 | 2.11043400 | -0.43550500 |
| H | -3.63967700 | 4.49968100 | -0.34792200 |
| H | -1.32992500 | 5.04481000 | 0.33458500 |
| H | 0.54814500 | -3.82830700 | 1.68194300 |
| H | -1.60621200 | -4.47037600 | 0.64678600 |
| H | -3.24859600 | -2.68289600 | 0.07483900 |
| H | 3.37623100 | 3.45447400 | 1.21751400 |
| H | 4.90859500 | 1.62277800 | 1.79484500 |
| H | 3.97163700 | -0.60586900 | 2.35633200 |
| H | 0.00277800 | 5.10868500 | 2.30540200 |
| H | 1.67933800 | 4.59958900 | 2.61533000 |

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|---|-------------|-------------|-------------|
| H | 0.32722100 | 3.60092000 | 3.18876700 |
| H | -0.04526300 | -0.08887400 | 3.76940700 |
| H | 0.17893700 | -1.75643900 | 4.33904500 |
| H | 1.47366900 | -0.54653100 | 4.56764900 |
| H | -1.14347700 | -2.66135100 | -2.16044400 |
| H | -0.86810900 | 1.65399900 | -2.36002000 |
| H | 2.02661700 | -5.23344500 | -0.57886600 |
| H | 4.18943100 | -5.73989700 | 0.56419300 |
| H | 5.84266800 | -3.91245400 | 0.94665500 |
| H | 5.33684400 | -1.62701500 | 0.17945800 |
| H | 5.78303700 | -0.07862200 | -0.98189100 |
| H | 6.84990700 | 2.12133000 | -1.25986300 |
| H | 5.46511300 | 4.09162000 | -1.90996300 |
| H | 3.02107700 | 3.82031800 | -2.27140700 |
| H | 1.80516100 | -3.27936200 | 3.27199000 |
| H | 3.07583000 | -2.09724200 | 3.50870500 |
| H | 2.80771800 | -2.77993900 | 1.89209200 |
| H | 2.26062500 | 4.62459700 | 0.03524400 |
| H | 0.65967000 | 5.33207100 | -0.10509000 |
| H | 1.07158500 | 3.89410400 | -1.06257400 |

DQAC-NBO (gas), S₁

| | | | |
|---|-------------|-------------|-------------|
| C | 4.79617300 | -0.37728900 | 1.49869400 |
| C | 5.40280700 | -0.46270700 | 0.15860600 |
| C | 4.38955800 | -0.33917200 | -0.80428000 |
| C | 3.02582300 | -0.10358700 | -0.13310400 |
| C | 3.40601800 | -0.23155500 | 1.35957200 |
| C | 2.55646700 | -0.22373900 | 2.46732000 |
| C | 3.15578900 | -0.29673500 | 3.73546400 |
| C | 4.54463200 | -0.39466000 | 3.88241000 |
| C | 5.37958500 | -0.45360700 | 2.76344700 |
| C | 6.72947400 | -0.64525400 | -0.23498000 |
| C | 7.02068200 | -0.70602100 | -1.60102300 |
| C | 6.00360800 | -0.58585900 | -2.55685400 |
| C | 4.67388500 | -0.39778100 | -2.16074100 |
| C | 2.54467500 | 1.30981700 | -0.41272600 |
| C | 1.22713400 | 1.60092400 | -0.83266400 |
| N | 0.32813000 | 0.55559800 | -1.17045700 |
| C | 0.75334300 | -0.78988000 | -1.09620100 |
| C | 2.01292500 | -1.13376300 | -0.56436900 |
| C | 3.44701200 | 2.34587700 | -0.18200100 |
| C | 3.07500400 | 3.67187300 | -0.34801000 |
| C | 1.76263400 | 3.95999700 | -0.69941600 |
| C | 0.81852900 | 2.95477400 | -0.91422800 |
| C | -0.11108500 | -1.83263200 | -1.53834800 |
| C | 0.21386700 | -3.15071200 | -1.25792400 |
| C | 1.43659700 | -3.48055800 | -0.66815200 |
| C | 2.34637700 | -2.47590700 | -0.38177400 |
| C | -1.00646500 | 0.84915800 | -1.46526500 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.52057000 | 2.16762800 | -1.31025500 |
| C | -2.89398700 | 2.36059900 | -1.40476500 |
| C | -3.76254900 | 1.30469800 | -1.65694300 |
| C | -3.24487700 | 0.03906100 | -1.94249500 |
| C | -1.88313800 | -0.19060200 | -1.90460800 |
| C | -0.61501700 | 3.37651800 | -1.18058000 |
| C | -1.27256600 | -1.46720900 | -2.43597000 |
| C | -0.68219500 | 4.14343800 | -2.53707100 |
| C | -0.65930400 | -1.12312700 | -3.83942700 |
| C | 1.07465700 | -0.27796500 | 2.28554100 |
| C | 0.49990200 | -1.54938900 | 2.11198300 |
| C | -0.84028300 | -1.64839700 | 1.76487700 |
| C | -1.67681500 | -0.52165000 | 1.65583400 |
| C | -1.07942500 | 0.72601800 | 1.90962400 |
| C | 0.27874400 | 0.87403900 | 2.18750200 |
| B | -3.13043700 | -0.65011100 | 1.26528500 |
| C | -3.51171200 | -2.05020800 | 0.78164600 |
| C | -3.91489900 | 0.65827700 | 1.35006600 |
| C | -2.55082400 | -3.09165700 | 0.94117900 |
| C | -2.77501900 | -4.40021300 | 0.52115700 |
| C | -3.98426100 | -4.73937400 | -0.10435600 |
| C | -4.94577600 | -3.74652600 | -0.31111900 |
| C | -4.70771100 | -2.44043400 | 0.11978200 |
| C | -5.30873500 | 0.84272400 | 1.14683600 |
| C | -5.92213100 | 2.09528000 | 1.19646400 |
| C | -5.16621500 | 3.23287700 | 1.48762100 |
| C | -3.79137600 | 3.09679000 | 1.73784000 |
| C | -3.19092200 | 1.84497500 | 1.65821100 |
| O | -1.32520300 | -2.89469700 | 1.52565600 |
| O | -1.82791600 | 1.86361300 | 1.84569100 |
| C | -2.28795300 | -2.60061100 | -2.64640400 |
| C | -1.08444100 | 4.31234500 | -0.03289800 |
| H | 2.51375300 | -0.29787600 | 4.61079700 |
| H | 4.97317700 | -0.45073900 | 4.87814500 |
| H | 6.45386300 | -0.56636500 | 2.87318200 |
| H | 7.51752700 | -0.74208000 | 0.50567000 |
| H | 8.04599900 | -0.85084600 | -1.92621200 |
| H | 6.24920400 | -0.64014100 | -3.61251000 |
| H | 3.87964400 | -0.30284900 | -2.89543500 |
| H | 4.45197000 | 2.09732000 | 0.13890500 |
| H | 3.78940700 | 4.47061000 | -0.18071000 |
| H | 1.45757900 | 4.99479900 | -0.79053600 |
| H | -0.49057300 | -3.93500500 | -1.50024700 |
| H | 1.67593900 | -4.51647300 | -0.45410800 |
| H | 3.31674600 | -2.70846500 | 0.04499500 |
| H | -3.30953500 | 3.34537000 | -1.24034600 |
| H | -4.83301600 | 1.46793300 | -1.62902500 |
| H | -3.91993500 | -0.77925300 | -2.15479900 |
| H | -0.03926100 | 5.02743900 | -2.50805500 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.70904200 | 4.46554200 | -2.73070700 |
| H | -0.35682100 | 3.50048400 | -3.36032600 |
| H | 0.07937400 | -0.31940400 | -3.77395300 |
| H | -0.17146000 | -2.01366200 | -4.24742300 |
| H | -1.46019600 | -0.80777300 | -4.51505400 |
| H | 1.10479900 | -2.44624500 | 2.16828600 |
| H | 0.70376800 | 1.86521700 | 2.31018900 |
| H | -1.99892700 | -5.13793400 | 0.69733500 |
| H | -4.16177900 | -5.76052800 | -0.42435100 |
| H | -5.88156000 | -3.99155000 | -0.80479600 |
| H | -5.46344800 | -1.68583300 | -0.06610800 |
| H | -5.92270700 | -0.03127200 | 0.96254100 |
| H | -6.99183400 | 2.18175600 | 1.02902600 |
| H | -5.63315700 | 4.21037000 | 1.54804500 |
| H | -3.17973500 | 3.95411700 | 1.99496200 |
| H | -1.79187800 | -3.46923600 | -3.08564700 |
| H | -3.05222000 | -2.28511400 | -3.36060500 |
| H | -2.77067500 | -2.89486000 | -1.71617900 |
| H | -2.11983100 | 4.62134100 | -0.18273300 |
| H | -0.47372000 | 5.21687600 | -0.00470000 |
| H | -1.01511700 | 3.79091600 | 0.92212900 |

DQAC-NBO (gas), T₁

| | | | |
|---|-------------|-------------|-------------|
| C | 4.77283600 | -0.40169700 | 1.54102500 |
| C | 5.40800400 | -0.52883900 | 0.21739600 |
| C | 4.41771600 | -0.41342600 | -0.77006400 |
| C | 3.04554700 | -0.13218500 | -0.13762400 |
| C | 3.38842700 | -0.24306300 | 1.36387100 |
| C | 2.51290400 | -0.20721200 | 2.44971800 |
| C | 3.07734200 | -0.25356400 | 3.73542500 |
| C | 4.46125300 | -0.35800700 | 3.91857400 |
| C | 5.32265600 | -0.45377700 | 2.82179400 |
| C | 6.74035900 | -0.74135300 | -0.14057700 |
| C | 7.06087400 | -0.84134100 | -1.49760300 |
| C | 6.06682100 | -0.72968000 | -2.47859700 |
| C | 4.73196500 | -0.51012500 | -2.11778300 |
| C | 2.60891400 | 1.29495900 | -0.44235600 |
| C | 1.29103400 | 1.61804800 | -0.82908500 |
| N | 0.35678400 | 0.59076500 | -1.13645100 |
| C | 0.74922800 | -0.75981400 | -1.08134100 |
| C | 2.00690700 | -1.13991200 | -0.56792700 |
| C | 3.54647700 | 2.30881400 | -0.24319800 |
| C | 3.20376100 | 3.64320500 | -0.40020200 |
| C | 1.88800600 | 3.96164400 | -0.71103700 |
| C | 0.91350500 | 2.97929300 | -0.90255800 |
| C | -0.13866800 | -1.77874500 | -1.53397400 |
| C | 0.16863500 | -3.10906900 | -1.28898800 |
| C | 1.39277600 | -3.47675500 | -0.72217200 |
| C | 2.32008000 | -2.49498300 | -0.41929000 |

| | | | |
|---|-------------|-------------|-------------|
| C | -0.97979700 | 0.92280700 | -1.42538600 |
| C | -1.45423700 | 2.24904200 | -1.27326800 |
| C | -2.82407900 | 2.48285900 | -1.37734200 |
| C | -3.72488400 | 1.45333100 | -1.61660100 |
| C | -3.24037600 | 0.17493200 | -1.89769100 |
| C | -1.88025800 | -0.08958900 | -1.86667900 |
| C | -0.51968800 | 3.43804700 | -1.12658400 |
| C | -1.29515700 | -1.37118900 | -2.42409000 |
| C | -0.59876900 | 4.25860700 | -2.44813900 |
| C | -0.67734900 | -1.01260300 | -3.82013600 |
| C | 1.03570700 | -0.27193600 | 2.23364000 |
| C | 0.47470200 | -1.54634300 | 2.04211500 |
| C | -0.87541100 | -1.66448800 | 1.70481800 |
| C | -1.73197800 | -0.55404700 | 1.61774500 |
| C | -1.14269200 | 0.69776200 | 1.85869100 |
| C | 0.22010600 | 0.86456100 | 2.12660900 |
| B | -3.18782000 | -0.70184300 | 1.25460600 |
| C | -3.55078900 | -2.10215700 | 0.76368600 |
| C | -3.98201400 | 0.60254800 | 1.33915500 |
| C | -2.56400000 | -3.12620400 | 0.88787000 |
| C | -2.75508000 | -4.42852700 | 0.43414100 |
| C | -3.96005600 | -4.78004400 | -0.18792600 |
| C | -4.95124400 | -3.80633100 | -0.35232200 |
| C | -4.74537200 | -2.50639900 | 0.10989500 |
| C | -5.37887000 | 0.77826600 | 1.16355400 |
| C | -5.99535200 | 2.02825900 | 1.21781100 |
| C | -5.23779100 | 3.17555900 | 1.47360000 |
| C | -3.85929200 | 3.05221200 | 1.68679200 |
| C | -3.25782200 | 1.79867300 | 1.61761700 |
| O | -1.33484900 | -2.91039900 | 1.46145200 |
| O | -1.89546200 | 1.82367800 | 1.78851500 |
| C | -2.32835700 | -2.48458700 | -2.65840000 |
| C | -0.95100500 | 4.33753300 | 0.06482800 |
| H | 2.41432900 | -0.23109400 | 4.59479700 |
| H | 4.86482100 | -0.39312900 | 4.92558800 |
| H | 6.39240100 | -0.57580700 | 2.96198700 |
| H | 7.51012900 | -0.83095000 | 0.62000900 |
| H | 8.09068300 | -1.01013600 | -1.79600400 |
| H | 6.33491500 | -0.81472400 | -3.52676700 |
| H | 3.95562600 | -0.41988900 | -2.87184900 |
| H | 4.55397600 | 2.03668300 | 0.04969800 |
| H | 3.94240900 | 4.42429000 | -0.25646600 |
| H | 1.60573200 | 5.00404900 | -0.79297300 |
| H | -0.54881600 | -3.87663100 | -1.54793000 |
| H | 1.61919400 | -4.52253500 | -0.54440400 |
| H | 3.29335100 | -2.75344200 | -0.01394200 |
| H | -3.20547700 | 3.48469400 | -1.22887700 |
| H | -4.79121300 | 1.64569500 | -1.58870200 |
| H | -3.93773800 | -0.62131800 | -2.12285200 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.05980000 | 5.13041100 | -2.40123200 |
| H | -1.62171000 | 4.60778700 | -2.61359600 |
| H | -0.30045800 | 3.64039100 | -3.29995000 |
| H | 0.07540300 | -0.22370700 | -3.73754900 |
| H | -0.20558700 | -1.90281700 | -4.24811800 |
| H | -1.47182000 | -0.66727600 | -4.48902900 |
| H | 1.08618300 | -2.43849900 | 2.09934900 |
| H | 0.63181200 | 1.86394500 | 2.23006400 |
| H | -1.95431900 | -5.14719400 | 0.57573600 |
| H | -4.11418000 | -5.79450200 | -0.53954100 |
| H | -5.88498800 | -4.06298000 | -0.84402400 |
| H | -5.52078900 | -1.76661300 | -0.05267700 |
| H | -5.99287400 | -0.09971200 | 0.99932500 |
| H | -7.06885300 | 2.10863800 | 1.07387100 |
| H | -5.70926700 | 4.15122900 | 1.52777300 |
| H | -3.24082900 | 3.91509200 | 1.90733600 |
| H | -1.84503500 | -3.34786800 | -3.12257700 |
| H | -3.09210000 | -2.14055500 | -3.36001100 |
| H | -2.81167500 | -2.80193500 | -1.73581300 |
| H | -1.98518900 | 4.66602900 | -0.05722100 |
| H | -0.32426300 | 5.23058100 | 0.11882300 |
| H | -0.87642400 | 3.78360100 | 1.00157100 |

Cartesian Coordinates of Optimized Structures (QM part).

AC-BO (crystal), S₀

| | | | |
|---|-------------|-------------|-------------|
| O | 2.00534000 | -2.28156500 | -0.80386000 |
| O | 3.01594900 | 2.04410800 | -2.57425500 |
| N | 3.92191800 | -3.70415800 | -3.92215200 |
| C | 6.69306600 | -3.17591900 | -3.07257700 |
| C | 7.97285900 | -3.94522800 | -3.43877200 |
| C | 8.07784400 | -5.10065500 | -4.20120600 |
| H | 7.18587400 | -5.58626500 | -4.58512900 |
| C | 9.35131900 | -5.60879100 | -4.47617800 |
| H | 9.45402100 | -6.51512500 | -5.06440300 |
| C | 10.49722300 | -4.93963000 | -4.02484800 |
| H | 11.47730300 | -5.32863400 | -4.27642800 |
| C | 10.38814900 | -3.77226500 | -3.26566500 |
| H | 11.27724300 | -3.25043400 | -2.92320000 |
| C | 9.11241000 | -3.29766000 | -2.94963000 |
| C | 8.68373800 | -2.13383800 | -2.15501900 |
| C | 9.46462100 | -1.22340000 | -1.44336200 |
| H | 10.54499800 | -1.32912000 | -1.41723300 |
| C | 8.82577800 | -0.18101200 | -0.76985400 |
| H | 9.40270100 | 0.53801100 | -0.19653700 |
| C | 7.43720300 | -0.05380400 | -0.83356000 |
| H | 6.94732400 | 0.76570400 | -0.31587300 |
| C | 6.63652000 | -0.97069000 | -1.54501900 |
| C | 7.27637400 | -2.03413100 | -2.19846000 |

| | | | |
|---|-------------|-------------|-------------|
| C | 5.72399400 | -4.07854200 | -2.31546300 |
| C | 6.16423600 | -4.67705700 | -1.13041600 |
| H | 7.19512200 | -4.51119400 | -0.82950300 |
| C | 5.31758800 | -5.44869400 | -0.34222500 |
| H | 5.67590800 | -5.90554000 | 0.57370200 |
| C | 3.99587600 | -5.62312300 | -0.76125000 |
| H | 3.31419600 | -6.23668100 | -0.18854200 |
| C | 3.53278700 | -5.04187400 | -1.93238300 |
| H | 2.49977400 | -5.17841600 | -2.22577700 |
| C | 4.39604400 | -4.27556800 | -2.74137600 |
| C | 4.75734200 | -2.96313400 | -4.75863600 |
| C | 4.29617000 | -2.54050700 | -6.02404700 |
| H | 3.28367100 | -2.77085700 | -6.33019400 |
| C | 5.13603600 | -1.84328500 | -6.87984700 |
| H | 4.76989700 | -1.52841800 | -7.84758800 |
| C | 6.44087100 | -1.53307900 | -6.49599500 |
| H | 7.10600200 | -1.02154000 | -7.17331100 |
| C | 6.88509900 | -1.92455200 | -5.24286800 |
| H | 7.89703400 | -1.69929100 | -4.92515200 |
| C | 6.07119000 | -2.64963000 | -4.36948000 |
| C | 2.57229300 | -3.96213200 | -4.32232800 |
| C | 2.26399300 | -5.10785100 | -5.06106200 |
| H | 3.06590700 | -5.77228000 | -5.36610000 |
| C | 0.93419300 | -5.37868500 | -5.38888100 |
| H | 0.69114800 | -6.26525400 | -5.96657600 |
| C | -0.08293000 | -4.51507300 | -4.96602400 |
| H | -1.11825300 | -4.73625700 | -5.20735500 |
| C | 0.23238600 | -3.36202500 | -4.24388200 |
| H | -0.55120500 | -2.69066000 | -3.90413400 |
| C | 1.56526900 | -3.07815300 | -3.93972300 |
| H | 1.83900300 | -2.17978100 | -3.40352300 |
| C | 5.16420200 | -0.70569100 | -1.59602800 |
| C | 4.23284900 | -1.62717800 | -1.09637700 |
| H | 4.54008300 | -2.56053700 | -0.64485900 |
| C | 2.87684600 | -1.32968800 | -1.20309500 |
| C | 2.40630300 | -0.10596500 | -1.71821400 |
| C | 3.37982300 | 0.82373800 | -2.12867000 |
| C | 4.74034000 | 0.53207300 | -2.10768600 |
| H | 5.45172500 | 1.25818400 | -2.48424700 |
| C | 0.66859700 | -2.17140400 | -1.00670200 |
| C | -0.05553700 | -3.32897100 | -0.69097800 |
| H | 0.48084800 | -4.18090300 | -0.28731400 |
| C | -1.41972800 | -3.36450200 | -0.91595900 |
| H | -1.95788300 | -4.27406100 | -0.67586500 |
| C | -2.10961500 | -2.25729900 | -1.45948000 |
| C | -1.36118700 | -1.12174800 | -1.74676200 |
| H | -1.85851900 | -0.26896700 | -2.18447900 |
| C | 0.03680100 | -1.02365600 | -1.53267800 |
| C | -3.60806200 | -2.35605700 | -1.78725200 |

| | | | |
|---|-------------|-------------|-------------|
| C | -3.75829200 | -3.07956000 | -3.14851300 |
| H | -3.25190200 | -2.51634000 | -3.93971100 |
| H | -4.81623500 | -3.17688500 | -3.41868800 |
| H | -3.31518800 | -4.08026200 | -3.10637000 |
| C | -4.35703100 | -3.16095300 | -0.69816000 |
| H | -4.12873500 | -4.22560600 | -0.76024800 |
| H | -5.43692300 | -3.04989200 | -0.81803600 |
| H | -4.09375600 | -2.81134500 | 0.30179800 |
| C | -4.27052800 | -0.96709800 | -1.89128700 |
| H | -4.12875400 | -0.39247200 | -0.97130700 |
| H | -5.34370500 | -1.09833100 | -2.05548900 |
| H | -3.87784100 | -0.38427700 | -2.73001000 |
| C | 0.61621000 | 1.60521100 | -2.35572900 |
| C | 1.71988700 | 2.44249200 | -2.62762600 |
| C | 1.54948000 | 3.78957000 | -2.97613400 |
| H | 2.42280800 | 4.40950700 | -3.12771700 |
| C | 0.27571600 | 4.30583300 | -3.09072700 |
| H | 0.16343100 | 5.35303800 | -3.33793400 |
| C | -0.87361600 | 3.51751000 | -2.86302800 |
| C | -0.67014900 | 2.19510000 | -2.48930500 |
| H | -1.52853300 | 1.58531300 | -2.24745600 |
| C | -2.26014500 | 4.15539300 | -3.04040500 |
| C | -2.52416900 | 4.37852400 | -4.54863700 |
| H | -1.73648700 | 4.99060900 | -4.99950000 |
| H | -3.48123600 | 4.89514800 | -4.68414600 |
| H | -2.56006100 | 3.42278500 | -5.08236800 |
| C | -2.30301200 | 5.52423600 | -2.31732000 |
| H | -1.95119900 | 5.41928700 | -1.28780800 |
| H | -3.32728900 | 5.91056400 | -2.30752000 |
| H | -1.67486000 | 6.26938100 | -2.81272100 |
| C | -3.38942700 | 3.27591000 | -2.46770700 |
| H | -3.46083600 | 2.31240500 | -2.98357400 |
| H | -4.34592700 | 3.79236200 | -2.58793700 |
| H | -3.24270500 | 3.09083500 | -1.40073800 |
| B | 0.93231500 | 0.18050300 | -1.87327000 |

QAC-BO (crystal), S₀

| | | | |
|---|-------------|-------------|-------------|
| C | -2.70131400 | 2.13401300 | 3.39315300 |
| B | -0.15868500 | 2.31211200 | 0.41958900 |
| O | 2.05052500 | 2.76792800 | -1.37486800 |
| N | 4.67215900 | 0.58649400 | 1.75227400 |
| O | -0.65845600 | -0.48975700 | 0.86435700 |
| C | -2.85775200 | 0.72896200 | 3.44508900 |
| H | -3.52097200 | 0.29049400 | 4.18225800 |
| C | -2.17195900 | -0.11605700 | 2.59000100 |
| H | -2.28285100 | -1.19392900 | 2.64578600 |
| C | -1.30307700 | 0.42802200 | 1.62998500 |
| C | 0.33244900 | -0.14420000 | 0.01204600 |
| C | 1.03905000 | -1.17428600 | -0.59734000 |

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|---|-------------|-------------|-------------|
| H | 0.81290300 | -2.20200300 | -0.35159600 |
| C | 2.13060400 | -0.86152300 | -1.41639900 |
| C | 2.47458500 | 0.47296600 | -1.67989400 |
| H | 3.33313800 | 0.72255100 | -2.29047300 |
| C | 1.70887100 | 1.48656600 | -1.09921000 |
| C | 0.63437600 | 1.20854400 | -0.23235400 |
| C | -0.66581000 | 7.47788900 | 0.39750200 |
| C | -1.13802000 | 1.82309400 | 1.49775000 |
| C | -1.84953700 | 2.63607500 | 2.41762200 |
| H | -1.69166600 | 3.70265000 | 2.36105600 |
| C | 0.20386000 | 3.71628400 | -0.08243900 |
| C | -0.45630600 | 4.92227700 | 0.26247800 |
| H | -1.35310000 | 4.83719100 | 0.85806000 |
| C | -0.00708300 | 6.18306800 | -0.10760200 |
| C | 1.13819200 | 6.23570600 | -0.93696100 |
| H | 1.52264500 | 7.19689700 | -1.26636100 |
| C | 1.79251400 | 5.08650700 | -1.34841600 |
| H | 2.66763800 | 5.13777100 | -1.98656100 |
| C | 1.32964600 | 3.82880900 | -0.92353200 |
| C | 2.97647600 | -2.00377600 | -1.90819700 |
| C | 2.64323900 | -2.73773400 | -3.05694900 |
| H | 1.76528900 | -2.44889500 | -3.62427000 |
| C | 3.42518600 | -3.82502600 | -3.47147100 |
| H | 3.14752100 | -4.39014200 | -4.35362200 |
| C | 4.55293700 | -4.21882200 | -2.75000800 |
| H | 5.15154600 | -5.06562100 | -3.07115300 |
| C | 4.88296100 | -3.50309900 | -1.60077100 |
| C | 5.99391700 | -3.67230100 | -0.64761700 |
| C | 7.02752900 | -4.60666100 | -0.60214200 |
| H | 7.12519400 | -5.37149500 | -1.36750100 |
| C | 7.91756900 | -4.55614000 | 0.47288000 |
| H | 8.70490700 | -5.29287100 | 0.53942100 |
| C | 7.79427300 | -3.58129900 | 1.47062100 |
| H | 8.49755300 | -3.56361700 | 2.29495700 |
| C | 6.77538600 | -2.62485500 | 1.40743400 |
| H | 6.67795600 | -1.85049900 | 2.16466500 |
| C | 5.88609700 | -2.68568300 | 0.34481700 |
| C | 4.72436000 | -1.73990800 | 0.03703100 |
| C | 4.10060700 | -2.41323700 | -1.18794900 |
| C | 3.74755300 | -1.59876200 | 1.19760200 |
| C | 2.82962000 | -2.61963700 | 1.46782400 |
| H | 2.88644900 | -3.53377300 | 0.88422400 |
| C | 1.82614800 | -2.45385100 | 2.41360800 |
| H | 1.10979800 | -3.24742100 | 2.59817500 |
| C | 1.72743000 | -1.23705500 | 3.09643400 |
| H | 0.90911100 | -1.07104400 | 3.78631600 |
| C | 2.66474000 | -0.23335600 | 2.88184600 |
| H | 2.60240400 | 0.70533600 | 3.42041700 |
| C | 3.71088700 | -0.42335200 | 1.95894400 |

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|---|-------------|-------------|-------------|
| C | 5.24663000 | 1.32618800 | 2.80686200 |
| C | 5.34031300 | 0.80814300 | 4.10913700 |
| H | 4.91773100 | -0.16524500 | 4.33177800 |
| C | 5.98792900 | 1.53645700 | 5.10611900 |
| H | 6.06680000 | 1.12831500 | 6.10717100 |
| C | 6.55715300 | 2.77528400 | 4.81629800 |
| H | 7.06125900 | 3.34569600 | 5.58968300 |
| C | 6.47077600 | 3.27802100 | 3.51782800 |
| H | 6.90010800 | 4.24503700 | 3.30181100 |
| C | 5.81696700 | 2.57891500 | 2.49997000 |
| C | 5.65680500 | 3.11562000 | 1.07311500 |
| C | 5.83630300 | 1.94086100 | 0.11158200 |
| C | 6.42058800 | 2.05853600 | -1.14825600 |
| H | 6.85553500 | 3.00184800 | -1.45465800 |
| C | 6.41375900 | 0.98184900 | -2.04032500 |
| H | 6.80889100 | 1.08253800 | -3.04383600 |
| C | 5.85091100 | -0.22403800 | -1.65689700 |
| H | 5.81824900 | -1.05206700 | -2.35118300 |
| C | 5.29285400 | -0.38282700 | -0.38710900 |
| C | 5.27238400 | 0.70440100 | 0.48626900 |
| C | 6.63993000 | 4.25896500 | 0.77342600 |
| H | 6.44832500 | 4.66876400 | -0.22000600 |
| H | 7.67878100 | 3.91991000 | 0.82617000 |
| H | 6.50013900 | 5.07064700 | 1.48807300 |
| C | 4.20835000 | 3.65011500 | 0.87921100 |
| H | 4.03600400 | 4.50664900 | 1.53799700 |
| H | 3.46524100 | 2.87471100 | 1.09313300 |
| H | 4.07010800 | 3.96459900 | -0.15897600 |
| C | 0.37724400 | 8.30909800 | 1.18387400 |
| H | 1.21633600 | 8.59888900 | 0.54735900 |
| H | 0.76851900 | 7.73702200 | 2.02937100 |
| H | -0.08418000 | 9.22491600 | 1.57028200 |
| C | -1.19250200 | 8.31967900 | -0.78570900 |
| H | -1.95270200 | 7.75770900 | -1.33540200 |
| H | -0.38827300 | 8.59564400 | -1.47485800 |
| H | -1.65156900 | 9.24262700 | -0.41354700 |
| C | -1.85052400 | 7.19077100 | 1.33979500 |
| H | -2.24942300 | 8.14384200 | 1.69498600 |
| H | -1.54069300 | 6.60496700 | 2.21198700 |
| H | -2.65851700 | 6.65756200 | 0.82756400 |
| C | -3.14934200 | 4.52757500 | 4.18384000 |
| H | -2.08536700 | 4.73679700 | 4.34125200 |
| H | -3.71609100 | 5.11842300 | 4.91014300 |
| H | -3.42779500 | 4.87116000 | 3.18125500 |
| C | -3.08482400 | 2.65185300 | 5.83840500 |
| H | -3.39460900 | 1.63067600 | 6.07206900 |
| H | -3.59019000 | 3.31802300 | 6.54623900 |
| H | -2.00489900 | 2.73357800 | 5.99632800 |
| C | -4.98504500 | 2.81462200 | 4.19266700 |

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|---|-------------|------------|------------|
| H | -5.28761600 | 3.13206800 | 3.19300500 |
| H | -5.55215900 | 3.39776800 | 4.92418300 |
| H | -5.26334600 | 1.76340700 | 4.31500200 |
| C | -3.46461500 | 3.02963300 | 4.38618800 |

AC-BO (thin film), S₀

| | | | |
|---|-------------|-------------|-------------|
| C | 10.96306300 | 6.55597900 | -3.54598800 |
| C | 10.29620700 | 7.78032700 | -3.42518200 |
| C | 10.07159800 | 8.57920300 | -4.54516000 |
| C | 10.48631800 | 8.16733600 | -5.81471400 |
| C | 11.13027500 | 6.93818600 | -5.93798000 |
| C | 11.37197200 | 6.14130300 | -4.81029200 |
| C | 11.57129900 | 6.20102500 | -7.13510800 |
| C | 12.00532400 | 4.92674700 | -6.73430900 |
| C | 12.05781900 | 4.81864500 | -5.20464800 |
| C | 11.55305300 | 6.55493100 | -8.48516100 |
| C | 11.91894200 | 5.59268900 | -9.43116100 |
| C | 12.28669900 | 4.30150500 | -9.03077600 |
| C | 12.34144900 | 3.96475900 | -7.67253900 |
| C | 13.51661600 | 4.84085900 | -4.72894000 |
| C | 14.02580700 | 3.86485900 | -3.85740700 |
| N | 13.25610700 | 2.76165600 | -3.46335200 |
| C | 11.89023600 | 2.67967200 | -3.78061300 |
| C | 11.29537800 | 3.62205100 | -4.64283200 |
| C | 11.07270200 | 1.66450200 | -3.23373200 |
| C | 9.71426800 | 1.60899600 | -3.51784100 |
| C | 9.12609200 | 2.53966900 | -4.37806500 |
| C | 9.92888500 | 3.52823700 | -4.93328700 |
| C | 14.32194700 | 5.93191700 | -5.08000100 |
| C | 15.60174300 | 6.09553100 | -4.56539000 |
| C | 16.08612100 | 5.14894400 | -3.65715900 |
| C | 15.31213200 | 4.05263900 | -3.30578200 |
| C | 13.92256200 | 1.67849600 | -2.80881100 |
| C | 13.61892400 | 1.34964600 | -1.48849200 |
| C | 14.27145000 | 0.29304100 | -0.85381800 |
| C | 15.24808300 | -0.43515200 | -1.53578000 |
| C | 15.57508800 | -0.08874700 | -2.85151100 |
| C | 14.91979800 | 0.96658300 | -3.48456200 |
| C | 11.21911000 | 5.71183400 | -2.35106800 |
| C | 12.52063600 | 5.64461600 | -1.84827700 |
| C | 12.76895200 | 4.78652500 | -0.78667700 |
| C | 11.76018800 | 4.00005900 | -0.20640000 |
| C | 10.47488500 | 4.08069600 | -0.77324800 |
| C | 10.17643900 | 4.95081900 | -1.81121700 |
| B | 12.07470000 | 3.02687900 | 0.90676300 |
| C | 11.03466100 | 1.88737600 | 0.97668400 |
| C | 9.82014200 | 2.09452200 | 0.27660000 |

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|---|-------------|-------------|--------------|
| O | 9.49385100 | 3.26294300 | -0.33535300 |
| O | 14.04296300 | 4.68742400 | -0.35852500 |
| C | 14.32909300 | 4.13330500 | 0.84701100 |
| C | 13.43469500 | 3.31287700 | 1.57785000 |
| C | 11.29005400 | 0.56255300 | 1.40218300 |
| C | 10.42645500 | -0.50873500 | 1.13463400 |
| C | 9.19335700 | -0.20856700 | 0.52613200 |
| C | 8.88001100 | 1.07821200 | 0.11393200 |
| C | 15.59004100 | 4.47158400 | 1.33960500 |
| C | 15.92082300 | 4.14093900 | 2.64256200 |
| C | 15.02235500 | 3.44902400 | 3.47704700 |
| C | 13.83097400 | 2.99202700 | 2.89945000 |
| C | 10.82924500 | -1.95933400 | 1.45793400 |
| C | 10.80113400 | -2.16471600 | 2.98436600 |
| C | 12.25866200 | -2.22149300 | 0.93108800 |
| C | 9.88603900 | -2.99646000 | 0.81389600 |
| C | 15.27799800 | 3.34969800 | 4.99144000 |
| C | 16.73411000 | 3.69261500 | 5.37326000 |
| C | 14.98039300 | 1.93737700 | 5.51984200 |
| C | 14.33946400 | 4.36656500 | 5.68793400 |
| H | 9.95901200 | 8.10299400 | -2.44498300 |
| H | 9.56331400 | 9.52204700 | -4.40275700 |
| H | 10.28292400 | 8.76295500 | -6.69706900 |
| H | 11.23666500 | 7.54752200 | -8.79376800 |
| H | 11.90017400 | 5.84165300 | -10.48747700 |
| H | 12.53013300 | 3.55678800 | -9.78163400 |
| H | 12.62020500 | 2.97002500 | -7.34428200 |
| H | 11.49318600 | 0.91634700 | -2.57694400 |
| H | 9.11631700 | 0.82562700 | -3.06259200 |
| H | 8.06812600 | 2.49229500 | -4.60872300 |
| H | 9.49660600 | 4.27218800 | -5.59783600 |
| H | 13.91493200 | 6.67473000 | -5.75868400 |
| H | 16.20363200 | 6.95090200 | -4.85209200 |
| H | 17.06810200 | 5.26821900 | -3.21060000 |
| H | 15.68560400 | 3.34660700 | -2.57616900 |
| H | 12.85372100 | 1.91193900 | -0.97825400 |
| H | 14.01535100 | 0.05476000 | 0.17320100 |
| H | 15.75844100 | -1.25781400 | -1.04556600 |
| H | 16.34170400 | -0.64022200 | -3.38688400 |
| H | 15.19794300 | 1.27570600 | -4.48642600 |
| H | 13.33145500 | 6.21092000 | -2.29182800 |
| H | 9.19252200 | 4.94423800 | -2.26480400 |
| H | 12.23747100 | 0.37831000 | 1.90370600 |
| H | 8.47553600 | -0.99375000 | 0.32545400 |
| H | 7.95496500 | 1.30496500 | -0.40545600 |
| H | 16.25397400 | 5.05610100 | 0.71254800 |
| H | 16.87953600 | 4.46921800 | 3.02369600 |
| H | 13.12908600 | 2.42520700 | 3.50132000 |
| H | 11.40389500 | -1.39682200 | 3.47431500 |

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|---|-------------|-------------|-------------|
| H | 9.77593200 | -2.08506800 | 3.36033900 |
| H | 11.19555700 | -3.15022000 | 3.25557400 |
| H | 12.32763800 | -2.01325700 | -0.14139100 |
| H | 12.97941700 | -1.58365600 | 1.44486300 |
| H | 12.54272800 | -3.26370000 | 1.11135900 |
| H | 9.86982600 | -2.90270000 | -0.27692000 |
| H | 10.23685600 | -4.00031600 | 1.06984400 |
| H | 8.86339900 | -2.90290900 | 1.19049700 |
| H | 16.98367100 | 4.73243600 | 5.14292100 |
| H | 16.86483100 | 3.55487600 | 6.45122900 |
| H | 17.44440600 | 3.03724800 | 4.85761500 |
| H | 13.94391800 | 1.65122600 | 5.33632700 |
| H | 15.63160900 | 1.20142300 | 5.03672000 |
| H | 15.14998900 | 1.89932500 | 6.60066700 |
| H | 14.45541100 | 4.31044400 | 6.77642100 |
| H | 14.57074700 | 5.38621000 | 5.36277400 |
| H | 13.29511000 | 4.16549900 | 5.43527100 |

AC-BO (thin film), S₁

| | | | |
|---|-------------|-------------|-------------|
| C | 10.93745800 | 6.54888800 | -3.53864500 |
| C | 10.26429900 | 7.77504900 | -3.44330200 |
| C | 10.05469700 | 8.57168800 | -4.56821500 |
| C | 10.48589900 | 8.16294200 | -5.83404500 |
| C | 11.12644300 | 6.93077500 | -5.94526900 |
| C | 11.34804000 | 6.14395100 | -4.80736000 |
| C | 11.56054800 | 6.17895400 | -7.13473800 |
| C | 11.97294700 | 4.89879200 | -6.72909800 |
| C | 12.01673000 | 4.80383800 | -5.19440800 |
| C | 11.55057800 | 6.51915500 | -8.48804200 |
| C | 11.90056000 | 5.54247500 | -9.42598000 |
| C | 12.24624900 | 4.24871800 | -9.01789500 |
| C | 12.29536900 | 3.92229700 | -7.65623600 |
| C | 13.46135600 | 4.81065300 | -4.71362300 |
| C | 13.94134800 | 3.84190900 | -3.80205900 |
| N | 13.15050600 | 2.76413900 | -3.42804900 |
| C | 11.80462700 | 2.68586400 | -3.74739500 |
| C | 11.22838500 | 3.63760200 | -4.63299200 |
| C | 10.98609800 | 1.65877100 | -3.20042800 |
| C | 9.64220600 | 1.60505800 | -3.51092500 |
| C | 9.08390300 | 2.52524300 | -4.40950300 |
| C | 9.88176200 | 3.52155700 | -4.96690400 |
| C | 14.30909100 | 5.85019900 | -5.09184400 |
| C | 15.58274700 | 5.97890500 | -4.54482100 |
| C | 16.02221000 | 5.06624800 | -3.57433300 |
| C | 15.21778100 | 4.00810400 | -3.20283600 |
| C | 13.80870700 | 1.67209900 | -2.75384300 |
| C | 13.48245100 | 1.34540600 | -1.44169200 |
| C | 14.14937600 | 0.29124000 | -0.81958400 |
| C | 15.12273300 | -0.43308500 | -1.50963600 |

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|---|-------------|-------------|--------------|
| C | 15.45590600 | -0.08342000 | -2.82366700 |
| C | 14.81203200 | 0.98325100 | -3.44496200 |
| C | 11.19289200 | 5.70763800 | -2.34686100 |
| C | 12.49537100 | 5.62523400 | -1.83249000 |
| C | 12.74562000 | 4.75906200 | -0.77962000 |
| C | 11.73572400 | 3.99927500 | -0.16065000 |
| C | 10.45028000 | 4.09137500 | -0.73340400 |
| C | 10.15641500 | 4.93346700 | -1.79336300 |
| B | 12.04536500 | 3.03089300 | 0.96556100 |
| C | 11.03903300 | 1.86478100 | 0.97451200 |
| C | 9.82653800 | 2.06176900 | 0.24527800 |
| O | 9.45972800 | 3.29206000 | -0.25074000 |
| O | 14.04305300 | 4.58839700 | -0.40504500 |
| C | 14.32570800 | 4.12527500 | 0.86250200 |
| C | 13.42298300 | 3.31645200 | 1.60892900 |
| C | 11.27659300 | 0.52286000 | 1.37457000 |
| C | 10.42823600 | -0.55449300 | 1.05424200 |
| C | 9.24049000 | -0.27665400 | 0.36388800 |
| C | 8.94270100 | 1.03423500 | -0.03232700 |
| C | 15.56268300 | 4.51589400 | 1.34843400 |
| C | 15.92585500 | 4.20476100 | 2.66148900 |
| C | 15.04706900 | 3.49835200 | 3.49147900 |
| C | 13.84445800 | 3.02925100 | 2.93048700 |
| C | 10.81416800 | -1.99774800 | 1.43367100 |
| C | 10.78805700 | -2.14611800 | 2.96761400 |
| C | 12.23814000 | -2.30522600 | 0.91559500 |
| C | 9.85614600 | -3.05093300 | 0.83953200 |
| C | 15.31191000 | 3.38888600 | 5.00419700 |
| C | 16.76641100 | 3.74236500 | 5.38176700 |
| C | 15.03026400 | 1.96872300 | 5.52326200 |
| C | 14.36800500 | 4.38762800 | 5.71895800 |
| H | 9.91774300 | 8.10176400 | -2.46805300 |
| H | 9.54707900 | 9.51630000 | -4.43328000 |
| H | 10.29564200 | 8.75916800 | -6.71903400 |
| H | 11.24945200 | 7.51347000 | -8.80516300 |
| H | 11.88477900 | 5.78360000 | -10.48402600 |
| H | 12.47554900 | 3.49339100 | -9.76215700 |
| H | 12.55715200 | 2.92409100 | -7.32466200 |
| H | 11.39421400 | 0.92808800 | -2.51848100 |
| H | 9.02722600 | 0.84494500 | -3.04334300 |
| H | 8.03200500 | 2.46652300 | -4.66413100 |
| H | 9.45584500 | 4.24887800 | -5.65152700 |
| H | 13.94496100 | 6.58525700 | -5.80131200 |
| H | 16.21802500 | 6.80522900 | -4.84528700 |
| H | 16.98518600 | 5.19718700 | -3.09442800 |
| H | 15.53068300 | 3.34303600 | -2.41140900 |
| H | 12.73630000 | 1.91305400 | -0.90327900 |
| H | 13.89650900 | 0.05702300 | 0.20758800 |
| H | 15.63171000 | -1.25844200 | -1.02286700 |

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|---|-------------|-------------|-------------|
| H | 16.22136000 | -0.63226900 | -3.36240400 |
| H | 15.09278000 | 1.30401200 | -4.44208000 |
| H | 13.31114000 | 6.19124800 | -2.26889500 |
| H | 9.16288300 | 4.93342200 | -2.22753300 |
| H | 12.19456300 | 0.33397300 | 1.92741900 |
| H | 8.54255400 | -1.06261100 | 0.10853200 |
| H | 8.03336600 | 1.27036400 | -0.57642800 |
| H | 16.20788500 | 5.11178900 | 0.71179500 |
| H | 16.87748900 | 4.56198600 | 3.03288700 |
| H | 13.14965800 | 2.47977100 | 3.55546600 |
| H | 11.40174100 | -1.37152400 | 3.43265300 |
| H | 9.76418500 | -2.03364100 | 3.33875100 |
| H | 11.16462600 | -3.12846800 | 3.27533700 |
| H | 12.30213500 | -2.14129300 | -0.16535900 |
| H | 12.96922700 | -1.65666000 | 1.40073500 |
| H | 12.50840600 | -3.34440500 | 1.13484800 |
| H | 9.86120400 | -3.02702700 | -0.25529700 |
| H | 10.17145100 | -4.04637200 | 1.16702300 |
| H | 8.83056200 | -2.89770600 | 1.18707500 |
| H | 17.00344400 | 4.78549900 | 5.15341000 |
| H | 16.90614200 | 3.59967300 | 6.45843300 |
| H | 17.47856300 | 3.09793300 | 4.85497200 |
| H | 13.99299600 | 1.67944200 | 5.34814600 |
| H | 15.67833200 | 1.24141900 | 5.02268600 |
| H | 15.21470100 | 1.91971300 | 6.60177600 |
| H | 14.48813400 | 4.32043400 | 6.80693600 |
| H | 14.58873700 | 5.41234800 | 5.40255400 |
| H | 13.32538400 | 4.17958500 | 5.46556400 |

AC-BO (thin film), T₁

| | | | |
|---|-------------|------------|-------------|
| C | 10.91909000 | 6.56538600 | -3.55600000 |
| C | 10.26318300 | 7.79697200 | -3.44338300 |
| C | 10.04777600 | 8.59072700 | -4.56850500 |
| C | 10.46367900 | 8.17099800 | -5.83561300 |
| C | 11.09867000 | 6.93674600 | -5.95211900 |
| C | 11.32408100 | 6.14452200 | -4.81866700 |
| C | 11.54973400 | 6.19078600 | -7.13981600 |
| C | 11.97997800 | 4.91862100 | -6.72656200 |
| C | 12.01373500 | 4.82073800 | -5.19546100 |
| C | 11.54437700 | 6.53578700 | -8.49214400 |
| C | 11.91732700 | 5.56671500 | -9.42828800 |
| C | 12.28126000 | 4.27841700 | -9.01610900 |
| C | 12.32588000 | 3.95070400 | -7.65510200 |
| C | 13.46341200 | 4.85709900 | -4.69352100 |
| C | 13.94319700 | 3.92693100 | -3.75987800 |
| N | 13.14875700 | 2.85939500 | -3.31057200 |
| C | 11.80798200 | 2.74095800 | -3.69018600 |
| C | 11.24251100 | 3.63128900 | -4.63081500 |
| C | 10.97797900 | 1.74751400 | -3.11786200 |

| | | | |
|---|-------------|-------------|--------------|
| C | 9.64456900 | 1.63561200 | -3.48795700 |
| C | 9.09490600 | 2.49233000 | -4.44583000 |
| C | 9.90084300 | 3.48039400 | -5.00121200 |
| C | 14.28911500 | 5.92154300 | -5.07824500 |
| C | 15.56014200 | 6.09294500 | -4.54307200 |
| C | 16.01802400 | 5.18408800 | -3.58342600 |
| C | 15.22242800 | 4.11614500 | -3.19471200 |
| C | 13.82749900 | 1.74386300 | -2.71020600 |
| C | 13.58971200 | 1.39092600 | -1.38551700 |
| C | 14.24609600 | 0.29360700 | -0.82519200 |
| C | 15.15410000 | -0.44380700 | -1.58594300 |
| C | 15.41778500 | -0.06622600 | -2.90798900 |
| C | 14.76247300 | 1.02897900 | -3.46730300 |
| C | 11.17570200 | 5.72247900 | -2.36450500 |
| C | 12.44240600 | 5.67761500 | -1.79312100 |
| C | 12.68174300 | 4.81622300 | -0.70044500 |
| C | 11.69639400 | 3.99663300 | -0.11784700 |
| C | 10.45783900 | 4.02506900 | -0.76933100 |
| C | 10.17142100 | 4.87429900 | -1.85787500 |
| B | 12.00330300 | 3.03724300 | 1.00894200 |
| C | 11.02350300 | 1.84741600 | 0.98697300 |
| C | 9.82692000 | 2.00099200 | 0.21883900 |
| O | 9.49074500 | 3.17732400 | -0.40732600 |
| O | 13.93614700 | 4.77943200 | -0.25793000 |
| C | 14.25941000 | 4.19930100 | 0.94589000 |
| C | 13.37550200 | 3.34312600 | 1.66607100 |
| C | 11.26629300 | 0.51776300 | 1.41372900 |
| C | 10.43199400 | -0.57267300 | 1.09546300 |
| C | 9.23456400 | -0.32016700 | 0.40594500 |
| C | 8.93135400 | 0.97075800 | -0.02401700 |
| C | 15.51383400 | 4.57427800 | 1.40583600 |
| C | 15.90568100 | 4.21967600 | 2.69471500 |
| C | 15.04121100 | 3.48462300 | 3.51635500 |
| C | 13.83115400 | 3.01230300 | 2.96142000 |
| C | 10.84836800 | -2.00963300 | 1.45731500 |
| C | 10.82305700 | -2.17605000 | 2.98881500 |
| C | 12.28033400 | -2.26622100 | 0.93363100 |
| C | 9.91939100 | -3.07918200 | 0.84717900 |
| C | 15.33187800 | 3.34578500 | 5.01968700 |
| C | 16.79520500 | 3.68175500 | 5.37882900 |
| C | 15.04350700 | 1.92231200 | 5.52267600 |
| C | 14.40492700 | 4.34431900 | 5.75868000 |
| H | 9.93025500 | 8.13170800 | -2.46577900 |
| H | 9.54938300 | 9.53893600 | -4.43009700 |
| H | 10.27011500 | 8.76632900 | -6.72024700 |
| H | 11.23158900 | 7.52652100 | -8.81003500 |
| H | 11.90710200 | 5.80817400 | -10.48641200 |
| H | 12.52916400 | 3.52856800 | -9.76016400 |
| H | 12.60414000 | 2.95821200 | -7.31955900 |

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|---|-------------|-------------|-------------|
| H | 11.37018400 | 1.06726600 | -2.37391100 |
| H | 9.03594900 | 0.87164800 | -3.01498100 |
| H | 8.05802200 | 2.39398700 | -4.74568300 |
| H | 9.49151800 | 4.17396300 | -5.73135900 |
| H | 13.90875300 | 6.63547700 | -5.80183700 |
| H | 16.17829000 | 6.92682600 | -4.85724000 |
| H | 16.99482100 | 5.31109700 | -3.12809600 |
| H | 15.56915500 | 3.43386200 | -2.42923800 |
| H | 12.88860500 | 1.96349500 | -0.79598000 |
| H | 14.04096300 | 0.03312100 | 0.20763200 |
| H | 15.66341500 | -1.29822100 | -1.15205300 |
| H | 16.13459500 | -0.62291000 | -3.50358500 |
| H | 14.99148700 | 1.36445300 | -4.47307200 |
| H | 13.27017200 | 6.24893700 | -2.20227600 |
| H | 9.20002200 | 4.80501900 | -2.33812600 |
| H | 12.18433600 | 0.34153700 | 1.96919400 |
| H | 8.54884000 | -1.11996700 | 0.16243900 |
| H | 8.03805300 | 1.18800500 | -0.60061800 |
| H | 16.13774900 | 5.19270300 | 0.76979400 |
| H | 16.86398200 | 4.56408600 | 3.05928800 |
| H | 13.16710900 | 2.42068600 | 3.57933300 |
| H | 11.41120900 | -1.38765200 | 3.46235800 |
| H | 9.79561600 | -2.10467000 | 3.36021600 |
| H | 11.23264700 | -3.14877000 | 3.28302900 |
| H | 12.34137300 | -2.08530500 | -0.14442000 |
| H | 12.99066800 | -1.60145800 | 1.42640100 |
| H | 12.57959100 | -3.29953000 | 1.14033100 |
| H | 9.91775900 | -3.03585900 | -0.24674900 |
| H | 10.27235300 | -4.06795700 | 1.15430300 |
| H | 8.89170500 | -2.97307600 | 1.20582800 |
| H | 17.03762200 | 4.72728000 | 5.16849400 |
| H | 16.94996600 | 3.51729500 | 6.44992500 |
| H | 17.49398500 | 3.04137200 | 4.82989100 |
| H | 13.99885500 | 1.64843500 | 5.36910500 |
| H | 15.67204900 | 1.19392100 | 4.99964500 |
| H | 15.25143200 | 1.85887300 | 6.59558800 |
| H | 14.54166500 | 4.25971800 | 6.84303200 |
| H | 14.62985600 | 5.37179200 | 5.45474500 |
| H | 13.35711300 | 4.14650800 | 5.51926100 |

QAC-BO (thin film), S₀

| | | | |
|---|------------|------------|------------|
| C | 1.58918200 | 7.39231800 | 3.04712800 |
| C | 2.47543000 | 8.40042100 | 2.62442500 |
| C | 3.45095800 | 8.92092900 | 3.47401400 |
| C | 3.44649500 | 8.50014000 | 4.80586700 |
| C | 2.48624400 | 7.60662200 | 5.29976400 |
| C | 1.61713300 | 7.01259900 | 4.39984200 |
| B | 0.70927300 | 6.67527100 | 2.06648200 |
| C | 0.69764800 | 7.30464600 | 0.67589200 |

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|---|-------------|-------------|-------------|
| C | 1.58642200 | 8.37137000 | 0.42704600 |
| O | 2.44441900 | 8.86575200 | 1.35683200 |
| O | 0.81029200 | 6.03419500 | 4.86483800 |
| C | 0.11388500 | 5.22452400 | 4.03031100 |
| C | 0.01146300 | 5.43367000 | 2.63852800 |
| C | -0.08612700 | 6.87679000 | -0.40548000 |
| C | 0.02021900 | 7.38939500 | -1.69306000 |
| C | 0.93878800 | 8.43810200 | -1.89346400 |
| C | 1.68938600 | 8.95014600 | -0.84109900 |
| C | -0.49785500 | 4.12831500 | 4.65020000 |
| C | -1.21943300 | 3.22022600 | 3.88818900 |
| C | -1.33335200 | 3.36379200 | 2.48963100 |
| C | -0.69989100 | 4.45801100 | 1.90863300 |
| C | -0.87523700 | 6.79831000 | -2.78921000 |
| C | -0.59391500 | 5.28136700 | -2.90025100 |
| C | -2.03290700 | 2.32205000 | 1.60393700 |
| C | -2.98418600 | 1.42956800 | 2.42527000 |
| C | 6.41430700 | 8.18123700 | 7.11334700 |
| C | 7.30219700 | 7.01342700 | 7.23677100 |
| C | 7.01952400 | 6.12722700 | 6.18754900 |
| C | 5.53883800 | 7.96740700 | 6.03660500 |
| C | 4.52078300 | 8.87996600 | 5.76435200 |
| C | 4.44365500 | 10.04814200 | 6.53161900 |
| C | 5.31390300 | 10.25364000 | 7.60557300 |
| C | 6.30185600 | 9.31719200 | 7.91275300 |
| C | 8.22190600 | 6.67440900 | 8.23009800 |
| C | 8.82690400 | 5.41642400 | 8.17492600 |
| C | 8.51873400 | 4.52134300 | 7.14200500 |
| C | 7.62183800 | 4.87801200 | 6.12894800 |
| C | -2.37014400 | 6.96992300 | -2.42424200 |
| C | -0.62381000 | 7.46805700 | -4.15151800 |
| C | -2.86671800 | 3.00498400 | 0.49482000 |
| C | -0.94135100 | 1.44824700 | 0.93969100 |
| C | 4.44503700 | 5.19217600 | 3.80834100 |
| C | 4.83583300 | 5.65682400 | 5.06952900 |
| C | 5.93303900 | 6.69571400 | 5.25719500 |
| C | 6.54042500 | 7.11081500 | 3.91017400 |
| C | 6.06353300 | 6.62034300 | 2.68003700 |
| N | 4.93851100 | 5.76493300 | 2.61806000 |
| C | 3.53908300 | 4.10455800 | 3.71810700 |
| C | 2.89941300 | 3.65419100 | 4.86785200 |
| C | 3.22643400 | 4.17305600 | 6.12303300 |
| C | 4.23129300 | 5.12128600 | 6.21192700 |
| C | 7.62414000 | 8.00269600 | 3.92642000 |
| C | 8.24997000 | 8.42516800 | 2.76355800 |
| C | 7.82071400 | 7.88907200 | 1.54775400 |
| C | 6.77427900 | 6.97813700 | 1.51161300 |
| C | 4.16937700 | 5.59227200 | 1.43280800 |
| C | 4.13443000 | 6.56013300 | 0.41573000 |

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|---|-------------|-------------|-------------|
| C | 3.45579000 | 6.31955400 | -0.77471800 |
| C | 2.69550800 | 5.16575300 | -0.93335200 |
| C | 2.62919900 | 4.25576800 | 0.11776800 |
| C | 3.38026900 | 4.43067200 | 1.28493400 |
| C | 3.44555200 | 3.37447200 | 2.38033500 |
| C | 4.77166800 | 2.57423900 | 2.19281500 |
| C | 2.27283700 | 2.38116100 | 2.33295700 |
| H | 4.19618600 | 9.61420500 | 3.10142000 |
| H | 2.50423000 | 7.28209600 | 6.33205600 |
| H | -0.81839200 | 6.10359300 | -0.21976700 |
| H | 1.06346700 | 8.88255000 | -2.87402300 |
| H | 2.39301800 | 9.76227800 | -0.99017500 |
| H | -0.38690100 | 4.00937400 | 5.72278200 |
| H | -1.68285200 | 2.38277800 | 4.39629400 |
| H | -0.70879200 | 4.54590600 | 0.83107500 |
| H | 0.41736500 | 5.09649800 | -3.27380600 |
| H | -0.69530400 | 4.78062000 | -1.93247400 |
| H | -1.31902500 | 4.82581500 | -3.58024500 |
| H | -3.71582000 | 2.03731700 | 2.96866500 |
| H | -2.43792600 | 0.81784500 | 3.14982000 |
| H | -3.52873000 | 0.75790500 | 1.75613000 |
| H | 3.65276200 | 10.76269000 | 6.32499600 |
| H | 5.17981300 | 11.12463700 | 8.23688400 |
| H | 6.95169200 | 9.45316700 | 8.77161100 |
| H | 8.43511000 | 7.35944700 | 9.04539500 |
| H | 9.52584500 | 5.11926300 | 8.95043700 |
| H | 8.95851900 | 3.53069300 | 7.14822700 |
| H | 7.36471600 | 4.18250700 | 5.33552200 |
| H | -2.97339600 | 6.36112100 | -3.10046000 |
| H | -2.69422600 | 8.00698200 | -2.52915900 |
| H | -2.58592800 | 6.63910300 | -1.40529400 |
| H | -0.82071400 | 8.54355100 | -4.10410000 |
| H | 0.40641800 | 7.31491400 | -4.48922900 |
| H | -1.29104800 | 7.04719900 | -4.90496700 |
| H | -2.23992100 | 3.57541800 | -0.19733200 |
| H | -3.60658900 | 3.68581900 | 0.92526300 |
| H | -3.39014200 | 2.24211500 | -0.09039300 |
| H | -0.28188200 | 2.06777300 | 0.32083500 |
| H | -0.32067800 | 0.96128300 | 1.69689500 |
| H | -1.39433600 | 0.67983800 | 0.30335200 |
| H | 2.14495400 | 2.88241900 | 4.79230200 |
| H | 2.72980500 | 3.80750800 | 7.01544000 |
| H | 4.55530300 | 5.49227700 | 7.17504200 |
| H | 7.96719800 | 8.37523600 | 4.88583000 |
| H | 9.06593300 | 9.13858900 | 2.80191700 |
| H | 8.30400000 | 8.17831200 | 0.62049300 |
| H | 6.49822000 | 6.54075400 | 0.56275900 |
| H | 4.61833600 | 7.51557300 | 0.55741100 |
| H | 3.47665400 | 7.06931600 | -1.55496300 |

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|---|------------|------------|-------------|
| H | 2.13105800 | 4.99759100 | -1.84257800 |
| H | 1.99787800 | 3.38122000 | 0.01650300 |
| H | 5.63511800 | 3.24578200 | 2.20117600 |
| H | 4.88344700 | 1.84513300 | 3.00226400 |
| H | 4.74981100 | 2.04761400 | 1.23267700 |
| H | 1.31483700 | 2.87990700 | 2.49216200 |
| H | 2.40832700 | 1.61890700 | 3.10024300 |
| H | 2.24573100 | 1.85845300 | 1.37390900 |

QAC-BO (thin film), S₁

| | | | |
|---|-------------|-------------|-------------|
| C | 1.62468000 | 7.34367600 | 3.06810900 |
| C | 2.47724500 | 8.39344300 | 2.67280400 |
| C | 3.45565000 | 8.92054500 | 3.51379400 |
| C | 3.52703200 | 8.44662000 | 4.83174900 |
| C | 2.61202000 | 7.48598400 | 5.29831100 |
| C | 1.71489200 | 6.92019700 | 4.40837700 |
| B | 0.70324600 | 6.66098800 | 2.09683000 |
| C | 0.68622300 | 7.29577700 | 0.71388000 |
| C | 1.55035900 | 8.39536500 | 0.46375700 |
| O | 2.41528100 | 8.89404200 | 1.40721700 |
| O | 0.92288200 | 5.92141900 | 4.87814800 |
| C | 0.18749000 | 5.12826600 | 4.03609200 |
| C | 0.03090700 | 5.40590500 | 2.65024300 |
| C | -0.07622000 | 6.86601400 | -0.38913700 |
| C | 0.04195200 | 7.38715100 | -1.68208200 |
| C | 0.93729200 | 8.44515600 | -1.87992500 |
| C | 1.65562700 | 8.97597200 | -0.79131300 |
| C | -0.38911500 | 4.01771000 | 4.63851100 |
| C | -1.15141900 | 3.11517100 | 3.87953700 |
| C | -1.31975800 | 3.31859100 | 2.50256500 |
| C | -0.71678000 | 4.44369100 | 1.92798600 |
| C | -0.84223500 | 6.78456200 | -2.78246100 |
| C | -0.55960700 | 5.26706700 | -2.88593000 |
| C | -2.04837100 | 2.30543600 | 1.60613700 |
| C | -3.00020900 | 1.41113400 | 2.42467700 |
| C | 6.47444700 | 8.15991000 | 7.18548900 |
| C | 7.36763300 | 6.99971000 | 7.33364800 |
| C | 7.10494600 | 6.09489800 | 6.29472100 |
| C | 5.60446600 | 7.93163100 | 6.10807400 |
| C | 4.59134800 | 8.83785200 | 5.79071500 |
| C | 4.52131600 | 10.02156600 | 6.53794500 |
| C | 5.37327800 | 10.24099900 | 7.62333100 |
| C | 6.35671700 | 9.31028500 | 7.96255500 |
| C | 8.28778400 | 6.68309200 | 8.33342300 |
| C | 8.91203000 | 5.43365900 | 8.29439300 |
| C | 8.62486100 | 4.52260900 | 7.27055200 |
| C | 7.72600200 | 4.85448600 | 6.24986400 |
| C | -2.34091700 | 6.95310700 | -2.42982000 |
| C | -0.58870500 | 7.44706200 | -4.14781500 |

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|---|-------------|-------------|-------------|
| C | -2.88947300 | 3.01041000 | 0.51651100 |
| C | -0.97766800 | 1.42844400 | 0.91244600 |
| C | 4.51959800 | 5.17988900 | 3.87173600 |
| C | 4.94633600 | 5.59667100 | 5.14841900 |
| C | 6.01975600 | 6.64908300 | 5.34936800 |
| C | 6.64513900 | 7.06659100 | 4.02104500 |
| C | 6.14264300 | 6.62713800 | 2.78012000 |
| N | 4.97850500 | 5.82590800 | 2.71784600 |
| C | 3.59058300 | 4.11007800 | 3.73849300 |
| C | 2.97860300 | 3.61373300 | 4.87627600 |
| C | 3.34613500 | 4.07514500 | 6.14410500 |
| C | 4.36217400 | 5.01026500 | 6.26870000 |
| C | 7.74778700 | 7.92779200 | 4.03916900 |
| C | 8.36694700 | 8.34854600 | 2.86974200 |
| C | 7.91970500 | 7.84701300 | 1.64404700 |
| C | 6.84849900 | 6.97065400 | 1.60089100 |
| C | 4.23358800 | 5.70258600 | 1.53089300 |
| C | 4.24298900 | 6.72713500 | 0.55602700 |
| C | 3.59692900 | 6.54474000 | -0.65101100 |
| C | 2.82086800 | 5.40261500 | -0.86359400 |
| C | 2.71327200 | 4.43926500 | 0.13973600 |
| C | 3.42365000 | 4.55351100 | 1.32966200 |
| C | 3.44753900 | 3.45384000 | 2.37458500 |
| C | 4.75038800 | 2.61516800 | 2.13725500 |
| C | 2.24606300 | 2.49660200 | 2.28980600 |
| H | 4.14208300 | 9.67596900 | 3.14587200 |
| H | 2.64422200 | 7.13814600 | 6.32299200 |
| H | -0.80210900 | 6.08404500 | -0.21815000 |
| H | 1.06712600 | 8.89999100 | -2.85417600 |
| H | 2.34305100 | 9.80518900 | -0.92612000 |
| H | -0.24362100 | 3.87146300 | 5.70427800 |
| H | -1.59721200 | 2.26724600 | 4.38382400 |
| H | -0.79542600 | 4.57729800 | 0.85921400 |
| H | 0.45470900 | 5.08077100 | -3.25463800 |
| H | -0.66804300 | 4.77404800 | -1.91534500 |
| H | -1.27936400 | 4.80538000 | -3.56813600 |
| H | -3.71658700 | 2.02266400 | 2.98329700 |
| H | -2.45198900 | 0.78967400 | 3.13894100 |
| H | -3.55874500 | 0.75100600 | 1.75497600 |
| H | 3.73506200 | 10.73393000 | 6.30788600 |
| H | 5.22767200 | 11.11984000 | 8.24122200 |
| H | 6.99430100 | 9.45980500 | 8.82821800 |
| H | 8.48756400 | 7.38046900 | 9.14131000 |
| H | 9.61191600 | 5.15625400 | 9.07624700 |
| H | 9.08395400 | 3.54095400 | 7.28814300 |
| H | 7.48852500 | 4.14476500 | 5.46296100 |
| H | -2.94121000 | 6.34723700 | -3.11267900 |
| H | -2.66130700 | 7.99161400 | -2.53318100 |
| H | -2.56150400 | 6.62183300 | -1.41244100 |

| | | | |
|---|-------------|------------|-------------|
| H | -0.78721800 | 8.52211400 | -4.10309800 |
| H | 0.44418200 | 7.29735700 | -4.47933800 |
| H | -1.25377200 | 7.02225400 | -4.90166500 |
| H | -2.26619800 | 3.57043800 | -0.18656800 |
| H | -3.60210900 | 3.70727000 | 0.96586800 |
| H | -3.44299900 | 2.26189200 | -0.06000700 |
| H | -0.32834200 | 2.05302400 | 0.28816800 |
| H | -0.34788700 | 0.93054600 | 1.65577600 |
| H | -1.44505500 | 0.66909100 | 0.27493000 |
| H | 2.19590900 | 2.87439700 | 4.78289500 |
| H | 2.85148600 | 3.68479000 | 7.02685400 |
| H | 4.69318100 | 5.33846000 | 7.24241600 |
| H | 8.10990200 | 8.28132000 | 4.99781500 |
| H | 9.20297800 | 9.03836100 | 2.91107200 |
| H | 8.41149600 | 8.13589800 | 0.72241900 |
| H | 6.55550900 | 6.54333000 | 0.65284300 |
| H | 4.69092000 | 7.68394900 | 0.78190600 |
| H | 3.60272400 | 7.33642100 | -1.38689800 |
| H | 2.23898700 | 5.30890500 | -1.77307600 |
| H | 2.05395000 | 3.59411200 | -0.00951500 |
| H | 5.64418800 | 3.24559400 | 2.16681400 |
| H | 4.83560000 | 1.84529000 | 2.91030300 |
| H | 4.69504100 | 2.13604200 | 1.15489300 |
| H | 1.30334900 | 3.01191200 | 2.47450300 |
| H | 2.36784200 | 1.69003900 | 3.01435100 |
| H | 2.20349800 | 2.02257300 | 1.30657000 |

QAC-BO (thin film), T₁

| | | | |
|---|-------------|------------|-------------|
| C | 1.63751500 | 7.31739900 | 3.02482500 |
| C | 2.48337300 | 8.37269500 | 2.63830000 |
| C | 3.47944900 | 8.90562900 | 3.48449000 |
| C | 3.57574000 | 8.44134800 | 4.79632200 |
| C | 2.67062900 | 7.45515500 | 5.24839900 |
| C | 1.75389000 | 6.88565500 | 4.35360800 |
| B | 0.69944500 | 6.65360500 | 2.06883700 |
| C | 0.68088000 | 7.29592000 | 0.68828600 |
| C | 1.55672500 | 8.38798400 | 0.44109500 |
| O | 2.41211500 | 8.88262500 | 1.39713300 |
| O | 0.98864300 | 5.89406400 | 4.83051500 |
| C | 0.22685600 | 5.10556100 | 4.00660200 |
| C | 0.04047200 | 5.39651500 | 2.62515400 |
| C | -0.08435200 | 6.88194100 | -0.41083000 |
| C | 0.04119400 | 7.41045500 | -1.70071600 |
| C | 0.95084800 | 8.45938300 | -1.89578200 |
| C | 1.67714600 | 8.97497400 | -0.81094100 |
| C | -0.33121100 | 3.99180300 | 4.62286400 |
| C | -1.10307200 | 3.09570600 | 3.87511400 |
| C | -1.30116900 | 3.30977400 | 2.49879900 |
| C | -0.71784900 | 4.43877100 | 1.91432500 |

| | | | |
|---|-------------|-------------|-------------|
| C | -0.84113500 | 6.81408200 | -2.80393400 |
| C | -0.55994700 | 5.29568500 | -2.90466100 |
| C | -2.04026200 | 2.29624700 | 1.61374300 |
| C | -2.99477600 | 1.41354700 | 2.44216300 |
| C | 6.48083300 | 8.17511600 | 7.19036800 |
| C | 7.37249200 | 7.01501100 | 7.35338600 |
| C | 7.12085600 | 6.10973900 | 6.31184400 |
| C | 5.63451100 | 7.94255000 | 6.09566600 |
| C | 4.62369400 | 8.84591000 | 5.76742700 |
| C | 4.52400000 | 10.02771700 | 6.51440500 |
| C | 5.35950200 | 10.25227300 | 7.61152800 |
| C | 6.34133700 | 9.32496300 | 7.96519900 |
| C | 8.28285400 | 6.70453900 | 8.36411900 |
| C | 8.91356600 | 5.45838700 | 8.33168300 |
| C | 8.64090800 | 4.54663800 | 7.30370500 |
| C | 7.74980200 | 4.87287500 | 6.27478200 |
| C | -2.34002700 | 6.98808000 | -2.45201900 |
| C | -0.58103300 | 7.47532800 | -4.16862800 |
| C | -2.87959900 | 2.99779400 | 0.52018200 |
| C | -0.96994100 | 1.41337800 | 0.92588800 |
| C | 4.55143000 | 5.20876500 | 3.85291900 |
| C | 4.96263700 | 5.62108700 | 5.13632500 |
| C | 6.05447500 | 6.65982200 | 5.34743500 |
| C | 6.69643800 | 7.06869800 | 4.01682900 |
| C | 6.19137600 | 6.64547200 | 2.77436500 |
| N | 5.02104300 | 5.84523900 | 2.69985500 |
| C | 3.64450900 | 4.12057800 | 3.72445800 |
| C | 3.03196000 | 3.61726100 | 4.86252800 |
| C | 3.38673500 | 4.07011300 | 6.13814800 |
| C | 4.38846100 | 5.01539100 | 6.26120700 |
| C | 7.82066600 | 7.90616800 | 4.05619800 |
| C | 8.45945800 | 8.33396300 | 2.90183800 |
| C | 7.99833800 | 7.86235200 | 1.67147100 |
| C | 6.90673100 | 7.00714400 | 1.61071700 |
| C | 4.27434200 | 5.69246700 | 1.49478000 |
| C | 4.25491800 | 6.69844100 | 0.51532500 |
| C | 3.58380700 | 6.50628200 | -0.68462300 |
| C | 2.81513100 | 5.36196600 | -0.88381100 |
| C | 2.74712800 | 4.40702900 | 0.12485800 |
| C | 3.49003100 | 4.53507400 | 1.30268800 |
| C | 3.53157300 | 3.44229400 | 2.36220800 |
| C | 4.84228100 | 2.62077100 | 2.14764400 |
| C | 2.34012300 | 2.47007600 | 2.28181200 |
| H | 4.16314400 | 9.65519700 | 3.09864400 |
| H | 2.69707000 | 7.10489800 | 6.27274200 |
| H | -0.81162300 | 6.10016000 | -0.24603300 |
| H | 1.08841500 | 8.91065500 | -2.87040200 |
| H | 2.37847900 | 9.79281400 | -0.94118000 |
| H | -0.14740600 | 3.83500200 | 5.68090100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.53023300 | 2.23812200 | 4.37852000 |
| H | -0.81808900 | 4.57597300 | 0.84820900 |
| H | 0.45432100 | 5.10705600 | -3.27020200 |
| H | -0.67057900 | 4.80087400 | -1.93553900 |
| H | -1.28121600 | 4.83852300 | -3.58773900 |
| H | -3.70241000 | 2.03245800 | 3.00397100 |
| H | -2.44925900 | 0.78604200 | 3.15277800 |
| H | -3.56391000 | 0.75799200 | 1.77728400 |
| H | 3.73539900 | 10.73473800 | 6.27523200 |
| H | 5.20185100 | 11.13142900 | 8.22597800 |
| H | 6.96317300 | 9.47856100 | 8.84165200 |
| H | 8.47349100 | 7.40453200 | 9.17215800 |
| H | 9.60863200 | 5.18494000 | 9.11927000 |
| H | 9.10948900 | 3.56919800 | 7.32316800 |
| H | 7.52492100 | 4.16481300 | 5.48270500 |
| H | -2.93804500 | 6.36653900 | -3.12190100 |
| H | -2.66319600 | 8.02343100 | -2.57709100 |
| H | -2.56158600 | 6.67588400 | -1.42890700 |
| H | -0.77469900 | 8.55147500 | -4.12624100 |
| H | 0.45115600 | 7.31864200 | -4.49858900 |
| H | -1.24667200 | 7.05244000 | -4.92314500 |
| H | -2.25477900 | 3.54137400 | -0.19402000 |
| H | -3.58565000 | 3.70573800 | 0.96308600 |
| H | -3.44135200 | 2.24665000 | -0.04416100 |
| H | -0.31149400 | 2.03248900 | 0.30610300 |
| H | -0.34785400 | 0.90968000 | 1.67089400 |
| H | -1.44188500 | 0.65854400 | 0.28690900 |
| H | 2.26134900 | 2.86507300 | 4.76342400 |
| H | 2.90644300 | 3.65611100 | 7.01822000 |
| H | 4.73313600 | 5.33192900 | 7.23499200 |
| H | 8.18401200 | 8.23412900 | 5.02408200 |
| H | 9.30909600 | 9.00575100 | 2.95775400 |
| H | 8.49110700 | 8.16043700 | 0.75241100 |
| H | 6.60138700 | 6.61936700 | 0.64976600 |
| H | 4.73599800 | 7.64781300 | 0.70029100 |
| H | 3.59549000 | 7.28876200 | -1.43180600 |
| H | 2.23034000 | 5.24759400 | -1.78934000 |
| H | 2.10323500 | 3.54659800 | -0.00774700 |
| H | 5.72414900 | 3.26718400 | 2.17774000 |
| H | 4.93579900 | 1.86020700 | 2.92999700 |
| H | 4.80736400 | 2.12970900 | 1.16949900 |
| H | 1.39045200 | 2.97580200 | 2.46569900 |
| H | 2.46580200 | 1.66692500 | 3.00990800 |
| H | 2.30147200 | 1.99137400 | 1.30055200 |

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