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# Supporting Information

# Understanding CO Capture Reaction through Electronic Structure Analysis of Four-Membered-Ring Group-13/N- and B/Group-15-Based Lewis Acid-Base Pairs

Zheng-Feng Zhang[1] and Ming-Der Su[1,2,a)]

[1]Department of Applied Chemistry, National Chiayi University, Chiayi 60004, Taiwan
[2]Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 80708, Taiwan

[a)] E-mail: midesu@mail.ncyu.edu.tw

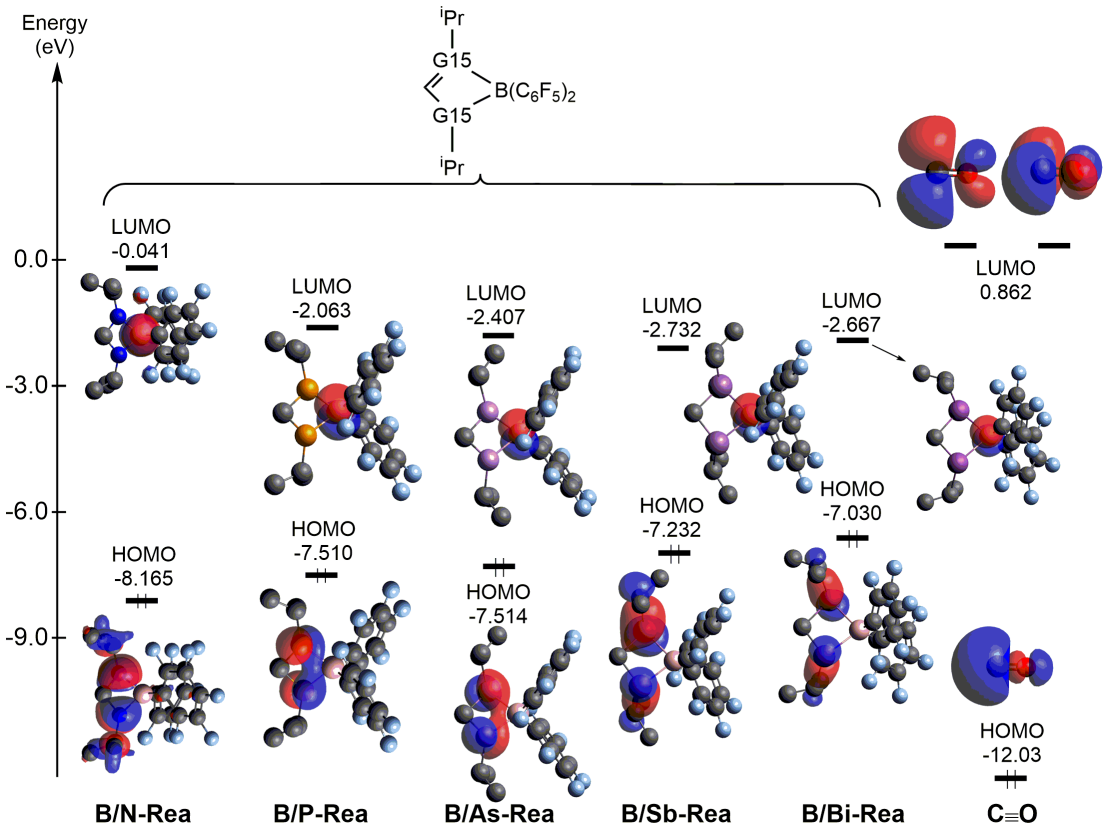



**Figure S1.** Energies of the frontier orbitals (HOMO and LUMO) of the model molecules **B/G15-Rea** and CO for comparison, computed at the M06-2X-D3/def2-TZVP level.

| System | Energy difference \| CO (LUMO) – FLP (HOMO) \| | Energy difference \| FLP (LUMO) – CO (HOMO) \| |
|---|---|---|
| **B/N-Rea** + **CO** | 9.027 | 11.99 |
| **B/P-Rea** + **CO** | 8.372 | 9.975 |
| **B/As-Rea** + **CO** | 8.376 | 9.631 |
| **B/Sb-Rea** + **CO** | 8.094 | 9.306 |
| **B/Bi-Rea** + **CO** | 7.892 | 9.371 |

**Table S1.** The energy difference between the HOMO of **B/G15-Rea** and the LUMO of CO, as well as the energy difference between the HOMO of CO and the LUMO of **B/G15-Rea**. The energy values (in eV) see Figure S1. Energies of the frontier orbitals (HOMO and LUMO) of the model molecules **B/G15-Rea** and CO for comparison, computed at the M06-2X-D3/def2-TZVP level.

**Table S2.** EDA-NOCV results (kcal/mol) of **B/G15-TS** using both singlet-singlet and triplet-triplet models at the ZORA-M06-2X-D3/TZ2P//M06-2X-D3/def2-TZVP level.[a]

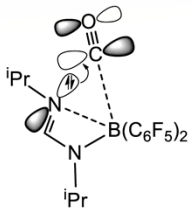
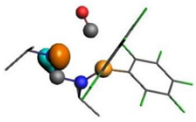
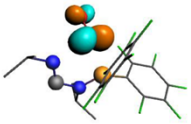
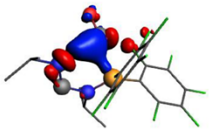
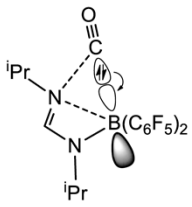
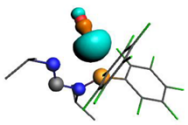
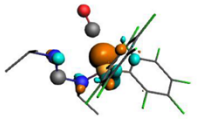
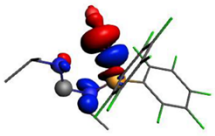
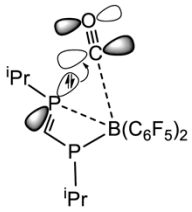
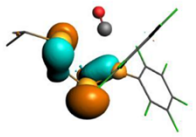
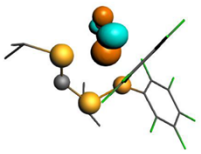
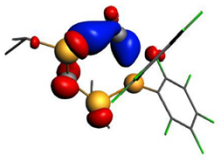
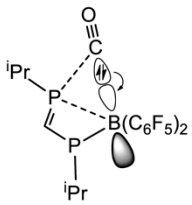
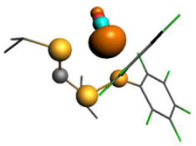
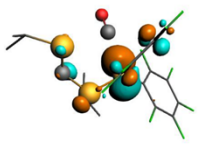
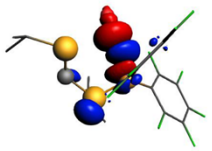
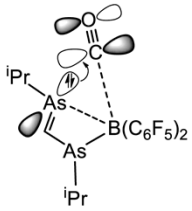
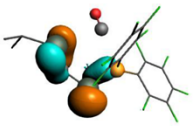
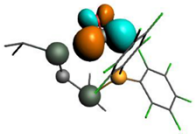
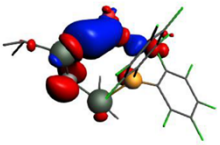
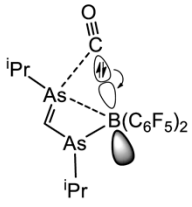
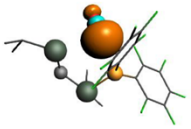
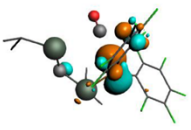
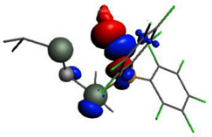
| Fragments | B/N-TS | | B/P-TS | | B/As-TS | | B/Sb-TS | | B/Bi-TS | |
|---|---|---|---|---|---|---|---|---|---|---|
| | B/N-Rea (S) + CO (S) | B/N-Rea (T) + CO (T) | B/P-Rea (S) + CO (S) | B/P-Rea (T) + CO (T) | B/As-Rea (S) + CO (S) | B/As-Rea (T) + CO (T) | B/Sb-Rea (S) + CO (S) | B/Sb-Rea (T) + CO (T) | B/Bi-Rea (S) + CO (S) | B/Bi-Rea (T) + CO (T) |
| $\Delta E_{INT}$ [a] | -6.6 | -215.6 | -6.5 | -190.2 | -6.2 | -189.2 | -6.0 | -182.9 | -5.6 | -175.8 |
| $\Delta E_{Pauli}$ | 59.1 | 49.4 | 33.3 | 48.5 | 26.1 | 42.7 | 22.9 | 22.1 | 38.6 | 34.6 |
| $\Delta E_{Elstat}$ [b] | -30.2 (45.9%) | -34.7 (13.1%) | -16.2 (40.7%) | -22.2 (9.3%) | -12.6 (38.9%) | -17.5 (7.6%) | -11.0 (38.0%) | -14.2 (6.9%) | -18.9 (42.7%) | -19.7 (9.4%) |
| $\Delta E_{Orb}$ [b] | -27.8 (42.3%) | -222.6 (84.0 %) | -15.2 (38.2%) | -208.2 (87.2%) | -11.4 (35.3%) | -206.1 (88.8%) | -9.2 (31.9%) | -182.1 (88.8%) | -15.1 (34.3%) | -180.6 (85.8%) |
| $\Delta E_{Orb\ (1)}$ [c] | -18.7 (67.2%) | -209.8 (94.2 %) | -9.1 (59.6%) | -193.5 (93.0%) | -6.3 (55.6%) | -194.7 (94.5%) | -5.0 (54.3%) | -177.0 (97.2%) | -8.5 (56.4%) | -172.8 (95.7%) |
| $\Delta E_{Orb\ (2)}$ [c] | -4.1 (14.7%) | -7.6 (3.4 %) | -2.6 (17.0%) | -13.7 (6.6%) | -2.2 (19.2%) | -10.5 (5.1%) | -1.8 (19.1%) | -4.7 (2.6%) | -2.5 (16.3%) | -3.5 (1.9%) |
| $\Delta E_{Rest}$ [c] | -5.0 (18.1%) | -5.2 (2.3 %) | -3.6 (23.4%) | -1.0 (0.5%) | -2.9 (25.2%) | -0.9 (0.4%) | -2.5 (26.6%) | -0.4 (0.2%) | -4.1 (27.4%) | -4.3 (2.4%) |
| $\Delta E_{Disper}$ [b] | -7.7 (11.7 %) | -7.7 (2.9%) | -8.4 (21.1%) | -8.4 (3.5%) | -8.3 (25.8%) | -8.3 (3.6%) | -8.7 (30.1%) | -8.7 (4.3%) | -10.2 (23.0%) | -10.2 (4.8%) |

(a) All energy values are given in kcal/mol.

(b) $\Delta E_{INT} = \Delta E_{Elstat} + \Delta E_{Pauli} + \Delta E_{Orb} + \Delta E_{Disper}$.

(c) The values, shown in parentheses, reflect the percentage contribution of attractive interactions to the overall total ($\Delta E_{Elstat} + \Delta E_{Orb} + \Delta E_{Disper}$).

(d) The percentages shown in parentheses denote the contribution of each value to the overall orbital interactions ($\Delta E_{ORB}$).

| (a) Donor- Acceptor Interaction | (b) Donor Orbital | Acceptor Orbital | (c) Deformation Densities Δρ |
|---|---|---|---|
|  |  |  |  |
| HOMO of CO to LUMO of B/N-FLP | HOMO of B/N-FLP | LUMO of CO | $\Delta\rho_1$<br>$\Delta E_1$ = -18.7 kcal/mol; $\nu$ = ±0.44 |
|  |  |  |  |
| HOMO of B/N-FLP to LUMO of CO | HOMO of CO | LUMO of B/N-FLP | $\Delta\rho_2$<br>$\Delta E_2$ = -4.1 kcal/mol; $\nu$ = ±0.23 |
|  |  |  |  |
| HOMO of CO to LUMO of B/P-FLP | HOMO of B/P-FLP | LUMO of CO | $\Delta E_1$ = -8.3 kcal/mol; $\nu$ = ±0.27 |
|  |  |  |  |
| HOMO of B/P-FLP to LUMO of CO | HOMO of CO | LUMO of B/P-FLP | $\Delta E_2$ = -2.5 kcal/mol; $\nu$ = ±0.13 |
|  |  |  |  |
| HOMO of CO to LUMO of B/As-FLP | HOMO of B/As-FLP | LUMO of CO | $\Delta E_1$ = -5.9 kcal/mol; $\nu$ = ±0.22 |
|  |  |  |  |
| HOMO of B/As-FLP to LUMO of CO | HOMO of CO | LUMO of B/As-FLP | $\Delta E_2$ = -2.0 kcal/mol; $\nu$ = ±0.12 |

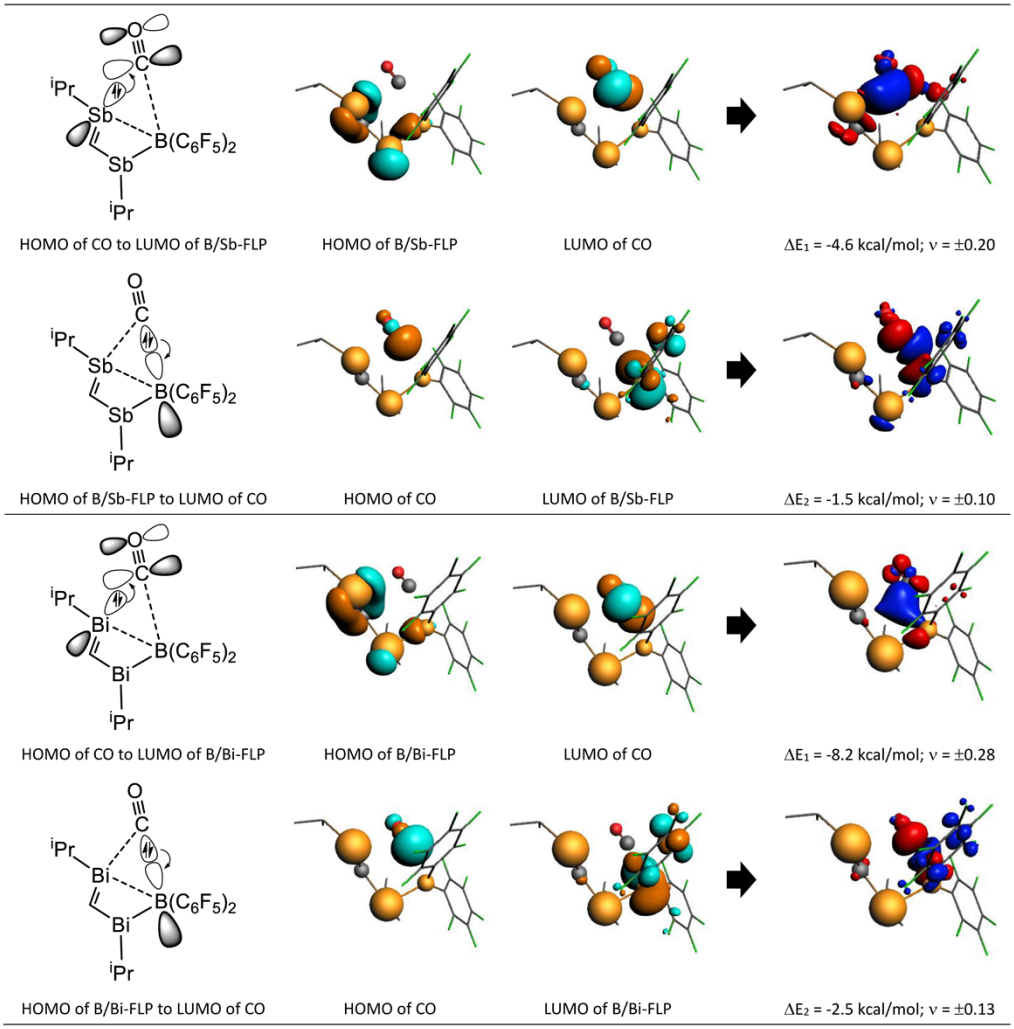



**Figure S2.** The analysis of **B/G15-TS** using EDA-NOCV involved the following components: (a) a qualitative illustration of the orbital interactions between **B/G15-Rea** and CO; (b) the shape of the most significant interaction between occupied and empty orbitals of **B/G15-Rea** and CO; (c) a plot indicating the deformation densities ($\Delta\rho_{(1)}$ and $\Delta\rho_{(2)}$) of the pairwise orbital interactions between the two fragments in their closed-shell state, along with the corresponding interaction energies (kcal/mol) $\Delta E_{Orb(1)}$ and $\Delta E_{Orb(2)}$, respectively. The deformation densities show the direction of charge flow from red to blue.

Table S1
M06-2X-D3/def2-TZVP
**B/N-Rea**

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| F | 5.19235800 | 4.80212100 | 0.67866200 |
| F | 3.24912800 | 5.00713800 | -1.13885400 |
| F | 1.16146200 | 3.27627300 | -1.12223400 |
| F | 1.03427300 | 1.31704500 | 0.75626400 |
| F | 2.99464300 | 1.09961400 | 2.59956400 |
| F | 5.30242500 | 0.22615500 | 4.54812200 |
| F | 6.77065900 | -1.94591200 | 4.04411300 |
| F | 8.40527900 | -2.03018500 | 1.88269500 |
| F | 8.56322500 | 0.10781600 | 0.21237600 |
| F | 7.08508900 | 2.31017400 | 0.71367800 |
| N | 4.77833100 | 2.97375400 | 4.32458300 |
| N | 6.18161800 | 3.98465000 | 3.17336500 |
| C | 5.60783700 | 3.99976700 | 4.36191500 |
| C | 3.68421100 | 2.62029100 | 5.21367600 |
| H | 3.41178800 | 1.59193700 | 4.94493700 |
| C | 2.47414200 | 3.52525000 | 4.98353400 |
| H | 2.71783900 | 4.56853700 | 5.23919300 |
| H | 1.62861300 | 3.20615900 | 5.60912000 |
| H | 2.15704800 | 3.49358400 | 3.93177100 |
| C | 4.15094000 | 2.63567100 | 6.66529300 |
| H | 5.00660900 | 1.96008300 | 6.79817300 |
| H | 3.33923000 | 2.30822200 | 7.32898400 |
| H | 4.44522000 | 3.64965900 | 6.97960100 |
| C | 8.63911300 | 4.05431700 | 3.24124300 |
| H | 8.68027200 | 4.15498600 | 4.33728300 |
| H | 9.52571200 | 4.54623900 | 2.81690100 |
| H | 8.68469300 | 2.98504900 | 2.99158000 |
| C | 7.36020700 | 4.68615300 | 2.69239400 |
| H | 7.34624200 | 4.56418300 | 1.60216900 |
| C | 7.26385700 | 6.17326400 | 3.01541900 |

| | | | |
|---|---|---|---|
| H | 6.34484100 | 6.59733000 | 2.58896600 |
| H | 8.12539900 | 6.70992200 | 2.59552600 |
| H | 7.26534400 | 6.34684300 | 4.10327100 |
| C | 4.16347200 | 2.93735400 | 1.71686100 |
| C | 3.07734000 | 2.06794600 | 1.68220300 |
| C | 2.05452700 | 2.15964600 | 0.74488500 |
| C | 2.11892000 | 3.16484300 | -0.21846700 |
| C | 3.18971800 | 4.05303500 | -0.22353600 |
| C | 4.19142400 | 3.92417200 | 0.73880300 |
| C | 6.14258800 | 1.35883100 | 2.64459800 |
| C | 6.08937700 | 0.24407500 | 3.47262200 |
| C | 6.84457100 | -0.90385500 | 3.23154100 |
| C | 7.68261700 | -0.95019300 | 2.12186400 |
| C | 7.76268100 | 0.14631700 | 1.26530700 |
| C | 6.98978100 | 1.26778400 | 1.54434600 |
| B | 5.29177700 | 2.71436900 | 2.84826300 |
| H | 5.78031200 | 4.70226900 | 5.18909300 |

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Table S2

M06-2X-D3/def2-TZVP

**Al/N-Rea**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| Al | -0.00005200 | -0.58292800 | -0.00007700 |
| N | -0.14345600 | -2.14762200 | 1.09439900 |
| N | 0.14337200 | -2.14713700 | -1.09525400 |
| C | 1.67052500 | 0.45692400 | 0.13420100 |
| C | -1.67060700 | 0.45701200 | -0.13394100 |
| C | 1.95737500 | 1.17099500 | 1.28865500 |
| C | 2.61421100 | 0.51523100 | -0.88113200 |
| C | -1.95714700 | 1.17192100 | -1.28795400 |
| C | -2.61454500 | 0.51460800 | 0.88119900 |
| C | 3.12008400 | 1.91835700 | 1.45094000 |
| F | 1.08545300 | 1.14448700 | 2.30318900 |
| C | 3.79443900 | 1.24697400 | -0.77276800 |

| | | | |
|---|---|---|---|
| F | 2.40528000 | -0.14654800 | -2.02465700 |
| C | -0.39842000 | -2.67994200 | 2.42686300 |
| C | -0.00002100 | -2.87867300 | -0.00058700 |
| C | 0.39838100 | -2.67885400 | -2.42795000 |
| C | -3.11979500 | 1.91942400 | -1.44999700 |
| F | -1.08496400 | 1.14611500 | -2.30228100 |
| C | -3.79473100 | 1.24645400 | 0.77305900 |
| F | -2.40591100 | -0.14798500 | 2.02430500 |
| C | 4.04163300 | 1.95003300 | 0.40501500 |
| F | 3.36542200 | 2.58618700 | 2.56635100 |
| F | 4.67654200 | 1.28367100 | -1.75866500 |
| C | 0.73181800 | -3.59901000 | 2.88655900 |
| C | -1.76248100 | -3.36389200 | 2.49850000 |
| H | -0.42228900 | -1.80317900 | 3.09028600 |
| H | 0.00000900 | -3.98152700 | -0.00082700 |
| C | -0.73163500 | -3.59804700 | -2.88794300 |
| C | 1.76262300 | -3.36240500 | -2.49995600 |
| H | 0.42196600 | -1.80182100 | -3.09102700 |
| C | -4.04161000 | 1.95036400 | -0.40428100 |
| F | -3.36484100 | 2.58807400 | -2.56498100 |
| F | -4.67708600 | 1.28246900 | 1.75875800 |
| F | 5.15461000 | 2.64936500 | 0.53153700 |
| H | 0.57096800 | -3.91826600 | 3.92564300 |
| H | 0.78172900 | -4.50611800 | 2.26371700 |
| H | 1.70004100 | -3.08348100 | 2.82498000 |
| H | -1.97379800 | -3.70140600 | 3.52293100 |
| H | -1.79190300 | -4.24624700 | 1.83952200 |
| H | -2.55288900 | -2.66713800 | 2.19037500 |
| H | -0.57077000 | -3.91682100 | -3.92717200 |
| H | -0.78124200 | -4.50543500 | -2.26548600 |
| H | -1.69999900 | -3.08281700 | -2.82607800 |
| H | 1.97395400 | -3.69946600 | -3.52453300 |
| H | 1.79233400 | -4.24500100 | -1.84131500 |
| H | 2.55286400 | -2.66555100 | -2.19162500 |
| F | -5.15453900 | 2.64981200 | -0.53058800 |

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Table S3

M06-2X-D3/def2-TZVP

**Ga/N-Rea**

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Ga | -0.00000500 | 0.48077500 | 0.00001300 |
| N | -0.14759600 | 2.14393600 | -1.09437700 |
| N | 0.14759200 | 2.14389500 | 1.09446800 |
| C | 1.70820200 | -0.53600100 | -0.14165000 |
| C | -1.70821100 | -0.53600900 | 0.14163100 |
| C | 1.99579800 | -1.26941300 | -1.28294300 |
| C | 2.66037600 | -0.54361500 | 0.86661600 |
| C | -1.99578000 | -1.26951700 | 1.28286900 |
| C | -2.66041100 | -0.54353600 | -0.86661200 |
| C | 3.17726300 | -1.98890900 | -1.43849500 |
| F | 1.11295900 | -1.29016600 | -2.28580600 |
| C | 3.85777700 | -1.24737100 | 0.76028300 |
| F | 2.44428400 | 0.13901100 | 1.99490900 |
| C | -0.42466400 | 2.67607000 | -2.42168500 |
| C | 0.00000200 | 2.87006900 | 0.00005800 |
| C | 0.42467400 | 2.67598100 | 2.42179200 |
| C | -3.17724400 | -1.98902400 | 1.43839000 |
| F | -1.11291700 | -1.29035800 | 2.28570800 |
| C | -3.85781100 | -1.24729800 | -0.76030800 |
| F | -2.44434700 | 0.13918300 | -1.99485300 |
| C | 4.11043600 | -1.97238300 | -0.40283900 |
| F | 3.42705700 | -2.67697800 | -2.54014900 |
| F | 4.75011100 | -1.23767800 | 1.73702300 |
| C | 0.69569800 | 3.59868600 | -2.89950300 |
| C | -1.79129400 | 3.35749000 | -2.47468300 |
| H | -0.45680900 | 1.80063500 | -3.08694800 |
| H | 0.00000700 | 3.97259300 | 0.00007800 |
| C | -0.69565500 | 3.59862500 | 2.89963300 |
| C | 1.79132900 | 3.35735000 | 2.47481400 |
| H | 0.45678500 | 1.80052600 | 3.08703000 |
| C | -4.11044200 | -1.97240900 | 0.40275900 |
| F | -3.42701100 | -2.67718400 | 2.53999300 |

| | | | |
|---|---|---|---|
| F | -4.75016900 | -1.23752000 | -1.73702500 |
| F | 5.23945800 | -2.64587800 | -0.52525200 |
| H | 0.51845300 | 3.91815800 | -3.93600200 |
| H | 0.75236500 | 4.50520900 | -2.27648000 |
| H | 1.66630100 | 3.08616500 | -2.85217100 |
| H | -2.01963600 | 3.69249100 | -3.49642500 |
| H | -1.81200100 | 4.24089600 | -1.81690500 |
| H | -2.57570000 | 2.66038700 | -2.15219600 |
| H | -0.51840200 | 3.91805900 | 3.93614200 |
| H | -0.75228600 | 4.50516900 | 2.27663700 |
| H | -1.66627700 | 3.08614200 | 2.85228200 |
| H | 2.01968100 | 3.69231500 | 3.49656500 |
| H | 1.81207000 | 4.24077200 | 1.81705800 |
| H | 2.57571000 | 2.66022600 | 2.15230900 |
| F | -5.23946300 | -2.64591000 | 0.52514300 |

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Table S4

M06-2X-D3/def2-TZVP

**In/N-Rea**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | 4.91088100 | 4.74295700 | 0.20931200 |
| F | 2.93096500 | 5.35221300 | -1.53022300 |
| F | 0.66659500 | 3.86895500 | -1.57102000 |
| F | 0.36667900 | 1.77348300 | 0.12043000 |
| F | 2.34936100 | 1.15849400 | 1.86417200 |
| F | 5.42390100 | -0.25586400 | 4.36935400 |
| F | 6.99082600 | -2.45815300 | 4.26211200 |
| F | 8.82042600 | -2.71716600 | 2.28293700 |
| F | 9.09521500 | -0.78392400 | 0.40506700 |
| F | 7.52622700 | 1.42476500 | 0.50857400 |
| N | 4.79414700 | 3.13293700 | 4.60239200 |
| N | 6.28491000 | 4.22643000 | 3.34528800 |
| C | 5.65347200 | 4.12924800 | 4.50012000 |
| C | 3.95391400 | 2.81324700 | 5.74285200 |

| | | | |
|---|---|---|---|
| H | 4.26805300 | 1.82183700 | 6.11461300 |
| C | 2.50672700 | 2.69547600 | 5.26882300 |
| H | 2.14591400 | 3.67347800 | 4.91468700 |
| H | 1.85017700 | 2.34992700 | 6.07984000 |
| H | 2.42804900 | 1.98095800 | 4.43579900 |
| C | 4.08267600 | 3.80838900 | 6.89077300 |
| H | 5.11201300 | 3.85995700 | 7.27411900 |
| H | 3.43190700 | 3.50289800 | 7.72114100 |
| H | 3.77421200 | 4.81679900 | 6.57303400 |
| C | 8.52676900 | 4.46858900 | 2.45953100 |
| H | 8.98356300 | 3.88295800 | 3.27220700 |
| H | 9.27478400 | 5.17300600 | 2.06903500 |
| H | 8.25413800 | 3.77428800 | 1.65066600 |
| C | 7.29250600 | 5.20496900 | 2.97666300 |
| H | 6.88170600 | 5.80071500 | 2.14233400 |
| C | 7.65133700 | 6.16351600 | 4.10676000 |
| H | 6.77768300 | 6.73598400 | 4.45049700 |
| H | 8.40549500 | 6.88191400 | 3.75823300 |
| H | 8.07523200 | 5.61854800 | 4.96486500 |
| C | 3.68340500 | 2.93205200 | 1.08344800 |
| C | 2.51169400 | 2.19496500 | 1.03352900 |
| C | 1.47830100 | 2.48958200 | 0.14832000 |
| C | 1.63150800 | 3.56841900 | -0.72153300 |
| C | 2.79805000 | 4.33143000 | -0.69950700 |
| C | 3.80262900 | 3.99800400 | 0.20628600 |
| C | 6.43269000 | 0.64431200 | 2.44009900 |
| C | 6.32018800 | -0.36283700 | 3.38514600 |
| C | 7.11423100 | -1.50690600 | 3.35108800 |
| C | 8.05658400 | -1.64148200 | 2.33269200 |
| C | 8.19672300 | -0.64659400 | 1.36595300 |
| C | 7.37843600 | 0.47723900 | 1.44183300 |
| In | 5.22972800 | 2.45849300 | 2.54414100 |
| H | 5.83211900 | 4.83417400 | 5.32518700 |

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Table S5

M06-2X-D3/def2-TZVP

**Tl/N-Rea**

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| Tl | 0.00000700 | -0.09399600 | 0.00001900 |
| N | 0.18126000 | -2.11737900 | 1.11091400 |
| N | -0.18120800 | -2.11741200 | -1.11081700 |
| C | 2.00884900 | 0.76969400 | -0.12335600 |
| C | -2.00882500 | 0.76972000 | 0.12333200 |
| C | 2.93711900 | 0.55185700 | 0.88190300 |
| C | 2.40502900 | 1.50463900 | -1.22821700 |
| C | -2.93712600 | 0.55172900 | -0.88186700 |
| C | -2.40496600 | 1.50484600 | 1.22808600 |
| C | 4.23719200 | 1.04541500 | 0.79990600 |
| F | 2.60015900 | -0.14312700 | 1.96890500 |
| C | 3.69504700 | 2.01589800 | -1.34828200 |
| F | 1.54211300 | 1.73360400 | -2.21836400 |
| C | 0.51736900 | -2.73651300 | 2.38465400 |
| C | 0.00000600 | -2.80138500 | 0.00006100 |
| C | -0.51744100 | -2.73655400 | -2.38452100 |
| C | -4.23718800 | 1.04532300 | -0.79991600 |
| F | -2.60020700 | -0.14345300 | -1.96875500 |
| C | -3.69497100 | 2.01614900 | 1.34810000 |
| F | -1.54201900 | 1.73395700 | 2.21817300 |
| C | 4.61059400 | 1.78142600 | -0.32344900 |
| F | 5.11344700 | 0.82957600 | 1.76607100 |
| F | 4.06024700 | 2.71429700 | -2.40961900 |
| C | 1.88722900 | -3.41498800 | 2.34030700 |
| C | -0.57681000 | -3.69380300 | 2.85934800 |
| H | 0.58016500 | -1.91090200 | 3.11014200 |
| H | -0.00003700 | -3.90650400 | 0.00008300 |
| C | -1.88738400 | -3.41485300 | -2.34009000 |
| C | 0.57660000 | -3.69399800 | -2.85922500 |
| H | -0.58015900 | -1.91096400 | -3.11004000 |
| C | -4.61054700 | 1.78152700 | 0.32332600 |
| F | -5.11347400 | 0.82933900 | -1.76602100 |
| F | -4.06013300 | 2.71472900 | 2.40933100 |
| F | 5.83719500 | 2.25848400 | -0.41763900 |

| | | | |
|---|---|---|---|
| H | 2.16317300 | -3.80783500 | 3.32962500 |
| H | 1.88177800 | -4.25771100 | 1.63103400 |
| H | 2.65506400 | -2.69695400 | 2.02279700 |
| H | -0.35480800 | -4.07071500 | 3.86798700 |
| H | -0.65761000 | -4.56352900 | 2.18862800 |
| H | -1.55089400 | -3.18591200 | 2.88119900 |
| H | -2.16341700 | -3.80771600 | -3.32937700 |
| H | -1.88201000 | -4.25753700 | -1.63077100 |
| H | -2.65511700 | -2.69670500 | -2.02258800 |
| H | 0.35452000 | -4.07089600 | -3.86785200 |
| H | 0.65730100 | -4.56372600 | -2.18849500 |
| H | 1.55075000 | -3.18623500 | -2.88111000 |
| F | -5.83713500 | 2.25862900 | 0.41746300 |

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Table S6

M06-2X-D3/def2-TZVP

**B/P-Rea**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| B | 0.00000000 | 0.00000000 | 0.48070400 |
| P | -1.15657800 | 0.59766100 | 1.99858400 |
| P | 1.15657800 | -0.59766100 | 1.99858400 |
| C | 0.56058000 | 1.22208200 | -0.40355800 |
| C | -0.56058000 | -1.22208200 | -0.40355800 |
| C | 1.90427800 | 1.51982500 | -0.62188000 |
| C | -0.36215500 | 2.06151100 | -1.02677300 |
| C | 0.36215500 | -2.06151100 | -1.02677300 |
| C | -1.90427800 | -1.51982500 | -0.62188000 |
| C | 2.31015300 | 2.60877100 | -1.39458800 |
| F | 2.86805300 | 0.76567700 | -0.10477200 |
| C | 0.00000000 | 3.15772300 | -1.80051700 |
| F | -1.66735400 | 1.82394800 | -0.86594500 |
| C | -1.57517500 | 2.39296700 | 2.28131000 |
| C | 0.00000000 | 0.00000000 | 3.13714400 |
| C | 1.57517500 | -2.39296700 | 2.28131000 |

| | | | |
|---|---|---|---|
| C | 0.00000000 | -3.15772300 | -1.80051700 |
| F | 1.66735400 | -1.82394800 | -0.86594500 |
| C | -2.31015300 | -2.60877100 | -1.39458800 |
| F | -2.86805300 | -0.76567700 | -0.10477200 |
| C | 1.35417600 | 3.43201900 | -1.98099800 |
| F | 3.59545200 | 2.86280800 | -1.57746000 |
| F | -0.91444100 | 3.93372400 | -2.35891600 |
| C | -2.45611900 | 2.52134000 | 3.52494300 |
| C | -0.32777200 | 3.27204900 | 2.37481500 |
| H | -2.16018100 | 2.66710700 | 1.38875900 |
| H | 0.00000000 | 0.00000000 | 4.22983100 |
| C | 0.32777200 | -3.27204900 | 2.37481500 |
| C | 2.45611900 | -2.52134000 | 3.52494300 |
| H | 2.16018100 | -2.66710700 | 1.38875900 |
| C | -1.35417600 | -3.43201900 | -1.98099800 |
| F | 0.91444100 | -3.93372400 | -2.35891600 |
| F | -3.59545200 | -2.86280800 | -1.57746000 |
| F | 1.72844700 | 4.46617300 | -2.71248900 |
| H | -2.73544800 | 3.57374900 | 3.68236000 |
| H | -1.91503700 | 2.18479600 | 4.42333200 |
| H | -3.37785700 | 1.93004200 | 3.43773600 |
| H | -0.61866300 | 4.33018400 | 2.46402700 |
| H | 0.26429500 | 3.00364700 | 3.26285000 |
| H | 0.32178100 | 3.17080100 | 1.49379000 |
| H | -0.32178100 | -3.17080100 | 1.49379000 |
| H | -0.26429500 | -3.00364700 | 3.26285000 |
| H | 0.61866300 | -4.33018400 | 2.46402700 |
| H | 3.37785700 | -1.93004200 | 3.43773600 |
| H | 1.91503700 | -2.18479600 | 4.42333200 |
| H | 2.73544800 | -3.57374900 | 3.68236000 |
| F | -1.72844700 | -4.46617300 | -2.71248900 |

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Table S7

M06-2X-D3/def2-TZVP

**B/As-Rea**

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Atomic Coordinates (Angstroms)

| Number | X | Y | Z |
|---|---|---|---|
| C | -0.00005800 | -3.08365800 | -0.00114900 |
| As | -0.52499600 | -1.88919600 | -1.30881700 |
| B | 0.00001700 | -0.29242200 | -0.00002100 |
| As | 0.52508500 | -1.89025100 | 1.30744900 |
| C | 1.29447600 | 0.57999600 | -0.36666200 |
| C | -1.29454100 | 0.57959100 | 0.36726400 |
| C | 1.88505000 | 1.29206500 | 0.67761400 |
| C | 1.92921200 | 0.67369000 | -1.60352800 |
| C | -1.88489400 | 1.29277300 | -0.67638200 |
| C | -1.92956200 | 0.67196600 | 1.60408200 |
| C | 3.06503400 | 2.01332100 | 0.54504300 |
| F | 1.32582500 | 1.24668500 | 1.89016300 |
| C | 3.10545800 | 1.40240400 | -1.78379400 |
| F | 1.43961100 | 0.06195800 | -2.67585700 |
| C | -2.43354900 | -2.23799500 | -1.78003500 |
| C | 2.43373800 | -2.23961800 | 1.77789800 |
| C | -3.06488800 | 2.01391800 | -0.54329300 |
| F | -1.32543900 | 1.24865600 | -1.88886800 |
| C | -3.10583300 | 1.40051500 | 1.78487600 |
| F | -1.44022000 | 0.05908500 | 2.67587300 |
| C | 3.67994800 | 2.06681800 | -0.70416300 |
| F | 3.60484700 | 2.63191200 | 1.58232700 |
| F | 3.68082400 | 1.46643900 | -2.97305800 |
| C | -3.36541800 | -2.07186100 | -0.58104400 |
| C | -2.86615400 | -1.39240200 | -2.97510100 |
| H | -2.40685100 | -3.30065300 | -2.07311200 |
| H | -0.00013100 | -4.17633300 | -0.00155900 |
| C | 3.36532300 | -2.07250800 | 0.57882400 |
| C | 2.86677700 | -1.39516800 | 2.97361200 |
| H | 2.40698600 | -3.30253800 | 2.07001800 |
| C | -3.68007000 | 2.06610400 | 0.70583500 |
| F | -3.60444900 | 2.63364700 | -1.58003100 |
| F | -3.68143000 | 1.46329400 | 2.97409300 |
| F | 4.79782800 | 2.75123700 | -0.86495700 |
| H | -4.37495200 | -2.42613100 | -0.84386200 |
| H | -3.45319100 | -1.01443300 | -0.28913900 |

| | | | |
|---|---|---|---|
| H | -3.01873600 | -2.64020600 | 0.29366600 |
| H | -2.85844900 | -0.32026500 | -2.73059600 |
| H | -3.89191300 | -1.65995400 | -3.27131100 |
| H | -2.21048900 | -1.54184200 | -3.84446000 |
| H | 4.37489900 | -2.42706500 | 0.84109000 |
| H | 3.45308600 | -1.01483000 | 0.28782100 |
| H | 3.01839400 | -2.64007500 | -0.29629300 |
| H | 2.85930700 | -0.32282300 | 2.73002500 |
| H | 3.89252800 | -1.66323800 | 3.26938600 |
| H | 2.21124800 | -1.54519500 | 3.84297300 |
| F | -4.79795900 | 2.75039400 | 0.86711600 |

Table S8

M06-2X-D3/def2-TZVP

**B/Sb-Rea**

| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |
| C | 0.08123300 | 3.02763000 | -0.50616500 |
| Sb | 0.66585000 | 1.44227000 | -1.64335100 |
| B | -0.03362400 | 0.03069600 | 0.09955000 |
| Sb | -0.70709400 | 2.00244200 | 1.14185000 |
| C | -1.27901900 | -0.92989400 | -0.20712500 |
| C | 1.27822400 | -0.71469000 | 0.64977900 |
| C | -2.05688300 | -1.32903300 | 0.88062700 |
| C | -1.71072600 | -1.38052200 | -1.45433900 |
| C | 1.91771100 | -1.60999200 | -0.21186100 |
| C | 1.89454100 | -0.53031300 | 1.88779200 |
| C | -3.22446700 | -2.07249100 | 0.76215900 |
| F | -1.70625700 | -0.93611200 | 2.10987100 |
| C | -2.86711200 | -2.14405200 | -1.61588200 |
| F | -1.03837900 | -1.08668900 | -2.56384700 |
| C | 2.81830400 | 1.58732300 | -2.10673300 |
| C | -2.88957000 | 2.31968600 | 0.98389300 |
| C | 3.11479100 | -2.24805200 | 0.08737300 |
| F | 1.39992100 | -1.82632300 | -1.42390100 |

| | | | |
|---|---|---|---|
| C | 3.08539000 | -1.16801500 | 2.23703300 |
| F | 1.36946200 | 0.27978800 | 2.80128700 |
| C | -3.63169400 | -2.48529000 | -0.50429600 |
| F | -3.94781000 | -2.37359900 | 1.82811600 |
| F | -3.24371000 | -2.54603000 | -2.81832700 |
| C | 3.63848800 | 1.67763800 | -0.82139300 |
| C | 3.25613500 | 0.42584500 | -2.99481100 |
| H | 2.90035900 | 2.53456200 | -2.66327600 |
| H | 0.18787800 | 4.10335600 | -0.67324700 |
| C | -3.44696300 | 1.85864400 | -0.35922600 |
| C | -3.62920000 | 1.69308800 | 2.16307400 |
| H | -2.96449400 | 3.41754100 | 1.04809500 |
| C | 3.70263000 | -2.02466700 | 1.33048600 |
| F | 3.69884300 | -3.04190900 | -0.79501500 |
| F | 3.63360800 | -0.96329600 | 3.42275900 |
| F | -4.73265200 | -3.20002300 | -0.64891400 |
| H | 4.70308400 | 1.82821500 | -1.06624300 |
| H | 3.56807400 | 0.74734400 | -0.23525200 |
| H | 3.31556000 | 2.50911500 | -0.17917900 |
| H | 3.12870400 | -0.54276500 | -2.48769100 |
| H | 4.32389000 | 0.52563700 | -3.24769700 |
| H | 2.69174600 | 0.38392400 | -3.93761600 |
| H | -4.50094100 | 2.16888000 | -0.45581800 |
| H | -3.42290800 | 0.76136100 | -0.44776300 |
| H | -2.89202000 | 2.28162300 | -1.20964000 |
| H | -3.53996400 | 0.59624200 | 2.16384500 |
| H | -4.70326800 | 1.93332300 | 2.10662800 |
| H | -3.25564200 | 2.05730400 | 3.13118900 |
| F | 4.83592900 | -2.62319300 | 1.64687800 |

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Table S9

M06-2X-D3/def2-TZVP

**B/Bi-Rea**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| B | -0.00455900 | 0.40957300 | -0.00200700 |
| Bi | -0.67274600 | -1.37566000 | -1.53773600 |
| Bi | 0.68445200 | -1.37319200 | 1.53117100 |
| C | -1.20691900 | 1.27878900 | 0.59639200 |
| C | 1.19297100 | 1.28914400 | -0.59558400 |
| C | -1.07161700 | 1.89709700 | 1.84061200 |
| C | -2.40605700 | 1.52361000 | -0.07040900 |
| C | 2.38959900 | 1.54192800 | 0.07264900 |
| C | 1.05443500 | 1.90795900 | -1.83928500 |
| C | -2.06908500 | 2.67630900 | 2.41756000 |
| F | 0.06007300 | 1.73983500 | 2.52944500 |
| C | -3.43128700 | 2.29659200 | 0.46869600 |
| F | -2.62251300 | 1.00306600 | -1.28189100 |
| C | -2.88904700 | -1.99559600 | -1.69961600 |
| C | 0.01736200 | -2.74321000 | -0.00508600 |
| C | 2.90507100 | -1.97329700 | 1.71205500 |
| C | 3.40996400 | 2.32237200 | -0.46489900 |
| F | 2.60859200 | 1.02215400 | 1.28408200 |
| C | 2.04690700 | 2.69481200 | -2.41448000 |
| F | -0.07552400 | 1.74354700 | -2.52931900 |
| C | -3.25918000 | 2.87680000 | 1.72164000 |
| F | -1.89873200 | 3.22938400 | 3.60644400 |
| F | -4.55887900 | 2.48139100 | -0.19731700 |
| C | -2.94031900 | -3.41100500 | -2.25404800 |
| C | -3.58731300 | -1.87001300 | -0.35455000 |
| H | -3.31083300 | -1.27713800 | -2.41746900 |
| H | 0.03381000 | -3.84037600 | -0.01095600 |
| C | 3.61353900 | -1.83896100 | 0.37317000 |
| C | 2.96353600 | -3.38934600 | 2.26412800 |
| H | 3.31418200 | -1.25256900 | 2.43494800 |
| C | 3.23502800 | 2.90265400 | -1.71740100 |
| F | 4.53589300 | 2.51375300 | 0.20208100 |
| F | 1.87380400 | 3.24815600 | -3.60281900 |
| F | -4.21929900 | 3.61367300 | 2.24964100 |
| H | -3.98584800 | -3.75210400 | -2.34296500 |
| H | -2.42534700 | -4.11812800 | -1.58356200 |
| H | -2.48109700 | -3.48904100 | -3.25040400 |
| H | -4.64929500 | -2.15594000 | -0.45042200 |

| | | | |
|---|---|---|---|
| H | -3.12734800 | -2.53301900 | 0.39448400 |
| H | -3.56009700 | -0.84280500 | 0.03613300 |
| H | 3.58123900 | -0.81107300 | -0.01516400 |
| H | 3.16552600 | -2.50414000 | -0.38112200 |
| H | 4.67693800 | -2.11642400 | 0.47771200 |
| H | 2.49666000 | -3.47335100 | 3.25642300 |
| H | 2.46020200 | -4.09934000 | 1.58786600 |
| H | 4.01113200 | -3.72180300 | 2.36109100 |
| F | 4.19057000 | 3.64662600 | -2.24378600 |

Table S10

M06-2X-D3/def2-TZVP

CO

| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |
| C | 0.00000000 | 0.00000000 | -0.06194300 |
| O | 0.00000000 | 0.00000000 | 1.06194300 |

Table S11

M06-2X-D3/def2-TZVP

**B/N-TS**

| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |
| F | 1.12092300 | 0.86129900 | 2.27802800 |
| F | 3.65404800 | 1.61582500 | 2.74592200 |
| F | 5.61868700 | 0.92306700 | 1.00285600 |
| F | 5.01324700 | -0.51507400 | -1.21635100 |
| F | 2.50702000 | -1.25856200 | -1.70511800 |
| F | -2.14656500 | 0.04521200 | 1.88987200 |
| F | -3.64184700 | 2.23135200 | 1.79981700 |
| F | -3.11164400 | 4.19669800 | -0.00211900 |
| F | -1.05554500 | 3.89719600 | -1.75786900 |

| | | | |
|---|---|---|---|
| F | 0.43803600 | 1.67899400 | -1.71204700 |
| O | -0.27875300 | -1.25561000 | -3.12317800 |
| N | -2.31872400 | -1.58604200 | -0.65607900 |
| N | -0.37332600 | -1.81397100 | 0.59184500 |
| C | -0.07723300 | -0.95787600 | -2.05980700 |
| C | -1.69017800 | -2.15364700 | 0.28297500 |
| H | -2.11251900 | -2.94648200 | 0.92379700 |
| C | 0.41644000 | -2.91567400 | 1.17607900 |
| H | -0.33133500 | -3.56083400 | 1.66514700 |
| C | 1.39333700 | -2.48821200 | 2.27043400 |
| H | 2.34456200 | -2.12613000 | 1.85848900 |
| H | 1.62328100 | -3.35675300 | 2.90345300 |
| H | 0.95873900 | -1.70345100 | 2.90535000 |
| C | 1.09876400 | -3.74168700 | 0.08784500 |
| H | 0.36293000 | -4.11616700 | -0.63951400 |
| H | 1.62181200 | -4.60436300 | 0.52494000 |
| H | 1.83617200 | -3.13444500 | -0.45706300 |
| C | -3.73634200 | -1.81163100 | -0.88549600 |
| H | -3.83042600 | -2.06020900 | -1.95632700 |
| C | -4.45451100 | -0.47969300 | -0.65686600 |
| H | -4.38318300 | -0.19015800 | 0.40364500 |
| H | -5.51728800 | -0.55387400 | -0.92716100 |
| H | -3.98896700 | 0.31236400 | -1.26066000 |
| C | -4.37996100 | -2.93322200 | -0.07556300 |
| H | -3.86929600 | -3.89492300 | -0.23162100 |
| H | -5.42801700 | -3.05517800 | -0.38109400 |
| H | -4.37081400 | -2.70194900 | 1.00098500 |
| C | 1.69636200 | -0.20130800 | 0.25724200 |
| C | 2.05384600 | 0.54065700 | 1.38288000 |
| C | 3.36069300 | 0.92780000 | 1.65663800 |
| C | 4.37028700 | 0.56796300 | 0.76655000 |
| C | 4.05800600 | -0.17074600 | -0.37023600 |
| C | 2.73417100 | -0.53966200 | -0.60378500 |
| C | -0.79760400 | 0.74759800 | 0.07195100 |
| C | -1.84004900 | 0.95893700 | 0.97299900 |
| C | -2.63182100 | 2.10194300 | 0.95399900 |
| C | -2.36942400 | 3.10490100 | 0.02487600 |
| C | -1.31998600 | 2.94853800 | -0.87474600 |

| | | | |
|---|---|---|---|
| C | -0.55598700 | 1.78477300 | -0.82586700 |
| B | 0.14010000 | -0.55577000 | 0.10071600 |

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Table S12

M06-2X-D3/def2-TZVP

**Al/N-TS**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | -0.99137700 | 2.37241600 | -0.81429500 |
| F | -3.32123300 | 3.72193000 | -0.64613000 |
| F | -5.58339600 | 2.42395700 | 0.07887900 |
| F | -5.52507000 | -0.22598300 | 0.64623100 |
| F | -3.18662300 | -1.57842100 | 0.49150500 |
| F | 2.63210600 | -0.81816500 | -1.49529100 |
| F | 4.86026500 | 0.50969600 | -0.86038900 |
| F | 4.79930100 | 2.46309800 | 1.02242500 |
| F | 2.48424400 | 3.04434300 | 2.31148900 |
| F | 0.24307700 | 1.65638100 | 1.73222600 |
| O | -0.29935500 | -2.32252400 | 2.55885400 |
| N | 1.12893800 | -2.96449500 | 0.21546200 |
| N | -0.18502700 | -2.03748300 | -1.42085100 |
| C | -0.25871200 | -1.85531700 | 1.53036800 |
| C | 0.69528300 | -2.96234700 | -0.99841400 |
| H | 1.05656400 | -3.70484900 | -1.73691800 |
| C | -0.68926100 | -2.05206800 | -2.79199900 |
| H | -0.18504600 | -2.88047400 | -3.31986000 |
| C | -0.32114300 | -0.74277200 | -3.48856800 |
| H | -0.80069100 | 0.11075000 | -2.97743400 |
| H | -0.66418400 | -0.73411100 | -4.53253600 |
| H | 0.76663400 | -0.58941700 | -3.46887300 |
| C | -2.19410400 | -2.30674100 | -2.82122100 |
| H | -2.44178500 | -3.23935300 | -2.29628000 |
| H | -2.55961200 | -2.37507500 | -3.85582000 |
| H | -2.72945300 | -1.48273200 | -2.32468800 |
| C | 2.20478900 | -3.85515900 | 0.61475700 |

| | | | |
|---|---|---|---|
| H | 2.43711500 | -4.53325100 | -0.23081100 |
| C | 1.78956300 | -4.70786500 | 1.81124900 |
| H | 1.60721600 | -4.07794500 | 2.69356200 |
| H | 2.58303100 | -5.42551400 | 2.06309700 |
| H | 0.86973400 | -5.26779000 | 1.59138200 |
| C | 3.45157700 | -3.02573800 | 0.92079000 |
| H | 3.75500500 | -2.44366300 | 0.03926500 |
| H | 4.28955800 | -3.66843800 | 1.22673000 |
| H | 3.23789200 | -2.32092000 | 1.73997700 |
| C | -2.01102000 | 0.35278200 | -0.15857800 |
| C | -2.08723600 | 1.71125500 | -0.44001900 |
| C | -3.27790100 | 2.43013200 | -0.36693500 |
| C | -4.44352800 | 1.76295000 | 0.00612500 |
| C | -4.41335600 | 0.39962800 | 0.29616600 |
| C | -3.19662400 | -0.26989900 | 0.20959500 |
| C | 1.34455300 | 0.37052800 | 0.09891900 |
| C | 2.54968600 | 0.11963000 | -0.54590900 |
| C | 3.72569100 | 0.80057400 | -0.24343500 |
| C | 3.69675300 | 1.80043300 | 0.72632700 |
| C | 2.50680400 | 2.09823400 | 1.38779000 |
| C | 1.36405900 | 1.37472700 | 1.05925800 |
| Al | -0.31850600 | -0.65414800 | -0.19509000 |

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Table S13

M06-2X-D3/def2-TZVP

**Ga/N-TS**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | -1.02941000 | 2.42078300 | -0.77037700 |
| F | -3.36626700 | 3.76675300 | -0.62804500 |
| F | -5.64009000 | 2.45465300 | 0.03341500 |
| F | -5.58794300 | -0.20237600 | 0.56234700 |
| F | -3.24534800 | -1.55070800 | 0.43273200 |
| F | 2.62167400 | -0.79061600 | -1.48450500 |
| F | 4.87333300 | 0.48765300 | -0.82146400 |

| | | | |
|---|---|---|---|
| F | 4.83699100 | 2.42677900 | 1.07605400 |
| F | 2.52487300 | 3.04421000 | 2.35277100 |
| F | 0.25848900 | 1.70359200 | 1.74553800 |
| O | -0.27735800 | -2.33745900 | 2.58528400 |
| N | 1.16502400 | -2.96485000 | 0.21417200 |
| N | -0.17393300 | -2.05664200 | -1.41994600 |
| C | -0.25444100 | -1.85981100 | 1.56197400 |
| C | 0.70756300 | -2.97447400 | -0.99057800 |
| H | 1.04534700 | -3.73265600 | -1.72488100 |
| C | -0.69288500 | -2.08106600 | -2.78269700 |
| H | -0.19682900 | -2.91628900 | -3.30768900 |
| C | -0.32859300 | -0.77988100 | -3.49658400 |
| H | -0.80298000 | 0.07922300 | -2.98942400 |
| H | -0.68106000 | -0.78021100 | -4.53750400 |
| H | 0.75942000 | -0.62739700 | -3.48740500 |
| C | -2.19919300 | -2.33017700 | -2.79516800 |
| H | -2.44445700 | -3.25843500 | -2.26160500 |
| H | -2.57670600 | -2.40272500 | -3.82516800 |
| H | -2.72660000 | -1.50162000 | -2.29751600 |
| C | 2.23396000 | -3.87015100 | 0.59580500 |
| H | 2.44399700 | -4.55735700 | -0.24867900 |
| C | 1.82985500 | -4.71020100 | 1.80510300 |
| H | 1.66800300 | -4.07099700 | 2.68492200 |
| H | 2.61925400 | -5.43466400 | 2.05060400 |
| H | 0.90036800 | -5.26150300 | 1.60452400 |
| C | 3.49733800 | -3.05665400 | 0.87671500 |
| H | 3.78877300 | -2.47600400 | -0.00995400 |
| H | 4.33470300 | -3.70855800 | 1.16476000 |
| H | 3.30776900 | -2.35033000 | 1.70057100 |
| C | -2.06489300 | 0.39498200 | -0.16345500 |
| C | -2.13281900 | 1.75651100 | -0.42812100 |
| C | -3.32651100 | 2.47149500 | -0.36672200 |
| C | -4.49793400 | 1.79681900 | -0.02694100 |
| C | -4.47065900 | 0.42955800 | 0.24427800 |
| C | -3.25286700 | -0.24028800 | 0.17118700 |
| C | 1.35368100 | 0.41238600 | 0.11331300 |
| C | 2.55456800 | 0.13810800 | -0.52797000 |
| C | 3.74052700 | 0.79496000 | -0.20986900 |

| | | | |
|---|---|---|---|
| C | 3.72398800 | 1.78788400 | 0.76720400 |
| C | 2.53537400 | 2.10455900 | 1.42251300 |
| C | 1.37979100 | 1.40791200 | 1.08091600 |
| Ga | -0.33969100 | -0.59393600 | -0.20234800 |

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Table S14

M06-2X-D3/def2-TZVP

**In/N-TS**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | -1.31150300 | 2.65555500 | -0.58082200 |
| F | -3.70474100 | 3.91543400 | -0.53284200 |
| F | -5.96481400 | 2.49577400 | -0.08166700 |
| F | -5.84934100 | -0.17955700 | 0.32261200 |
| F | -3.45644500 | -1.44346400 | 0.28010900 |
| F | 2.66667100 | -0.71464100 | -1.46770100 |
| F | 5.03314100 | 0.33199500 | -0.77332900 |
| F | 5.17046600 | 2.22750500 | 1.16439800 |
| F | 2.92460500 | 3.02866400 | 2.45324200 |
| F | 0.54091600 | 1.91394600 | 1.81717700 |
| O | 0.08053400 | -2.41545100 | 2.65197800 |
| N | 1.18831000 | -2.93981600 | 0.21163000 |
| N | -0.17737800 | -2.10033800 | -1.45491300 |
| C | -0.04176900 | -1.94379000 | 1.62481400 |
| C | 0.71209900 | -2.97895600 | -0.99434500 |
| H | 1.06363400 | -3.75866100 | -1.70076900 |
| C | -0.71111300 | -2.20026400 | -2.80509700 |
| H | -0.20537600 | -3.04572400 | -3.30575400 |
| C | -0.39261400 | -0.92245700 | -3.57946400 |
| H | -0.89939500 | -0.05910000 | -3.11068400 |
| H | -0.74658100 | -0.98095400 | -4.61829900 |
| H | 0.68941800 | -0.73072200 | -3.58083600 |
| C | -2.21171900 | -2.47958500 | -2.77686300 |
| H | -2.42512700 | -3.40370700 | -2.22276900 |
| H | -2.61647600 | -2.57422700 | -3.79464400 |

| | | | |
|---|---|---|---|
| H | -2.74107300 | -1.65547100 | -2.27289400 |
| C | 2.28386100 | -3.82363600 | 0.58004000 |
| H | 2.56973900 | -4.41520700 | -0.31239200 |
| C | 1.88142500 | -4.80746000 | 1.67861700 |
| H | 1.67388500 | -4.28676700 | 2.62280200 |
| H | 2.69369600 | -5.52651800 | 1.85690700 |
| H | 0.98099200 | -5.36671000 | 1.38737300 |
| C | 3.48852400 | -2.97743500 | 0.99082800 |
| H | 3.79640300 | -2.32048400 | 0.16491600 |
| H | 4.34139200 | -3.61102800 | 1.27390400 |
| H | 3.22598900 | -2.34588900 | 1.85448900 |
| C | -2.31570100 | 0.57196100 | -0.14248000 |
| C | -2.41210000 | 1.94083800 | -0.34698700 |
| C | -3.63321100 | 2.61097500 | -0.33128100 |
| C | -4.79786700 | 1.88064600 | -0.10010000 |
| C | -4.73755000 | 0.50315300 | 0.10768800 |
| C | -3.49447900 | -0.12331300 | 0.08239400 |
| C | 1.52124900 | 0.57856000 | 0.14777600 |
| C | 2.68930000 | 0.20372400 | -0.49887300 |
| C | 3.93059200 | 0.73841800 | -0.16407700 |
| C | 4.00334200 | 1.70461400 | 0.83730400 |
| C | 2.84743500 | 2.11638600 | 1.49892900 |
| C | 1.63169600 | 1.53882600 | 1.14185300 |
| In | -0.38774400 | -0.42485700 | -0.15981200 |

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Table S15

M06-2X-D3/def2-TZVP

**Tl/N-TS**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | -1.65224800 | 2.80111600 | -0.69678500 |
| F | -4.18416300 | 3.75567800 | -0.67901900 |
| F | -6.24889300 | 2.08649200 | -0.14716600 |
| F | -5.79956600 | -0.53350100 | 0.36377200 |
| F | -3.27138800 | -1.49368500 | 0.34573500 |

| | | | |
|---|---|---|---|
| F | 2.65725400 | -0.70228100 | -1.52436500 |
| F | 5.11330600 | 0.04184600 | -0.76723900 |
| F | 5.43989500 | 1.85460100 | 1.22366800 |
| F | 3.28151200 | 2.87727300 | 2.50662100 |
| F | 0.79657000 | 2.06609900 | 1.81058000 |
| O | 0.34688300 | -2.15771500 | 2.67774200 |
| N | 1.20731200 | -2.80132100 | 0.22918600 |
| N | -0.16557300 | -1.96106600 | -1.44296400 |
| C | 0.11753900 | -1.75972500 | 1.63190000 |
| C | 0.69100300 | -2.85314600 | -0.96251600 |
| H | 0.98626600 | -3.67790300 | -1.64472400 |
| C | -0.72126300 | -2.10021700 | -2.77850100 |
| H | -0.26225100 | -2.99286900 | -3.24241500 |
| C | -0.35644800 | -0.88194800 | -3.62529300 |
| H | -0.82070800 | 0.02716700 | -3.20204600 |
| H | -0.72286800 | -0.98412200 | -4.65656500 |
| H | 0.73246900 | -0.73664900 | -3.64544900 |
| C | -2.23312000 | -2.30920400 | -2.72581000 |
| H | -2.48510500 | -3.17557800 | -2.09969900 |
| H | -2.64529500 | -2.46494400 | -3.73318200 |
| H | -2.72344900 | -1.42329500 | -2.29186000 |
| C | 2.24508800 | -3.75199500 | 0.59857200 |
| H | 2.52978200 | -4.32490200 | -0.30624900 |
| C | 1.76270800 | -4.75788500 | 1.64519500 |
| H | 1.53994500 | -4.26388200 | 2.59967300 |
| H | 2.53703400 | -5.51793600 | 1.82354900 |
| H | 0.85203900 | -5.26688100 | 1.29838300 |
| C | 3.47703900 | -2.98196500 | 1.07260600 |
| H | 3.84694200 | -2.32270600 | 0.27393100 |
| H | 4.28674700 | -3.66643100 | 1.36387200 |
| H | 3.21931200 | -2.36051000 | 1.94467200 |
| C | -2.39760200 | 0.63197100 | -0.16712800 |
| C | -2.65561900 | 1.96913300 | -0.42647300 |
| C | -3.95171400 | 2.47997200 | -0.42587800 |
| C | -5.01511600 | 1.62129800 | -0.15226000 |
| C | -4.78300800 | 0.27174300 | 0.11065600 |
| C | -3.47339600 | -0.20196500 | 0.10022900 |
| C | 1.64775000 | 0.67180900 | 0.11689200 |

| | | | |
|---|---|---|---|
| C | 2.76882600 | 0.17671000 | -0.53204700 |
| C | 4.05634000 | 0.55917800 | -0.16286500 |
| C | 4.22581500 | 1.48047700 | 0.86800700 |
| C | 3.11545900 | 2.00553800 | 1.52706500 |
| C | 1.84515400 | 1.58538500 | 1.14110600 |
| Tl | -0.36199800 | -0.13647300 | -0.19303100 |

Table S16

M06-2X-D3/def2-TZVP

**B/P-TS**

| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |
| F | 0.89737300 | -1.94540300 | 2.11832900 |
| F | -0.16697400 | -4.27730700 | 2.93311500 |
| F | -2.49776300 | -5.15440600 | 1.84627100 |
| F | -3.73113000 | -3.68642700 | -0.07200200 |
| F | -2.69622100 | -1.37649100 | -0.88560000 |
| F | 2.50103000 | 1.08978200 | 0.81208800 |
| F | 4.65175500 | 0.81416100 | -0.74508600 |
| F | 4.50464400 | -0.63326700 | -3.03060300 |
| F | 2.17318900 | -1.82165400 | -3.74489100 |
| F | 0.00676700 | -1.56755700 | -2.18070800 |
| O | -2.19496300 | 1.25904300 | -2.31896800 |
| P | 0.52851200 | 3.18980200 | -0.62894900 |
| P | -0.37966500 | 1.19586200 | 1.58715900 |
| C | -1.46270300 | 0.83241000 | -1.58121600 |
| C | -0.25454300 | 2.80962000 | 0.80157500 |
| H | -0.71040600 | 3.59476700 | 1.41769400 |
| C | -2.14435100 | 1.19750000 | 2.22066800 |
| H | -2.15541900 | 2.12120600 | 2.82490300 |
| C | -2.40944800 | 0.02619100 | 3.16874200 |
| H | -2.49877600 | -0.92255600 | 2.61944600 |
| H | -3.35915700 | 0.18538000 | 3.70114300 |
| H | -1.60997000 | -0.08326200 | 3.91537300 |
| C | -3.21499000 | 1.31527400 | 1.14018500 |

| | | | |
|---|---|---|---|
| H | -3.02338300 | 2.16780300 | 0.47114800 |
| H | -4.20709100 | 1.45821000 | 1.59647900 |
| H | -3.26154100 | 0.40251700 | 0.52738900 |
| C | 0.40935000 | 5.05848400 | -0.77723900 |
| H | -0.04070000 | 5.19792400 | -1.77583900 |
| C | 1.83503800 | 5.62129000 | -0.82317600 |
| H | 2.33246800 | 5.49347000 | 0.15038700 |
| H | 1.81639400 | 6.69631100 | -1.05790200 |
| H | 2.45002900 | 5.11799400 | -1.58331700 |
| C | -0.44749000 | 5.78193800 | 0.25066000 |
| H | -1.47761000 | 5.39812700 | 0.27284600 |
| H | -0.49185900 | 6.85620100 | 0.01591900 |
| H | -0.01979100 | 5.68263600 | 1.26030300 |
| C | -0.85628700 | -1.55570600 | 0.60071800 |
| C | -0.24315700 | -2.35367100 | 1.56690000 |
| C | -0.77732900 | -3.56099400 | 2.00614200 |
| C | -1.97158300 | -4.01134800 | 1.44998500 |
| C | -2.60449100 | -3.25498800 | 0.46722300 |
| C | -2.03816300 | -2.05016400 | 0.05734200 |
| C | 1.16556000 | -0.24312700 | -0.60939800 |
| C | 2.38317800 | 0.35705600 | -0.28479800 |
| C | 3.51559400 | 0.23008500 | -1.08424200 |
| C | 3.44233700 | -0.51241000 | -2.25926900 |
| C | 2.24487500 | -1.12416800 | -2.62423800 |
| C | 1.13918600 | -0.98500000 | -1.79345700 |
| B | -0.12601300 | -0.17073900 | 0.29734900 |

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Table S17

M06-2X-D3/def2-TZVP

**B/As-TS**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | 0.87994500 | -2.11483900 | 2.21841900 |
| F | -0.31426900 | -4.39235400 | 3.01716100 |
| F | -2.66157100 | -5.15890900 | 1.88037800 |

| | | | |
|---|---|---|---|
| F | -3.77570300 | -3.64126000 | -0.07150600 |
| F | -2.60929800 | -1.39124200 | -0.87180100 |
| F | 2.60862400 | 0.95076900 | 0.80577400 |
| F | 4.67999500 | 0.74589800 | -0.86487700 |
| F | 4.42990200 | -0.63898000 | -3.18074900 |
| F | 2.08057400 | -1.83483300 | -3.80962500 |
| F | -0.00616000 | -1.65122800 | -2.13307500 |
| O | -2.13929100 | 1.34432600 | -2.27043800 |
| As | 0.79489300 | 3.25408500 | -0.57197200 |
| As | -0.22707200 | 1.13024100 | 1.79366800 |
| C | -1.41786200 | 0.87468100 | -1.54764100 |
| C | -0.15429400 | 2.81458300 | 0.87509100 |
| H | -0.73539700 | 3.58163400 | 1.40151900 |
| C | -2.15031900 | 1.13959800 | 2.33420600 |
| H | -2.19026100 | 2.05442000 | 2.94890800 |
| C | -2.47624000 | -0.04920400 | 3.23697000 |
| H | -2.50218400 | -0.99058300 | 2.66750900 |
| H | -3.47152100 | 0.08473200 | 3.68836100 |
| H | -1.74529700 | -0.16159900 | 4.05066000 |
| C | -3.14245100 | 1.27968500 | 1.18652300 |
| H | -2.90554400 | 2.14159200 | 0.54468900 |
| H | -4.16274500 | 1.42097700 | 1.57841200 |
| H | -3.15476100 | 0.37764900 | 0.55653200 |
| C | 0.41317300 | 5.20671700 | -0.77984200 |
| H | 0.00400700 | 5.26795700 | -1.80232200 |
| C | 1.74431300 | 5.96157500 | -0.74928800 |
| H | 2.19692300 | 5.91481600 | 0.25323400 |
| H | 1.59109500 | 7.02274400 | -1.00049400 |
| H | 2.47028300 | 5.54793800 | -1.46465300 |
| C | -0.59517000 | 5.79814200 | 0.19177700 |
| H | -1.56524300 | 5.28219800 | 0.14739300 |
| H | -0.76842300 | 6.86033200 | -0.04199600 |
| H | -0.22459200 | 5.74580900 | 1.22745800 |
| C | -0.81654900 | -1.65161000 | 0.65961700 |
| C | -0.26724600 | -2.47330400 | 1.64423600 |
| C | -0.86870700 | -3.65145100 | 2.07484000 |
| C | -2.07069800 | -4.04502300 | 1.49256900 |
| C | -2.64189800 | -3.26339000 | 0.49178400 |

| | | | |
|---|---|---|---|
| C | -2.00795600 | -2.09037900 | 0.08867700 |
| C | 1.21562800 | -0.35737000 | -0.58377800 |
| C | 2.44295600 | 0.24826400 | -0.30544400 |
| C | 3.53565700 | 0.15753500 | -1.16273100 |
| C | 3.40877700 | -0.55266900 | -2.35288900 |
| C | 2.20028400 | -1.16913600 | -2.67445900 |
| C | 1.13661500 | -1.06831100 | -1.78623000 |
| B | -0.02319000 | -0.30198700 | 0.38257800 |

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Table S18

M06-2X-D3/def2-TZVP

**B/Sb-TS**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | 0.75068800 | -2.41948100 | 2.26781100 |
| F | -0.67991700 | -4.59823100 | 2.95986700 |
| F | -3.06538400 | -5.08811000 | 1.74848200 |
| F | -3.97366500 | -3.40357100 | -0.17248400 |
| F | -2.56761000 | -1.26037000 | -0.87491100 |
| F | 2.73529000 | 0.69496700 | 0.84303500 |
| F | 4.68894400 | 0.62931500 | -0.97081700 |
| F | 4.28989600 | -0.59169500 | -3.36068300 |
| F | 1.90461400 | -1.74083300 | -3.92351800 |
| F | -0.07649100 | -1.67190400 | -2.11701400 |
| O | -1.86360300 | 1.78571600 | -1.97383800 |
| Sb | 1.58373300 | 3.50063800 | -0.19411200 |
| Sb | 0.03610300 | 1.03556700 | 2.17321100 |
| C | -1.27255100 | 1.07105400 | -1.33767000 |
| C | 0.14316600 | 2.81652400 | 0.99208900 |
| H | -0.73539700 | 3.46139000 | 1.13343500 |
| C | -2.13213600 | 1.10396700 | 2.58163100 |
| H | -2.20525400 | 1.98578200 | 3.23997400 |
| C | -2.55466100 | -0.12856000 | 3.38041200 |
| H | -2.51598400 | -1.03963500 | 2.76173800 |
| H | -3.59478300 | -0.02215000 | 3.72951500 |

| | | | |
|---|---|---|---|
| H | -1.92098200 | -0.29341300 | 4.26471600 |
| C | -3.02841200 | 1.32378400 | 1.36990900 |
| H | -2.74064700 | 2.21594100 | 0.79366800 |
| H | -4.07658100 | 1.45930700 | 1.68599600 |
| H | -3.00524500 | 0.45871300 | 0.68930400 |
| C | 0.65478200 | 5.39221600 | -0.85210700 |
| H | 0.64793700 | 5.29727500 | -1.95108300 |
| C | 1.56759900 | 6.55921400 | -0.47186000 |
| H | 1.61773800 | 6.68349700 | 0.62155700 |
| H | 1.18680900 | 7.50422800 | -0.89283100 |
| H | 2.59602500 | 6.42460500 | -0.84020800 |
| C | -0.77105400 | 5.60508400 | -0.36620000 |
| H | -1.44040500 | 4.78696000 | -0.67141800 |
| H | -1.18068100 | 6.54358500 | -0.77488100 |
| H | -0.80984000 | 5.68389700 | 0.73195900 |
| C | -0.84735000 | -1.74831700 | 0.68361300 |
| C | -0.41126200 | -2.65102500 | 1.65455500 |
| C | -1.13553100 | -3.77582500 | 2.03230900 |
| C | -2.35640800 | -4.02771800 | 1.41131600 |
| C | -2.82135700 | -3.16044700 | 0.42626900 |
| C | -2.06306500 | -2.04654600 | 0.07231600 |
| C | 1.24649700 | -0.50482300 | -0.55084100 |
| C | 2.49248500 | 0.08023000 | -0.31144300 |
| C | 3.53116100 | 0.05505400 | -1.23722400 |
| C | 3.32558100 | -0.56775700 | -2.46462200 |
| C | 2.09606400 | -1.16088500 | -2.75254400 |
| C | 1.08794600 | -1.12375100 | -1.79695200 |
| B | 0.07534100 | -0.47634400 | 0.49024000 |

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Table S19

M06-2X-D3/def2-TZVP

**B/Bi-TS**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | -3.07587000 | 0.36452800 | -2.22180500 |

| | | | |
|---|---|---|---|
| F | -5.74040200 | -0.00148300 | -1.98857100 |
| F | -6.86090100 | -0.22503000 | 0.47959700 |
| F | -5.30317400 | -0.03874000 | 2.69083000 |
| F | -2.67860400 | 0.35083000 | 2.47390200 |
| F | 1.04784800 | 1.01917200 | -1.93361800 |
| F | 2.44997300 | 3.27808200 | -1.93548000 |
| F | 1.74990000 | 5.32133000 | -0.29084000 |
| F | -0.37231500 | 5.06764500 | 1.36941700 |
| F | -1.78317200 | 2.80293800 | 1.40503400 |
| O | 0.51156500 | -0.02889400 | 2.91387500 |
| Bi | 3.24360700 | -0.24261400 | -0.02841700 |
| Bi | -0.31125400 | -1.53407100 | -1.09715000 |
| C | 0.05969100 | 0.38880300 | 1.97184200 |
| C | 1.59212900 | -1.48685500 | 0.09294800 |
| H | 1.66436800 | -2.32814100 | 0.79706400 |
| C | -1.39744400 | -3.02010400 | 0.30005000 |
| H | -0.85519200 | -3.95317900 | 0.07567600 |
| C | -2.85194500 | -3.17863900 | -0.12899800 |
| H | -3.44558600 | -2.28752000 | 0.13067800 |
| H | -3.31837400 | -4.03349800 | 0.38974400 |
| H | -2.95960800 | -3.35332200 | -1.21083500 |
| C | -1.26233800 | -2.70878000 | 1.78176100 |
| H | -0.21034100 | -2.59687200 | 2.08187500 |
| H | -1.70054200 | -3.51565900 | 2.39477300 |
| H | -1.78772000 | -1.77830600 | 2.04715200 |
| C | 4.53733600 | -1.28375300 | 1.57715500 |
| H | 4.82457500 | -0.45226100 | 2.24131000 |
| C | 5.79123700 | -1.84125200 | 0.90859700 |
| H | 5.53976500 | -2.64151000 | 0.19416200 |
| H | 6.47447200 | -2.27712200 | 1.65784300 |
| H | 6.35534900 | -1.06969000 | 0.36229000 |
| C | 3.79942700 | -2.34217700 | 2.37907700 |
| H | 2.87440000 | -1.95691300 | 2.83313600 |
| H | 4.43737000 | -2.72634500 | 3.19345800 |
| H | 3.53131200 | -3.20267700 | 1.74521200 |
| C | -2.77440800 | 0.38156600 | 0.10638100 |
| C | -3.61574800 | 0.28527000 | -1.00290100 |
| C | -4.98735800 | 0.08348500 | -0.90666700 |

| | | | |
|---|---|---|---|
| C | -5.56129700 | -0.03254000 | 0.35726200 |
| C | -4.75900400 | 0.06387300 | 1.49155800 |
| C | -3.38965700 | 0.27729100 | 1.35273600 |
| C | -0.43984800 | 1.79893000 | -0.25986700 |
| C | 0.66459000 | 1.98454600 | -1.09977200 |
| C | 1.40898800 | 3.15845700 | -1.13222100 |
| C | 1.05273900 | 4.20531500 | -0.28656500 |
| C | -0.04079700 | 4.07188200 | 0.56797000 |
| C | -0.76721500 | 2.88613000 | 0.56235800 |
| B | -1.23122600 | 0.45338600 | -0.21098700 |

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Table S20

M06-2X-D3/def2-TZVP

**B/N-Prod**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | 2.76795000 | -2.04193800 | 2.67676200 |
| F | 0.24413400 | -2.30177300 | 1.86708900 |
| F | -1.34789700 | -0.12143500 | 1.59989000 |
| F | -0.36162200 | 2.35144600 | 2.15415000 |
| F | 2.17204600 | 2.63019600 | 2.97984900 |
| F | 6.40525000 | -0.23015700 | 5.09869200 |
| F | 8.28855300 | -1.98309200 | 4.45648800 |
| F | 8.26300600 | -3.21774900 | 2.03196900 |
| F | 6.28487400 | -2.65605800 | 0.25763800 |
| F | 4.37235900 | -0.90406800 | 0.88328600 |
| O | 5.05096100 | 2.38652200 | 1.67050500 |
| N | 4.98463100 | 2.81785700 | 3.92616700 |
| N | 4.01160900 | 1.02270400 | 4.86206500 |
| C | 4.74365800 | 1.99492300 | 2.75896900 |
| C | 4.49894200 | 2.21544600 | 5.01613700 |
| H | 4.51464400 | 2.71773500 | 5.98917300 |
| C | 3.35139300 | 0.31992200 | 5.97314700 |
| H | 3.81910700 | 0.70022700 | 6.89693200 |
| C | 3.58553300 | -1.18309200 | 5.89378400 |

| | | | |
|---|---|---|---|
| H | 3.20891900 | -1.59122900 | 4.94474100 |
| H | 3.04686300 | -1.67643100 | 6.71388000 |
| H | 4.65100700 | -1.42443600 | 5.98177300 |
| C | 1.85849700 | 0.65341200 | 6.01769900 |
| H | 1.69090500 | 1.73932700 | 5.96887900 |
| H | 1.42306400 | 0.27543200 | 6.95324600 |
| H | 1.32636100 | 0.18285200 | 5.17921700 |
| C | 5.47976800 | 4.19170600 | 3.81886000 |
| H | 6.14412300 | 4.16137200 | 2.94276500 |
| C | 6.27873500 | 4.59536900 | 5.05005400 |
| H | 5.63314400 | 4.70918200 | 5.93473300 |
| H | 6.75764800 | 5.56752300 | 4.87369700 |
| H | 7.06371000 | 3.85961900 | 5.27421000 |
| C | 4.32309200 | 5.14001000 | 3.51734400 |
| H | 3.79136800 | 4.81688100 | 2.61281100 |
| H | 4.69730100 | 6.16101500 | 3.35959700 |
| H | 3.60897100 | 5.15705500 | 4.35555900 |
| C | 2.60897200 | 0.31816100 | 2.78962700 |
| C | 2.05213300 | -0.92901200 | 2.52020300 |
| C | 0.72923600 | -1.09637700 | 2.11400100 |
| C | -0.09068000 | 0.02027300 | 1.97916900 |
| C | 0.41727100 | 1.28649500 | 2.25719800 |
| C | 1.74399800 | 1.40204000 | 2.65772800 |
| C | 5.24624000 | -0.53681000 | 3.04538000 |
| C | 6.30326500 | -0.82961200 | 3.90369500 |
| C | 7.31686100 | -1.73315800 | 3.59111200 |
| C | 7.30864400 | -2.36108600 | 2.35123700 |
| C | 6.29157500 | -2.07370200 | 1.44519300 |
| C | 5.29996900 | -1.16372800 | 1.79934800 |
| B | 4.11226300 | 0.59147700 | 3.33830200 |

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Table S21

M06-2X-D3/def2-TZVP

**Al/N-Prod**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

| | | | |
|---|---|---|---|
| F | 2.59170800 | -2.09256500 | 2.54568500 |
| F | 0.01140700 | -2.37168100 | 1.83777300 |
| F | -1.54367000 | -0.18153200 | 1.49220700 |
| F | -0.51297200 | 2.30113700 | 1.85065200 |
| F | 2.07447700 | 2.59053200 | 2.55876900 |
| F | 6.80587500 | -0.49941300 | 4.76289500 |
| F | 8.44475100 | -2.58661500 | 4.32600400 |
| F | 8.12826400 | -4.11833100 | 2.10996300 |
| F | 6.16353700 | -3.55792800 | 0.33016600 |
| F | 4.52167400 | -1.46454300 | 0.75682700 |
| O | 5.43385000 | 3.04818600 | 1.73630900 |
| N | 4.98552000 | 3.15236400 | 3.97752900 |
| N | 4.15686900 | 1.20371500 | 4.90972300 |
| C | 5.03516300 | 2.44019400 | 2.69045800 |
| C | 4.49823800 | 2.45468000 | 5.01136700 |
| H | 4.39056000 | 2.98124200 | 5.97071700 |
| C | 3.52415500 | 0.52490800 | 6.05040800 |
| H | 3.97420800 | 0.92922500 | 6.97381200 |
| C | 3.81811900 | -0.96760700 | 5.97213300 |
| H | 3.38573000 | -1.39904600 | 5.05315500 |
| H | 3.36995000 | -1.49046000 | 6.82732100 |
| H | 4.90014900 | -1.15105900 | 5.97064500 |
| C | 2.02224700 | 0.80459300 | 6.06891000 |
| H | 1.81879800 | 1.88523100 | 6.09606900 |
| H | 1.55921000 | 0.34235000 | 6.95194600 |
| H | 1.54542300 | 0.38760900 | 5.16924700 |
| C | 5.29374700 | 4.58754700 | 4.04792600 |
| H | 5.90257200 | 4.76015500 | 3.14975800 |
| C | 6.11464000 | 4.93907400 | 5.28232500 |
| H | 5.52591200 | 4.85532300 | 6.20902700 |
| H | 6.45424600 | 5.98117400 | 5.21126200 |
| H | 6.99984300 | 4.29361600 | 5.36605100 |
| C | 4.01046700 | 5.40451300 | 3.92972500 |
| H | 3.46064100 | 5.12433000 | 3.02111300 |
| H | 4.24057100 | 6.47801100 | 3.88358900 |
| H | 3.35604100 | 5.23195500 | 4.79922800 |
| C | 2.44745200 | 0.26256600 | 2.50395800 |

| | | | |
|---|---|---|---|
| C | 1.86952400 | -0.98943800 | 2.33607200 |
| C | 0.53176100 | -1.16481400 | 1.98778000 |
| C | -0.27136100 | -0.03894700 | 1.81555400 |
| C | 0.26032400 | 1.23688700 | 1.99592400 |
| C | 1.60300500 | 1.35392200 | 2.34250700 |
| C | 5.57853300 | -0.92546000 | 2.79125400 |
| C | 6.61119900 | -1.24161600 | 3.66382000 |
| C | 7.47737700 | -2.31272400 | 3.46429000 |
| C | 7.31612200 | -3.09978200 | 2.32603000 |
| C | 6.30312400 | -2.81229000 | 1.41353300 |
| C | 5.46408400 | -1.72934700 | 1.66244400 |
| Al | 4.31929200 | 0.57138800 | 3.08008600 |

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Table S22

M06-2X-D3/def2-TZVP

**Ga/N-Prod**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | 2.57553200 | -2.06089900 | 2.64748700 |
| F | -0.01193300 | -2.44859500 | 2.01506400 |
| F | -1.61750300 | -0.32415300 | 1.51544700 |
| F | -0.63111900 | 2.19682900 | 1.64154400 |
| F | 1.96323800 | 2.59609300 | 2.26231200 |
| F | 6.79498800 | -0.28508600 | 4.64358400 |
| F | 8.46060100 | -2.38021500 | 4.35273200 |
| F | 8.13532900 | -4.09114800 | 2.27248200 |
| F | 6.13720000 | -3.70339900 | 0.48436600 |
| F | 4.46851300 | -1.60466800 | 0.76558400 |
| O | 5.39870900 | 3.14264500 | 1.71269600 |
| N | 4.96679500 | 3.18552900 | 3.95685400 |
| N | 4.10410400 | 1.24340000 | 4.87744800 |
| C | 4.99660200 | 2.52527000 | 2.65991900 |
| C | 4.47919000 | 2.47456700 | 4.99250700 |
| H | 4.40871300 | 2.99219000 | 5.96083800 |
| C | 3.49445400 | 0.53973300 | 6.01056400 |

| | | | |
|---|---|---|---|
| H | 3.91572800 | 0.96492900 | 6.93878100 |
| C | 3.85548700 | -0.93808800 | 5.93449300 |
| H | 3.44669300 | -1.38618800 | 5.01326600 |
| H | 3.43079600 | -1.48063300 | 6.78954000 |
| H | 4.94526100 | -1.07065900 | 5.93493800 |
| C | 1.98187500 | 0.75492500 | 6.01249900 |
| H | 1.73407400 | 1.82541700 | 6.05752900 |
| H | 1.52719500 | 0.25595700 | 6.87970800 |
| H | 1.53517100 | 0.33643400 | 5.09815900 |
| C | 5.32658700 | 4.60594400 | 4.08251600 |
| H | 5.81457000 | 4.82783200 | 3.12383700 |
| C | 6.32197200 | 4.84126000 | 5.21246800 |
| H | 5.86944900 | 4.67341400 | 6.20231700 |
| H | 6.66930500 | 5.88310400 | 5.18795700 |
| H | 7.19567100 | 4.18340500 | 5.10983600 |
| C | 4.07014700 | 5.46308000 | 4.20252000 |
| H | 3.38556100 | 5.25918700 | 3.36771300 |
| H | 4.33069900 | 6.53042800 | 4.18884300 |
| H | 3.53959800 | 5.25728100 | 5.14615700 |
| C | 2.37616300 | 0.27904000 | 2.41077400 |
| C | 1.82515400 | -0.99460300 | 2.35982800 |
| C | 0.48512600 | -1.22347900 | 2.05509800 |
| C | -0.34311400 | -0.13147900 | 1.80243600 |
| C | 0.16610600 | 1.16431600 | 1.86419400 |
| C | 1.51284100 | 1.33983000 | 2.17105100 |
| C | 5.55365500 | -0.89009800 | 2.72990200 |
| C | 6.60118900 | -1.11609900 | 3.61092400 |
| C | 7.47870300 | -2.18923500 | 3.48528200 |
| C | 7.31265300 | -3.06839500 | 2.41725300 |
| C | 6.28201700 | -2.86963400 | 1.50062600 |
| C | 5.42978200 | -1.78143700 | 1.67163100 |
| Ga | 4.27282500 | 0.62738100 | 2.95044500 |

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Table S23

M06-2X-D3/def2-TZVP

**In/N-Prod**

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| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| F | 2.22365600 | -1.74640100 | 3.16577300 |
| F | -0.21388200 | -2.63756400 | 2.40499000 |
| F | -1.82391200 | -1.04662500 | 0.91348900 |
| F | -1.00619500 | 1.42738000 | 0.17951600 |
| F | 1.43098300 | 2.31811000 | 0.92302700 |
| F | 6.77392200 | 0.40897100 | 4.08700700 |
| F | 8.49761500 | -1.66856100 | 4.21467400 |
| F | 8.00955800 | -3.91661400 | 2.77756300 |
| F | 5.80259400 | -4.09497200 | 1.22043400 |
| F | 4.07503100 | -2.02354500 | 1.08699700 |
| O | 5.12978400 | 3.70022800 | 1.77897100 |
| N | 4.86891500 | 3.42010400 | 4.02698600 |
| N | 3.91328600 | 1.45601700 | 4.86646400 |
| C | 4.75165100 | 2.97524200 | 2.65895600 |
| C | 4.44867100 | 2.61310700 | 5.03304700 |
| H | 4.59323400 | 3.01330400 | 6.04896900 |
| C | 3.51945500 | 0.65699300 | 6.02585500 |
| H | 3.71720800 | 1.25270100 | 6.93634400 |
| C | 4.35741100 | -0.61731900 | 6.07662900 |
| H | 4.14807600 | -1.24203700 | 5.19378800 |
| H | 4.10955500 | -1.20201500 | 6.97327800 |
| H | 5.43053400 | -0.38154900 | 6.08876600 |
| C | 2.02890400 | 0.34444600 | 5.95038500 |
| H | 1.43378600 | 1.26514800 | 5.87888000 |
| H | 1.71000300 | -0.21311400 | 6.84183800 |
| H | 1.82123600 | -0.27967500 | 5.06862000 |
| C | 5.49756500 | 4.71876500 | 4.33169200 |
| H | 5.71555000 | 5.13376100 | 3.33915600 |
| C | 6.81070800 | 4.52584500 | 5.08371300 |
| H | 6.64328800 | 4.11957100 | 6.09384900 |
| H | 7.32683300 | 5.48925600 | 5.19617400 |
| H | 7.47187200 | 3.83793400 | 4.53923200 |
| C | 4.52989600 | 5.65174200 | 5.05164800 |
| H | 3.59997000 | 5.76719200 | 4.47860100 |
| H | 4.98660400 | 6.64372800 | 5.17221600 |

| | | | |
|---|---|---|---|
| H | 4.27758400 | 5.28159900 | 6.05793500 |
| C | 1.90775800 | 0.30734700 | 2.05473600 |
| C | 1.45173700 | -0.95319500 | 2.41047800 |
| C | 0.19997500 | -1.43460100 | 2.04183000 |
| C | -0.62965800 | -0.61586800 | 1.27654500 |
| C | -0.20762800 | 0.65765700 | 0.90087900 |
| C | 1.05539000 | 1.09494900 | 1.29715400 |
| C | 5.37340500 | -0.74167400 | 2.57845600 |
| C | 6.51725800 | -0.68842300 | 3.35887500 |
| C | 7.41975000 | -1.74361800 | 3.44909300 |
| C | 7.16763000 | -2.90092200 | 2.71362100 |
| C | 6.03024200 | -2.99125400 | 1.91311200 |
| C | 5.15504100 | -1.90767900 | 1.86085300 |
| In | 3.92050400 | 0.89735500 | 2.66285200 |

Table S24

M06-2X-D3/def2-TZVP

**Tl/N-Prod**

| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |
| F | 2.29144200 | -1.68158100 | 3.17297400 |
| F | -0.11038900 | -2.74148300 | 2.53360000 |
| F | -1.83452700 | -1.33879900 | 0.98289800 |
| F | -1.16636200 | 1.12041800 | 0.06987200 |
| F | 1.23629500 | 2.18473300 | 0.69499700 |
| F | 6.69528400 | 0.65572900 | 3.96008900 |
| F | 8.39620700 | -1.41084100 | 4.30316700 |
| F | 7.94427300 | -3.76156400 | 3.02643900 |
| F | 5.78591500 | -4.05321600 | 1.41801700 |
| F | 4.07135800 | -1.99374600 | 1.07387600 |
| O | 5.05563100 | 3.84269300 | 1.78905700 |
| N | 4.85051500 | 3.45824300 | 4.02541900 |
| N | 3.84860600 | 1.50543000 | 4.85213600 |
| C | 4.68941100 | 3.10873100 | 2.66468300 |
| C | 4.44047500 | 2.62035700 | 5.03093300 |

| | | | |
|---|---|---|---|
| H | 4.66468700 | 2.98650700 | 6.04594500 |
| C | 3.49510400 | 0.67695400 | 5.99941000 |
| H | 3.71493600 | 1.24362900 | 6.92473500 |
| C | 4.34211100 | -0.59296900 | 5.98586100 |
| H | 4.12009400 | -1.18279700 | 5.08296000 |
| H | 4.11714600 | -1.21195000 | 6.86557700 |
| H | 5.41391100 | -0.34855700 | 5.98795800 |
| C | 2.00536000 | 0.35646900 | 5.95380100 |
| H | 1.40331300 | 1.27509500 | 5.93075500 |
| H | 1.71347800 | -0.23381400 | 6.83339800 |
| H | 1.78067500 | -0.23648400 | 5.05523600 |
| C | 5.57514700 | 4.69965800 | 4.36984000 |
| H | 5.74653700 | 5.17700500 | 3.39718500 |
| C | 6.92480300 | 4.37497300 | 5.00256900 |
| H | 6.80507200 | 3.90148900 | 5.98976000 |
| H | 7.50763200 | 5.29561300 | 5.14397300 |
| H | 7.49869600 | 3.69244500 | 4.36095300 |
| C | 4.72074500 | 5.62871800 | 5.22486700 |
| H | 3.75578900 | 5.82914300 | 4.73993600 |
| H | 5.24163400 | 6.58581800 | 5.36544700 |
| H | 4.53011800 | 5.20985500 | 6.22515000 |
| C | 1.83536200 | 0.27809900 | 1.94256000 |
| C | 1.46369100 | -0.97938600 | 2.39212900 |
| C | 0.23028200 | -1.54520400 | 2.08413700 |
| C | -0.65840600 | -0.82299000 | 1.28874700 |
| C | -0.31368400 | 0.44331700 | 0.82091600 |
| C | 0.93138200 | 0.97309000 | 1.15640600 |
| C | 5.33664700 | -0.60622400 | 2.49834500 |
| C | 6.45519000 | -0.49022500 | 3.30554800 |
| C | 7.34584500 | -1.54056700 | 3.50680000 |
| C | 7.11089400 | -2.75069700 | 2.85612300 |
| C | 5.99827400 | -2.89946400 | 2.02964200 |
| C | 5.13072100 | -1.82079500 | 1.86535800 |
| Tl | 3.83503100 | 1.05037900 | 2.45376400 |

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Table S25

M06-2X-D3/def2-TZVP

**B/P-Prod**

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| F | 3.01451800 | -1.99197500 | 1.82198900 |
| F | 0.57199400 | -2.19687600 | 0.80089200 |
| F | -1.20833500 | -0.16573300 | 1.05607700 |
| F | -0.49008600 | 2.10466700 | 2.37206200 |
| F | 1.96331800 | 2.33050700 | 3.41338800 |
| F | 5.61372100 | -1.38404700 | 5.13114100 |
| F | 7.51242300 | -3.08977400 | 4.39231800 |
| F | 8.18129300 | -3.36395100 | 1.77217500 |
| F | 6.89542600 | -1.89035700 | -0.11097500 |
| F | 4.97742100 | -0.15842100 | 0.62002100 |
| O | 4.39462800 | 2.50713800 | 1.72865800 |
| P | 6.06162900 | 2.67040900 | 3.88685400 |
| P | 4.05709200 | 0.94285200 | 5.13478600 |
| C | 4.72076900 | 1.91810700 | 2.71572500 |
| C | 5.08841600 | 2.21239700 | 5.35965900 |
| H | 5.22020800 | 2.71605300 | 6.32210100 |
| C | 3.00355400 | 0.39395000 | 6.53569800 |
| H | 3.20080600 | 1.14119200 | 7.32096700 |
| C | 3.38341000 | -1.00133800 | 7.03516800 |
| H | 3.24892700 | -1.75249800 | 6.24357300 |
| H | 2.72877300 | -1.27066400 | 7.87689200 |
| H | 4.42686100 | -1.04825900 | 7.37129900 |
| C | 1.53232700 | 0.46896900 | 6.10680700 |
| H | 1.26118300 | 1.46312400 | 5.72538600 |
| H | 0.89113800 | 0.23739600 | 6.96953800 |
| H | 1.31947800 | -0.27165600 | 5.32081300 |
| C | 5.66645500 | 4.48634900 | 3.65008200 |
| H | 5.76654800 | 4.57099000 | 2.55371300 |
| C | 6.72190800 | 5.35978000 | 4.32684200 |
| H | 6.67551700 | 5.25740400 | 5.42282500 |
| H | 6.54930700 | 6.42002800 | 4.08793500 |
| H | 7.73897100 | 5.09544400 | 4.00575100 |
| C | 4.24771100 | 4.88739800 | 4.04114000 |

| | | | |
|---|---|---|---|
| H | 3.49273500 | 4.25832100 | 3.55084700 |
| H | 4.05985000 | 5.93279200 | 3.75196700 |
| H | 4.10515000 | 4.81435100 | 5.13067900 |
| C | 2.61972100 | 0.19952400 | 2.63689800 |
| C | 2.20111300 | -0.95084100 | 1.96956600 |
| C | 0.92285900 | -1.08598900 | 1.42724500 |
| C | 0.00763500 | -0.04693000 | 1.55675100 |
| C | 0.37854300 | 1.11751900 | 2.22481200 |
| C | 1.66450100 | 1.21161700 | 2.74171000 |
| C | 5.23515000 | -0.65970700 | 2.90132800 |
| C | 5.91031500 | -1.45042900 | 3.82499300 |
| C | 6.90286400 | -2.36202800 | 3.46978000 |
| C | 7.24444000 | -2.50509000 | 2.13035100 |
| C | 6.58470500 | -1.74613100 | 1.16576900 |
| C | 5.60597200 | -0.84461700 | 1.56764900 |
| B | 4.09949100 | 0.45025800 | 3.22230200 |

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Table S26

M06-2X-D3/def2-TZVP

**B/As-Prod**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | 3.10131900 | -1.71153100 | 1.27808000 |
| F | 0.60152000 | -2.02398800 | 0.44478800 |
| F | -1.32500100 | -0.24839300 | 1.15351500 |
| F | -0.69241800 | 1.86782500 | 2.74262400 |
| F | 1.81215700 | 2.20170600 | 3.59856700 |
| F | 4.03453700 | -2.01131200 | 4.30350000 |
| F | 5.80549900 | -4.01365500 | 3.99529600 |
| F | 7.89614700 | -3.72225400 | 2.28215300 |
| F | 8.19289500 | -1.41419700 | 0.88821800 |
| F | 6.43350300 | 0.57681600 | 1.17959900 |
| O | 4.18691200 | 2.70337200 | 1.68071500 |
| As | 6.20979800 | 2.78895200 | 3.67778600 |
| As | 4.10822800 | 0.95767000 | 5.07299500 |

| | | | |
|---|---|---|---|
| C | 4.65396700 | 2.02604400 | 2.54618400 |
| C | 5.25125400 | 2.28010000 | 5.29433200 |
| H | 5.43938600 | 2.75687100 | 6.26107900 |
| C | 3.07337600 | 0.34426500 | 6.62568200 |
| H | 3.02757100 | 1.22768400 | 7.28021800 |
| C | 3.77808200 | -0.80750500 | 7.34006400 |
| H | 3.89674400 | -1.67037200 | 6.67016300 |
| H | 3.17054900 | -1.12409400 | 8.20158400 |
| H | 4.76966700 | -0.51427500 | 7.71050900 |
| C | 1.67292000 | -0.02830900 | 6.13790200 |
| H | 1.16868300 | 0.81908800 | 5.65211600 |
| H | 1.06027900 | -0.35048600 | 6.99287600 |
| H | 1.72007800 | -0.86366500 | 5.42221900 |
| C | 5.62630600 | 4.68801600 | 3.49021100 |
| H | 5.55370100 | 4.75947700 | 2.39181000 |
| C | 6.70069700 | 5.64213200 | 4.00340600 |
| H | 6.82464500 | 5.55096800 | 5.09416200 |
| H | 6.41796200 | 6.68497600 | 3.79044600 |
| H | 7.67739100 | 5.45197000 | 3.53670200 |
| C | 4.25590500 | 4.98106500 | 4.08845900 |
| H | 3.48677200 | 4.28783500 | 3.72059200 |
| H | 3.94310700 | 6.00384400 | 3.82489300 |
| H | 4.28120800 | 4.91571500 | 5.18746600 |
| C | 2.58343000 | 0.26672500 | 2.47935800 |
| C | 2.21083700 | -0.80389400 | 1.66620100 |
| C | 0.90490000 | -0.99115700 | 1.21288300 |
| C | -0.08384700 | -0.08131000 | 1.57098100 |
| C | 0.24236000 | 1.00482200 | 2.37919100 |
| C | 1.55697200 | 1.15610600 | 2.80153500 |
| C | 5.17625700 | -0.62798300 | 2.77637800 |
| C | 5.06240700 | -1.83687800 | 3.45971300 |
| C | 5.95684300 | -2.88789300 | 3.31677800 |
| C | 7.02919500 | -2.73884100 | 2.43803300 |
| C | 7.18086800 | -1.55356900 | 1.72690900 |
| C | 6.25436900 | -0.52513000 | 1.90242400 |
| B | 4.08241800 | 0.53787300 | 2.99265100 |

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Table S27

M06-2X-D3/def2-TZVP

**B/Sb-Prod**

| Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|
| F | 3.71746400 | 0.01237700 | 0.29783200 |
| F | 1.39122800 | -0.43541000 | -0.97037400 |
| F | -0.91133900 | -0.64466400 | 0.45005600 |
| F | -0.86146100 | -0.38614200 | 3.15702500 |
| F | 1.43100200 | 0.08211800 | 4.42884100 |
| F | 4.06325100 | -2.07078500 | 4.46689800 |
| F | 5.73732100 | -4.14824100 | 4.15297700 |
| F | 7.78314900 | -3.98587200 | 2.37077200 |
| F | 8.12942100 | -1.72879300 | 0.90868100 |
| F | 6.46507700 | 0.33803900 | 1.19866700 |
| O | 4.18409600 | 2.53689300 | 1.64525500 |
| Sb | 6.48003300 | 2.81908100 | 3.59433700 |
| Sb | 4.07741800 | 0.97694300 | 5.26888700 |
| C | 4.70253800 | 1.88192400 | 2.50430900 |
| C | 5.47434300 | 2.34382900 | 5.45164200 |
| H | 5.73941300 | 2.80183100 | 6.41090500 |
| C | 3.12800700 | 0.37162200 | 7.13309900 |
| H | 3.91009700 | 0.59505400 | 7.87475400 |
| C | 2.80962000 | -1.11947300 | 7.12921500 |
| H | 2.09011500 | -1.36658300 | 6.33587400 |
| H | 2.35487000 | -1.39303100 | 8.09431000 |
| H | 3.70264900 | -1.74135700 | 6.98356400 |
| C | 1.89748100 | 1.23696700 | 7.39619400 |
| H | 2.13984500 | 2.30813100 | 7.43442700 |
| H | 1.45974200 | 0.95514800 | 8.36713000 |
| H | 1.12877300 | 1.08006400 | 6.62626200 |
| C | 5.62651200 | 4.81350300 | 3.23464300 |
| H | 5.45725100 | 4.75517100 | 2.14589100 |
| C | 6.62658900 | 5.92110600 | 3.55122200 |
| H | 6.84302500 | 5.96937100 | 4.63037400 |
| H | 6.22081400 | 6.90286200 | 3.25635000 |

| | | | |
|---|---|---|---|
| H | 7.58215400 | 5.78300700 | 3.02458700 |
| C | 4.28491300 | 5.03018200 | 3.92078300 |
| H | 3.55655200 | 4.25057300 | 3.65365300 |
| H | 3.85769300 | 6.00109200 | 3.61938500 |
| H | 4.38957800 | 5.03680900 | 5.01722400 |
| C | 2.67657800 | 0.09309300 | 2.40576400 |
| C | 2.60493800 | -0.05716300 | 1.01978700 |
| C | 1.41302000 | -0.29969500 | 0.34392900 |
| C | 0.23006700 | -0.41054800 | 1.07150900 |
| C | 0.25603300 | -0.27651700 | 2.45581700 |
| C | 1.47236000 | -0.03191600 | 3.08705300 |
| C | 5.19894100 | -0.77384000 | 2.85799800 |
| C | 5.05733900 | -1.96111800 | 3.57502900 |
| C | 5.90992600 | -3.04926400 | 3.43701800 |
| C | 6.95986600 | -2.96592500 | 2.52461200 |
| C | 7.13720500 | -1.80515800 | 1.77801000 |
| C | 6.25926200 | -0.73585500 | 1.95265900 |
| B | 4.12758300 | 0.42178500 | 3.00911000 |

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Table S28

M06-2X-D3/def2-TZVP

**B/Bi-Prod**

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| Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|
| Number | X | Y | Z |

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| | | | |
|---|---|---|---|
| F | 3.68719900 | 0.11323100 | 0.18208500 |
| F | 1.34741000 | -0.30684300 | -1.07087800 |
| F | -0.93439400 | -0.57925400 | 0.37508300 |
| F | -0.84700800 | -0.41130700 | 3.08545600 |
| F | 1.44797200 | 0.03207700 | 4.34321700 |
| F | 3.82066500 | -2.00160000 | 4.32225000 |
| F | 5.43679300 | -4.14866500 | 4.21323500 |
| F | 7.65824100 | -4.09235800 | 2.65037400 |
| F | 8.24025300 | -1.87856900 | 1.19856500 |
| F | 6.63501300 | 0.25595900 | 1.28693900 |
| O | 4.23337800 | 2.56421100 | 1.51374300 |

| | | | |
|---|---|---|---|
| Bi | 6.62155700 | 2.87116300 | 3.45972200 |
| Bi | 4.05080400 | 1.09440100 | 5.24046600 |
| C | 4.74197200 | 1.89412000 | 2.36840500 |
| C | 5.69208200 | 2.30630000 | 5.44523800 |
| H | 6.03959700 | 2.66955300 | 6.42026700 |
| C | 3.19565000 | 0.35373300 | 7.22822800 |
| H | 4.00119600 | 0.60287300 | 7.93389800 |
| C | 2.95878600 | -1.14539500 | 7.16115300 |
| H | 2.22979600 | -1.39672900 | 6.37721900 |
| H | 2.54896200 | -1.49194500 | 8.12462400 |
| H | 3.87865100 | -1.71145400 | 6.96200500 |
| C | 1.93484600 | 1.14756400 | 7.53385300 |
| H | 2.12458500 | 2.22796800 | 7.60117900 |
| H | 1.52128900 | 0.81901800 | 8.50199300 |
| H | 1.16128200 | 0.97593300 | 6.77053900 |
| C | 5.58052000 | 4.90146800 | 3.17472100 |
| H | 5.41238500 | 4.87193300 | 2.08573800 |
| C | 6.51749200 | 6.04352000 | 3.54465700 |
| H | 6.73781800 | 6.04779300 | 4.62426000 |
| H | 6.05705800 | 7.01728300 | 3.30490800 |
| H | 7.47590500 | 5.99081600 | 3.00695200 |
| C | 4.23964700 | 4.99109200 | 3.88084500 |
| H | 3.55990000 | 4.18007000 | 3.57788700 |
| H | 3.74216600 | 5.94474700 | 3.63361800 |
| H | 4.35452100 | 4.94617500 | 4.97532600 |
| C | 2.67179300 | 0.14103000 | 2.30340500 |
| C | 2.58182000 | 0.02708500 | 0.91428000 |
| C | 1.38418800 | -0.20649200 | 0.24623500 |
| C | 0.21346700 | -0.35185100 | 0.98664000 |
| C | 0.25923700 | -0.26301400 | 2.37393000 |
| C | 1.48014700 | -0.02660400 | 3.00102300 |
| C | 5.16712800 | -0.78011900 | 2.82536400 |
| C | 4.90151700 | -1.95010400 | 3.53720200 |
| C | 5.72231900 | -3.07005200 | 3.50356100 |
| C | 6.86383400 | -3.04060000 | 2.70412400 |
| C | 7.16307700 | -1.90086700 | 1.96345900 |
| C | 6.31524700 | -0.79648700 | 2.03331800 |
| B | 4.14459100 | 0.45041200 | 2.85363100 |

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