Supporting Information

Sulfur Dioxide Activation: A Theoretical Investigation into S=O Dual Bond Cleavage by Three-Coordinate Molybdenum(III) Complexes

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Full citation for the Gaussian 09 program

Gaussian 09, revision A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

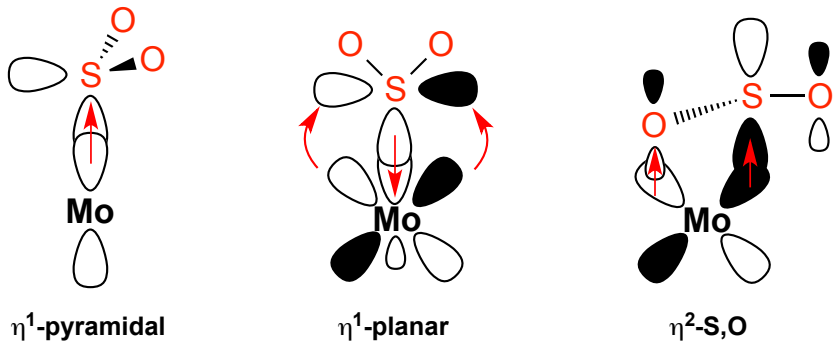

Figure S1. Illustrations of molecular orbital interactions between SO_2 and the Mo metal for three different binding modes.[1]

[1]Ryan, R. R.; Kubas, G. J.; Moody, D. C.; Eller, P. G. *Inorg. Chem.*; Springer Berlin Heidelberg: **1981**; *vol.* 46, p. 47.

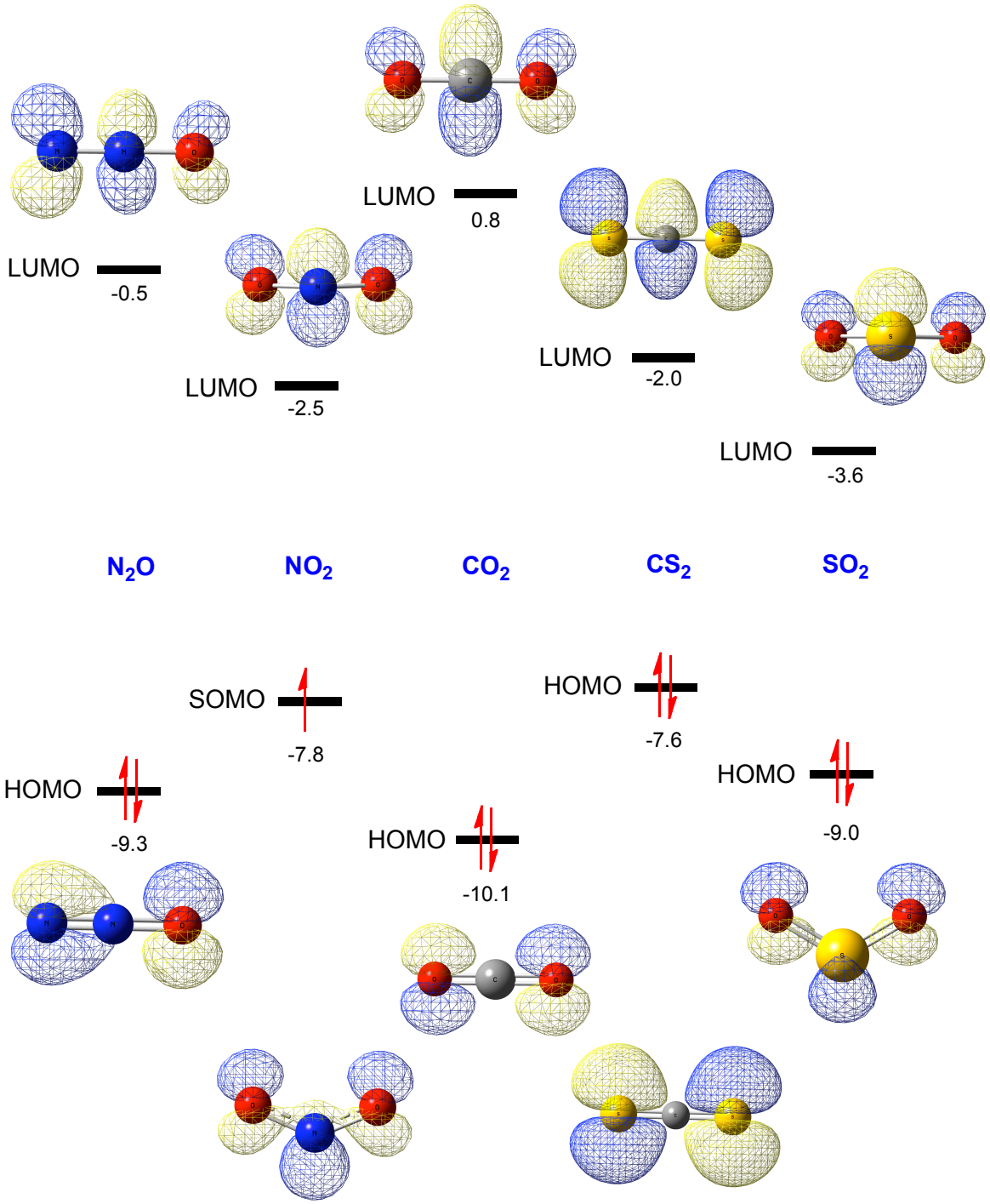

Figure S2. Diagram of frontier orbitals (isoval = 0.08) and their relative energies (eV) for common triatomic molecules: N_2O, NO_2, CO_2, CS_2 and SO_2 at the B3LYP/BS1 level of thoery.

As discussed in the computational details section, the calculated energy values throughout the article were obtained at the M06/BS2//B3LYP/BS1 level of theory. The validity of this was tested with respect to the calculated enthalpy (ΔH) for the removal of one oxygen atom from SO_2 by $Mo(NH_2)_3$ at the CCSD(T)/BS2//B3LYP/BS1 method. As such, calculations were carried out on the corresponding stationary points (**1_Q**, SO_2, **7_D** and SO) at different levels of theory and the results are shown below in Table S1.

Table S1. Effect of DFT functional method on thermal-corrected enthaply (ΔH) energies

Level of theory		**ΔH** (kJ/mol)
$\mathbf{H_{corr}}^a$	**SPE**^{b}	**1_Q**+SO_2 → **7_D**+SO
BPV86	B3LYP	-138.5
BPV86	M06	-120.1
M06	B3LYP	-136.8
M06	M06	-119.2
ωB97XD	B3LYP	-136.8
ωB97XD	M06	-118.4
B3LYP	B3LYP	-136.0
B3LYP	B3LYP-D3	-141.9
B3LYP	B3LYP-D3BJ	-142.1
B3LYP	M06	-116.9
B3LYP	CCSD(T)	-96.1

[a]All energies calculated with BS1 (SDD for Mo; 6-31G(d) for all other elements).
[b]All energies calculated with BS2 (def2-QZVP for Mo; 6-311+G(2d,p) for all other elements).

The experimental reaction enthalpy (ΔH) of -100.4 kJ/mol was reported by Cummins *et al.*[1] for the removal of one oxygen atom from SO_2 by $Mo(N[R]Ar)_3$. As such, calculations were carried out on the corresponding stationary points (**1Ar_Q**, SO_2, **7Ar_D** and SO) at different levels of theory and the results are shown below in Table S2.

Table S2. Effect of DFT functional method on thermal-corrected enthaply (ΔH) energies

Level of theory		**ΔH** (kJ/mol)
$\mathbf{H_{corr}}^a$	**SPE**^{b}	**1Ar_Q**+SO_2 → **7Ar_D**+SO
M06	M06	-36.6
M06	B3LYP-D3BJ	-119.9
B3LYP	B3LYP	-74.8
B3LYP	M06	-44.0
B3LYP	B3LYP-D3BJ	-118.5
B3LYP-D3BJ	B3LYP-D3BJ	-116.8

[a]All energies calculated with BS1 (SDD for Mo; 6-31G(d) for all other elements).
[b]All energies calculated with BS2 (def2-QZVP for Mo; 6-311+G(2d,p) for all other elements).

[1]Johnson, A. R.; Davis, W. M.; Cummins, C. C.; Serron, S.; Nolan, S. P.; Musaev, D. G.; Morokuma, K. *J. Am. Chem. Soc.* **1998**, *120*, 2071.

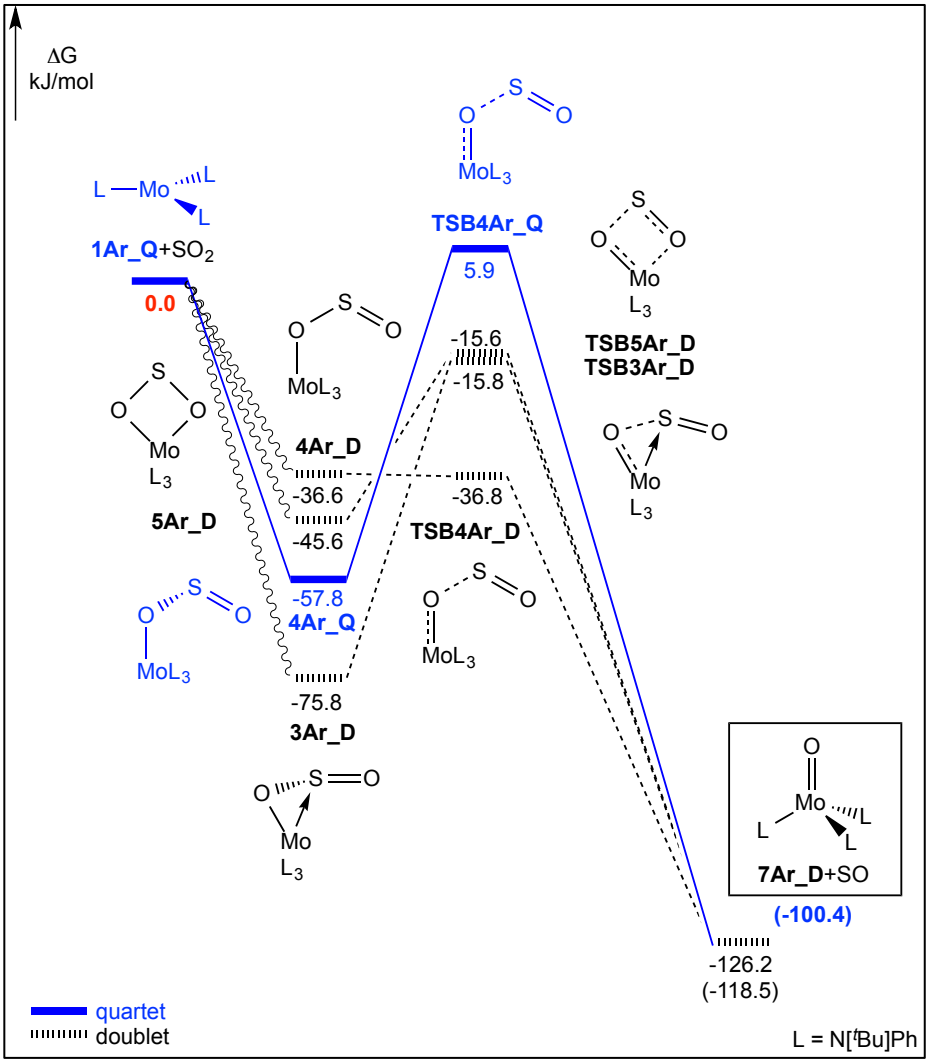

Figure S3. Energy profile for SO bond breaking from (N[^{t}Bu]Ph)$_3$ **(1Ar_Q)**. The thermal-corrected Gibbs energies (ΔG) obtained at the B3LYP-D3BJ/BS2//B3LYP/BS1 level in diethyl ether (Et_2O) are given in kJ/mol. Enthalpy energies (ΔH) in kJ/mol for formation of $L_3Mo{=}O$ + SO are given in parentheses for the experimental value[1] (blue) and the calculated value (black). All energies relative to **1Ar_Q** and free SO_2.

[1]Johnson, A. R.; Davis, W. M.; Cummins, C. C.; Serron, S.; Nolan, S. P.; Musaev, D. G.; Morokuma, K. *J. Am. Chem. Soc.* **1998**, *120*, 2071.

Cartesian coordinates, electronic energies (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for SO_2 and 1 (doublet/quartet)

SO_2

E_{elec} (B3LYP/BS1) = -548.5874633 au
H_{corr} (B3LYP/BS1) = 0.010818 au
G_{corr} (B3LYP/BS1) = -0.017436 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -548.59659247 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -548.69909457 au

0 1

O	0.00000000	1.26117200	-0.37142100
O	0.00000000	-1.26117200	-0.37142100
S	0.00000000	0.00000000	0.37142100

1_D

E_{elec} (B3LYP/BS1) = -236.0733183 au
H_{corr} (B3LYP/BS1) = 0.082904 au
G_{corr} (B3LYP/BS1) = 0.042519 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -236.0179984 au

0 2

N	0.07030500	1.92237100	0.09587300
N	1.66084300	-0.98855200	0.13813900
N	-1.72736300	-0.86919000	0.13808900
H	-2.16712200	-1.09143300	1.02751000
H	-2.14301400	-1.41678700	-0.61738200
H	0.92746000	2.45853000	0.20872700
H	-0.74219300	2.52297300	0.21411900
H	2.03848600	-1.56339000	-0.61698300
H	2.08259900	-1.24140400	1.02812800
Mo	-0.00054100	-0.00287800	-0.09163900

1_Q

E_{elec} (B3LYP/BS1) = -236.0955048 au
H_{corr} (B3LYP/BS1) = 0.082349 au
G_{corr} (B3LYP/BS1) = 0.039625 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -236.0373225 au

0 4

N	1.01802600	-1.69779600	0.00036200
N	-1.97949700	-0.03227000	0.00021500
N	0.96165800	1.73038900	0.00025900
H	1.16284800	2.28748300	0.82716100
H	1.33002200	2.19535200	-0.82601400
H	1.23851300	-2.24822200	-0.82612700
H	1.39883600	-2.15133400	0.82737900
H	-2.56632600	0.05120300	-0.82641600
H	-2.56270700	-0.13607100	0.82711100
Mo	-0.00005900	-0.00001600	-0.00021300

Cartesian coordinates, electronic energies (E_{elec}), thermal corrrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for 2, 4, 5, TS2 & TS4 (quartet)

2_Q

E_{elec} (B3LYP/BS1) = -784.70088877 au
H_{corr} (B3LYP/BS1) = 0.096187 au
G_{corr} (B3LYP/BS1) = 0.043644 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.65948299 au

0 4

Mo	-0.79333700	0.00676700	-0.08048900
O	2.21707100	-1.33397200	0.11236900
O	2.29958600	1.23609400	-0.05192000
N	-0.54651900	-1.61126300	-1.13212100
N	-2.15612900	-0.14586600	1.34058700
N	-0.60238600	1.80782400	-0.79435300
H	0.36296800	-2.07509700	-1.16033400
H	-1.14651700	-1.91877000	-1.89530400
H	-2.46397800	-1.03234400	1.73387300
H	-2.44061600	0.62441600	1.94159500
H	-1.25576800	2.25585800	-1.43456600
H	0.31526700	2.25523900	-0.82552100
S	1.68442500	0.00216500	0.53990200

4_Q

E_{elec} (B3LYP/BS1) = -784.7326939 au
H_{corr} (B3LYP/BS1) = 0.096161 au
G_{corr} (B3LYP/BS1) = 0.045499 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.67590906 au

0 4

Mo	-0.82436900	-0.03769100	-0.02305200
O	2.84589300	-0.57382000	-0.53956900
O	0.93749900	0.95926100	0.27759300
N	-2.17876900	-0.81889900	1.16297200
N	-1.55479400	1.60811600	-0.79728400
N	0.00314300	-1.49559600	-1.01159100
H	-2.09792600	-1.74542800	1.57758600
H	-2.84945600	-0.26153400	1.68896700
H	-2.34416700	1.65225300	-1.43825800
H	-0.93912300	2.40947700	-0.93198900
H	1.01380300	-1.47642600	-1.17632300
H	-0.47249300	-2.10030400	-1.67853000
S	2.38491600	0.31038200	0.59649000

5_Q

E_{elec} (B3LYP/BS1) = -784.7379426 au
H_{corr} (B3LYP/BS1) = 0.095351 au
G_{corr} (B3LYP/BS1) = 0.044327 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.67959386 au

0 4

Mo	0.52300700	-0.03268800	0.00324600
O	-1.11075100	1.29940700	-0.08070900
O	-1.63263200	-1.10828300	-0.00782200
N	1.19510700	-1.04428600	-1.51721300
N	1.90208900	1.40707400	-0.08171600
N	0.87782000	-0.81169400	1.74947300
H	0.83116200	-1.94898100	-1.80809600
H	1.99131000	-0.75864100	-2.08111600
H	1.66940500	2.35261400	0.21554100
H	2.90739900	1.26044100	-0.02592700
H	0.36289600	-1.61511600	2.10560800
H	1.69932700	-0.61509500	2.31491600
S	-2.33161500	0.26943900	-0.07517700

TS2_Q

E_{elec} (B3LYP/BS1) = -784.6979331 au
H_{corr} (B3LYP/BS1) = 0.094686 au
G_{corr} (B3LYP/BS1) = 0.044267 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.65458616 au

0 4

Mo	-0.70536100	-0.04191200	0.05799500
O	1.54396600	1.48296100	-0.26912300
O	2.66992700	-0.78874000	0.28041300
N	-0.40341700	0.51487400	1.89639400
N	-2.02323900	1.03472000	-0.93261300
N	-1.03717700	-1.93476600	-0.28789700
H	0.46303000	0.96439100	2.18922300
H	-0.99572300	0.28256600	2.68953000
H	-2.07328300	2.04998700	-0.87482000
H	-2.56085900	0.69655200	-1.72721000
H	-1.88910600	-2.42104200	-0.01247800
H	-0.28760500	-2.60845400	-0.43916500
S	1.71902400	-0.00382800	-0.56764900

TS4_Q

E_{elec} (B3LYP/BS1) = -784.7245637 au
H_{corr} (B3LYP/BS1) = 0.094043 au
G_{corr} (B3LYP/BS1) = 0.043001 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.66850139 au

0 4

Mo	0.68097400	0.00066200	0.13132400
O	-2.26716100	-0.81522400	-0.70966400
O	-1.01596300	0.88599900	0.72676400
N	0.83276900	-0.38066600	-1.80324000
N	2.11469800	1.34383100	-0.04649300
N	1.06693200	-1.70880900	0.98810700
H	-0.00817700	-0.75829000	-2.24156100
H	1.28258600	0.28132300	-2.43350600
H	2.78439900	1.33702900	-0.81325800
H	2.51097000	1.82971900	0.75569800
H	1.08664500	-2.58266500	0.46704200
H	1.46281200	-1.83533200	1.91727600
S	-2.47224600	0.39710900	0.17045500

Cartesian coordinates, electronic energies (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for 2-6, TS2-TS5 (doublet)

2_D

E_{elec} (B3LYP/BS1) = -784.7110827 au
H_{corr} (B3LYP/BS1) = 0.097260 au
G_{corr} (B3LYP/BS1) = 0.047436 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.67437304 au

0 2

Mo	0.69933900	0.04316500	0.00587700
O	-2.42856500	1.01877200	0.09230100
O	-2.16593300	-1.49109400	-0.27100500
N	0.63616900	1.77156200	-0.88602100
N	1.06911900	-0.05266600	1.92560400
N	1.80990300	-1.23929400	-0.97646800
H	-0.22033000	2.29239800	-1.07244600
H	1.44498000	2.39104000	-0.93375900
H	0.39546600	-0.08898300	2.68537000
H	1.98608600	0.20778300	2.28934000
H	2.06808800	-2.15527300	-0.61293600
H	1.91891200	-1.22174000	-1.98901500
S	-1.55098600	-0.17605100	0.02340300

3_D

E_{elec} (B3LYP/BS1) = -784.7470865 au
H_{corr} (B3LYP/BS1) = 0.095901 au
G_{corr} (B3LYP/BS1) = 0.047983 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.70164402 au

0 2

Mo	0.58022100	0.01645300	-0.02271100
O	-0.67419600	-0.44747200	1.37862200
O	-2.60871400	0.70046500	-0.11304600
N	-0.05259500	1.50814500	-1.05208300
N	2.16991800	0.68332000	0.93767600
N	1.27347700	-1.50604900	-1.02276900
H	-1.07343500	1.64754500	-1.09607600
H	0.48985100	2.19235300	-1.57443800
H	2.24735100	1.62124700	1.33040700
H	2.87773700	0.08391000	1.36278300
H	2.18932000	-1.50235500	-1.46883200
H	0.68517500	-2.23815900	-1.41348700
S	-1.82860100	-0.58233800	0.10307100

4_D

E_{elec} (B3LYP/BS1) = -784.7305616 au
H_{corr} (B3LYP/BS1) = 0.096025 au
G_{corr} (B3LYP/BS1) = 0.044773 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.67504926 au

0 2

Mo	0.72273900	-0.01767100	0.02256800
O	-0.95270000	-1.04636200	0.11510700
O	-2.56525300	0.96130200	0.24047700
N	0.47344800	1.86941900	-0.31466900
N	1.83186500	-0.34201700	1.59193100
N	1.75599300	-0.57129000	-1.50426800
H	-0.29590200	2.38791900	0.11052300
H	1.16368200	2.50647000	-0.71457800
H	1.49956500	-0.20036500	2.54682600
H	2.85053300	-0.29117700	1.57912200
H	2.33747600	-1.41025600	-1.53158800
H	1.62187400	-0.20535900	-2.44880900
S	-2.48861300	-0.50358400	-0.10906200

5_D

E_{elec} (B3LYP/BS1) = -784.7549263 au
H_{corr} (B3LYP/BS1) = 0.095630 au
G_{corr} (B3LYP/BS1) = 0.047341 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.70028488 au

0 2

Mo	0.47068000	-0.03334600	-0.03261600
O	-1.04091100	1.25519200	-0.26506200
O	-1.28652500	-1.02197700	0.33286700
N	1.82023000	1.38145100	-0.15682800
N	1.18265500	-0.66382500	1.67664800
N	0.83958400	-1.15842400	-1.58078100
H	1.57188700	2.31589500	-0.48268200
H	2.76550300	1.38663200	0.22616800
H	0.71890000	-1.39466600	2.20957600
H	1.90723000	-0.20358400	2.21951700
H	0.27368700	-1.96855900	-1.81553100
H	1.70632600	-1.12143300	-2.10775600
S	-2.31186800	0.22538300	0.06280400

6_D

E_{elec} (B3LYP/BS1) = -784.7414765 au
H_{corr} (B3LYP/BS1) = 0.095660 au
G_{corr} (B3LYP/BS1) = 0.047736 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.69526538 au

0 2

Mo	-0.37373200	-0.01301600	0.05439300
O	1.20398000	-0.88047600	-1.05973900
O	1.24545600	1.33976900	-0.09371700
N	-1.47184600	1.59539500	-0.04667600
N	-1.65010400	-0.90283700	-1.12154900
N	-0.73484200	-0.92705100	1.73547100
H	-1.06483100	2.50878400	0.13724000
H	-2.35760900	1.67726800	-0.53931000
H	-1.32849300	-1.62837800	-1.75919500
H	-2.55007300	-0.53039700	-1.41798700
H	-0.12706400	-0.84970300	2.54543000
H	-1.67071800	-1.22992900	1.99036300
S	2.01235000	-0.08961700	0.12599200

TS2_D

E_{elec} (B3LYP/BS1) = -784.7019784 au
H_{corr} (B3LYP/BS1) = 0.095230 au
G_{corr} (B3LYP/BS1) = 0.046560 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.66483018 au

0 2

Mo	0.64399100	-0.01409400	-0.00599000
O	-2.62837700	-1.12328100	0.11481000
O	-1.74018500	1.31046700	0.35234900
N	1.47749000	-1.54651600	-0.86917000
N	1.08165000	1.67962300	-0.84745100
N	1.16179500	-0.13974400	1.86159600
H	1.06521800	-2.02092900	-1.67141200
H	2.46346400	-1.79067700	-0.78903300
H	0.36963600	2.37273600	-1.07101400
H	2.01807000	1.99650300	-1.08364700
H	1.10609500	0.64798600	2.50581400
H	1.44840800	-0.98784400	2.34742100
S	-1.66353500	-0.06730400	-0.29616500

TS3_D

E_{elec} (B3LYP/BS1) = -784.7273480 au
H_{corr} (B3LYP/BS1) = 0.095012 au
G_{corr} (B3LYP/BS1) = 0.046175 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.67428653 au

0 2

Mo	0.64351400	-0.04359800	-0.03247700
O	-0.77833800	-0.76536100	1.14934100
O	-2.56647300	1.00604700	0.48423300
N	0.01509300	1.29570900	-1.27360300
N	2.04453800	0.72297700	1.06549700
N	1.40447400	-1.42714800	-1.13828400
H	-0.86938700	1.77240000	-1.07947200
H	0.54393700	1.76756000	-2.00703400
H	1.91202100	1.53450000	1.67118000
H	3.03897300	0.58134100	0.89163900
H	2.15719000	-2.05314300	-0.85107000
H	1.00251000	-1.73858100	-2.02379000
S	-2.27254300	-0.47563800	0.49295700

TS4_D

E_{elec} (B3LYP/BS1) = -784.7304939 au
H_{corr} (B3LYP/BS1) = 0.095104 au
G_{corr} (B3LYP/BS1) = 0.046605 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.67526684 au

0 2

Mo	0.69405100	-0.01221800	0.01540500
O	-2.44996300	0.99179600	0.20373100
O	-0.96150800	-1.09053600	0.08936100
N	1.66485900	-0.05879300	1.70347500
N	1.90711500	-0.80815700	-1.24551400
N	0.49697300	1.79303100	-0.64996400
H	1.26887900	0.25875100	2.58907000
H	2.68307200	-0.05078900	1.76678000
H	1.86512900	-0.66702800	-2.25640600
H	2.53640300	-1.58133900	-1.02293500
H	-0.30272700	2.35940700	-0.36424700
H	1.23244300	2.37343500	-1.05416400
S	-2.47651300	-0.49199600	-0.08161400

TS5_D

E_{elec} (B3LYP/BS1) = -784.7407725 au
H_{corr} (B3LYP/BS1) = 0.094702 au
G_{corr} (B3LYP/BS1) = 0.048548 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.69080991 au

0 2

Mo	-0.39829600	-0.01223700	0.07193000
O	1.17179100	-0.98372500	-0.87931800
O	1.13697600	1.31109000	-0.12325700
N	-1.51577900	1.55958500	-0.23142400
N	-1.54490700	-1.02442700	-1.12036400
N	-0.77907300	-0.77972600	1.82000900
H	-1.12125700	2.49330900	-0.14091100
H	-2.38159800	1.57964300	-0.76570700
H	-1.14076400	-1.80568100	-1.63710900
H	-2.31983600	-0.61776000	-1.64300900
H	-0.38752700	-0.36538900	2.66373900
H	-1.64537200	-1.27287200	2.01913300
S	2.13331000	-0.02526600	0.07661600

Cartesian coordinates and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for 4AF & 5AF

4AF

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.67692212 au

0 2

Mo	-0.82436900	-0.03769100	-0.02305200
O	2.84589300	-0.57382000	-0.53956900
O	0.93749900	0.95926100	0.27759300
N	-2.17876900	-0.81889900	1.16297200
N	-1.55479400	1.60811600	-0.79728400
N	0.00314300	-1.49559600	-1.01159100
H	-2.09792600	-1.74542800	1.57758600
H	-2.84945600	-0.26153400	1.68896700
H	-2.34416700	1.65225300	-1.43825800
H	-0.93912300	2.40947700	-0.93198900
H	1.01380300	-1.47642600	-1.17632300
H	-0.47249300	-2.10030400	-1.67853000
S	2.38491600	0.31038200	0.59649000

5AF

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.68637682 au

0 2

Mo	0.52300700	-0.03268800	0.00324600
O	-1.11075100	1.29940700	-0.08070900
O	-1.63263200	-1.10828300	-0.00782200
N	1.19510700	-1.04428600	-1.51721300
N	1.90208900	1.40707400	-0.08171600
N	0.87782000	-0.81169400	1.74947300
H	0.83116200	-1.94898100	-1.80809600
H	1.99131000	-0.75864100	-2.08111600
H	1.66940500	2.35261400	0.21554100
H	2.90739900	1.26044100	-0.02592700
H	0.36289600	-1.61511600	2.10560800
H	1.69932700	-0.61509500	2.31491600
S	-2.33161500	0.26943900	-0.07517700

Cartesian coordinates, electronic energies (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for TSB4 & TSB5 (quartet)

TSB4_Q

E_{elec} (B3LYP/BS1) = -784.7118325 au
H_{corr} (B3LYP/BS1) = 0.093581 au
G_{corr} (B3LYP/BS1) = 0.040572 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.64751566 au

0 4

Mo	0.74858400	-0.01491300	-0.00428900
O	-2.47554100	0.37465500	0.88955600
O	-0.72112400	-0.40245300	-1.07248400
N	2.44226900	0.13208300	-0.98395200
N	0.42843900	1.79706800	0.66531700
N	1.01428100	-1.45386600	1.29827900
H	2.95117000	-0.67861900	-1.33299800
H	2.67708700	0.95332900	-1.53951500
H	1.12591500	2.37891700	1.12443500
H	-0.51423000	2.05639600	0.95426000
H	0.25807200	-2.08163500	1.56338900
H	1.77604400	-1.51037500	1.97067600
S	-2.58351100	-0.22476600	-0.49713700

TSB5_Q
E_{elec} (B3LYP/BS1) = -784.7147194 au
H_{corr} (B3LYP/BS1) = 0.093506 au
G_{corr} (B3LYP/BS1) = 0.043620 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.65267277 au

0 4

Mo	-0.53466000	0.00007300	-0.00418900
N	-0.81563000	-1.73227100	-0.88648200
N	-2.25549000	-0.00058600	0.95781500
N	-0.81575400	1.73305200	-0.88523100
H	-0.12210600	-2.12418700	-1.52012000
H	-1.72839200	-2.15359600	-1.03837900
H	-2.61360300	0.83107400	1.42462600
H	-2.61376200	-0.83297500	1.42321900
H	-0.12242300	2.12509300	-1.51900500
H	-1.72870400	2.15382000	-1.03752600
O	1.67984400	0.00026600	-1.00436900
S	2.42491900	-0.00015000	0.34663500
O	0.79442300	-0.00042100	1.32864900

Cartesian coordinates, electronic energies (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for TSB3-TSB5 (doublet)

TSB3_D

E_{elec} (B3LYP/BS1) = -784.7305138 au
H_{corr} (B3LYP/BS1) = 0.094741 au
G_{corr} (B3LYP/BS1) = 0.047013 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.6805577 au

0 2

Mo	0.58018000	-0.07068500	0.04605600
O	-0.32258300	-0.52278900	1.52180800
O	-2.69847900	0.80674400	-0.24200400
N	0.02966100	1.56157400	-0.85334800
N	2.24572200	0.84619800	0.53394700
N	1.13415000	-1.54877100	-1.11453700
H	-0.96632000	1.74523000	-1.00498300
H	0.60188400	2.39397500	-0.97815700
H	2.40417000	1.85078300	0.49094000
H	2.96029500	0.40134800	1.10702200
H	1.78143500	-1.45273200	-1.89273800
H	0.69141500	-2.46345400	-1.11704800
S	-1.97116800	-0.48694000	0.07873400

TSB4_D

E_{elec} (B3LYP/BS1) = -784.7276197 au
H_{corr} (B3LYP/BS1) = 0.094595 au
G_{corr} (B3LYP/BS1) = 0.046510 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.66603503 au

0 2

Mo	-0.51257200	-0.04950100	-0.24546500
O	0.77192500	-1.24680400	-0.47028100
O	2.65029800	1.07546600	0.23893600
N	-0.04009700	1.69864700	-0.95477400
N	-2.23266300	-0.53166400	-1.04446900
N	-1.38753400	-0.08673800	1.51002400
H	0.93805700	1.99044100	-0.88640700
H	-0.67709600	2.48366600	-1.06225900
H	-2.31676700	-0.93076000	-1.97732000
H	-3.12856200	-0.56503000	-0.56034100
H	-2.31099800	-0.47157100	1.69507900
H	-0.93086100	0.19956500	2.37053900
S	1.86588800	0.03187800	1.02207700

TSB5_D

E_{elec} (B3LYP/BS1) = -784.7299867 au
H_{corr} (B3LYP/BS1) = 0.094394 au
G_{corr} (B3LYP/BS1) = 0.046924 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -784.67187569 au

0 2

Mo	-0.47422600	0.00223000	-0.01739300
O	1.38899800	0.52288100	0.79671000
O	0.63945400	-0.40566300	-1.37669700
N	-0.84323500	1.89347000	0.38143500
N	-2.21667400	-0.36028000	-0.82621500
N	-0.70873600	-1.37689100	1.35833800
H	-0.09990300	2.49030700	0.72985500
H	-1.76677200	2.29564600	0.49705500
H	-2.45363500	-0.18471800	-1.80170900
H	-3.05016100	-0.62259100	-0.30105700
H	-1.26415700	-2.21944900	1.23745000
H	-0.09316400	-1.44206300	2.16396400
S	2.42488600	-0.15266400	-0.22187900

Cartesian coordinates, electronic (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for SO (singlet/triplet), 7 & 8 (doublet)

SO_S

E_{elec} (B3LYP/BS1) = -473.3057342 au
H_{corr} (B3LYP/BS1) = 0.005885 au
G_{corr} (B3LYP/BS1) = -0.018309 au
SPE (M06/BS2//B3LYP/BS1, Solvent = (Et_2O) = -473.30247081 au

0 1

S	0.00000000	0.00000000	0.50590900
O	0.00000000	0.00000000	-1.01181700

SO_T

E_{elec} (B3LYP/BS1) = -473.3524890 au
H_{corr} (B3LYP/BS1) = 0.005886 au
G_{corr} (B3LYP/BS1) = -0.019344 au

SPE (M06/BS2//B3LYP/BS1, Solvent = (Et_2O) = -473.34276993 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = (Et_2O) = -473.41977809 au

0 3

S	0.00000000	0.00000000	0.50585600
O	0.00000000	0.00000000	-1.01171200

7_D

E_{elec} (B3LYP/BS1) = -311.3898273 au

H_{corr} (B3LYP/BS1) = 0.087987 au

G_{corr} (B3LYP/BS1) = 0.045261 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -311.33636357 au

0 2

Mo	-0.05140800	-0.06340500	0.07514000
O	-0.23938300	-0.66997500	1.66729000
N	1.39220300	-0.96668300	-0.90595200
N	-1.75087100	0.08364300	-0.90091200
N	0.76957000	1.72604900	0.04516900
H	1.59907300	-1.95921200	-0.84138000
H	2.04555200	-0.49732700	-1.52864300
H	-2.60404000	-0.38230600	-0.60427700
H	-1.89331400	0.57725200	-1.77830600
H	0.27781900	2.53878800	0.41169900
H	1.77280200	1.84454100	0.17859100

8_D

E_{elec} (B3LYP/BS1) = -634.3611455 au
H_{corr} (B3LYP/BS1) = 0.087161 au
G_{corr} (B3LYP/BS1) = 0.043596 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -634.30882269 au

0 2

Mo	0.04012000	-0.01945000	0.06195700
N	1.38423700	-1.05398700	-0.89566500
N	-1.67478100	0.12302500	-0.85132200
N	0.74398800	1.80434600	0.10109600
H	1.56562900	-2.04091600	-0.73257000
H	1.86391700	-0.72418700	-1.73074400
H	-2.46276700	-0.49565700	-0.67891800
H	-1.82872700	0.69319200	-1.68018400
H	0.15852000	2.59242800	0.37598600
H	1.71289100	1.99233400	0.35657100
S	-0.24927400	-0.84708400	2.03640500

Cartesian coordinates, electronic energies (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for 1Ar, 4Ar & TSB4Ar (quartet)

1Ar_Q

E_{elec} (B3LYP/BS1) = -1400.9642629 au
H_{corr} (B3LYP/BS1) = 0.695656 au
G_{corr} (B3LYP/BS1) = 0.584713 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1400.32178348 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -1401.60499034 au

0 4

Mo	0.01126900	0.01179900	-0.69875300
N	-0.65456400	1.90803800	-0.65028200
N	-1.30733400	-1.50422100	-0.65817300
N	1.98167600	-0.37902900	-0.62004500
C	-1.24479100	2.23508200	0.61555200
C	-2.64204100	2.21464200	0.80047200
C	-0.43592900	2.52911100	1.72970400
C	-3.20476000	2.48496400	2.04832000
H	-3.28040500	1.97125000	-0.04329800
C	-1.00117400	2.78879300	2.97957300
H	0.64259600	2.53691900	1.60434000
C	-2.38736700	2.77194300	3.14480900
H	-4.28556300	2.46281200	2.16562900
H	-0.35312500	3.00354100	3.82549200
H	-2.82704300	2.97612000	4.11738700
C	-1.31035200	-2.18260500	0.60504600
C	-0.59378800	-3.38126000	0.79265500
C	-1.98345300	-1.63441500	1.71327300
C	-0.56514100	-4.01340400	2.03614700
H	-0.04660300	-3.80023700	-0.04609200
C	-1.94505100	-2.26370800	2.95893400
H	-2.52638600	-0.70252800	1.58584700
C	-1.24131500	-3.45802400	3.12575000
H	-0.00594400	-4.93829100	2.15551000
H	-2.46783500	-1.81638600	3.80052200
H	-1.21469400	-3.94860700	4.09503500
C	2.53510600	-0.06929900	0.66638900
C	2.39183000	-0.96191600	1.74560900
C	3.18455600	1.15828000	0.90496800
C	2.87966100	-0.63920400	3.01317000
H	1.87854500	-1.90409500	1.57946200
C	3.67915000	1.47478600	2.17078300

H	3.28184500	1.86614700	0.08747300
C	3.52925900	0.57740400	3.23134500
H	2.74818100	-1.34209300	3.83189700
H	4.17639200	2.42856400	2.33018200
H	3.91007800	0.82684200	4.21810700
C	-2.28058400	-1.96323200	-1.69407700
C	2.89493900	-0.97393300	-1.64113700
C	-0.56160000	2.99457900	-1.67110500
C	-2.00852300	-3.42060200	-2.12495100
H	-2.70519400	-3.71805600	-2.91813100
H	-0.98762200	-3.52718900	-2.50978200
H	-2.13731800	-4.11747400	-1.29153100
C	-2.14465800	-1.05444000	-2.92619900
H	-1.13629600	-1.11059000	-3.35305100
H	-2.85413600	-1.36254900	-3.70327400
H	-2.35670300	-0.01039100	-2.66962500
C	-3.72310200	-1.85306400	-1.15625700
H	-3.87060900	-2.48817500	-0.27710100
H	-3.94927300	-0.81932400	-0.87144700
H	-4.44360700	-2.16508400	-1.92194800
C	3.50351000	-2.29142600	-1.11476400
H	4.10201100	-2.12343900	-0.21385100
H	2.71412000	-3.01089800	-0.86964400
H	4.15563100	-2.74178900	-1.87278000
C	2.07874500	-1.28175100	-2.90704100
H	2.72264100	-1.73472200	-3.67019400
H	1.26634000	-1.98520500	-2.69109800
H	1.64500200	-0.37010900	-3.33451200
C	4.03611100	-0.00246200	-2.01224800
H	3.63278400	0.94272500	-2.39332700
H	4.67193400	0.21840900	-1.14956500
H	4.67165000	-0.44153900	-2.79078400
C	0.14642000	2.43661600	-2.91628400
H	-0.41529400	1.60250800	-3.35331000
H	0.23494500	3.21696600	-3.68141500
H	1.15663400	2.08783500	-2.67328800
C	-1.95752100	3.50526400	-2.08761400
H	-1.86401300	4.27425900	-2.86401800
H	-2.56635600	2.68731700	-2.48999500
H	-2.49263200	3.94945100	-1.24313100
C	0.26632900	4.17524900	-1.11948900
H	0.36571900	4.96221100	-1.87687900
H	-0.20599700	4.61764600	-0.23656800
H	1.27107400	3.84142400	-0.83662400

4Ar_Q

E_{elec} (B3LYP/BS1) = -1949.5797022 au
H_{corr} (B3LYP/BS1) = 0.708841au
G_{corr} (B3LYP/BS1) = 0.591474 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1950.11767217 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -1950.34728036 au

0 4

Mo	-0.76545000	-0.16335800	-0.18828400
O	2.03856400	-0.28271100	2.77089100
O	0.96405200	0.60533600	0.58549600
N	-1.97305000	-0.82142100	1.26764500
N	-1.38243600	1.49757900	-1.12544300
N	0.12634100	-1.55825500	-1.31093500
S	1.62690600	0.95375800	2.01249300
C	-0.54190800	-1.74832500	-2.56561200
C	-1.65062100	-2.60729800	-2.65620500
C	-0.11047500	-1.08874700	-3.73385700
C	-2.31496700	-2.79096100	-3.87147300
H	-1.98190800	-3.13192700	-1.76670800
C	-0.76953500	-1.28104300	-4.94711000
H	0.74136400	-0.41945800	-3.67521600
C	-1.87861300	-2.13090200	-5.02086800
H	-3.17219400	-3.45765500	-3.91624100
H	-0.42032800	-0.76296300	-5.83676700
H	-2.39274600	-2.27748800	-5.96694500
C	-2.70268200	-1.98868300	0.85326100
C	-2.25772500	-3.28413600	1.17962900
C	-3.88526700	-1.85749100	0.10416500
C	-2.97326100	-4.40816100	0.76886800
H	-1.33996000	-3.39554600	1.74629100
C	-4.59767600	-2.98548100	-0.30986000
H	-4.24187900	-0.86414900	-0.14613600
C	-4.14658700	-4.26409100	0.02075500
H	-2.61207300	-5.39964300	1.02990600
H	-5.50807200	-2.85951400	-0.89002100
H	-4.70195500	-5.14174500	-0.29887600
C	-2.78394500	1.43842400	-1.42788500
C	-3.73779000	2.09795400	-0.62591700
C	-3.24284100	0.70640900	-2.53676900
C	-5.09774300	2.01735300	-0.91860200
H	-3.39994000	2.67212800	0.23038600
C	-4.60842200	0.61825300	-2.82186500
H	-2.51976200	0.21315500	-3.17682600
C	-5.54124700	1.27088900	-2.01610500

H	-5.81495000	2.53515800	-0.28663700
H	-4.93650400	0.04131200	-3.68245300
H	-6.60252800	1.20605700	-2.24031800
C	-2.23067300	-0.33996100	2.67579000
C	-0.64623800	2.77279600	-1.47463100
C	-0.49623900	3.65810800	-0.22070100
H	0.03814000	3.12100000	0.56701900
H	0.06599900	4.57027600	-0.45675000
H	-1.47433800	3.96043700	0.16876700
C	0.74590400	2.41875600	-2.03051300
H	1.29549200	3.33719500	-2.27005700
H	1.33382000	1.84965400	-1.30856700
H	0.65077400	1.83067700	-2.94933200
C	-1.39655700	3.56458000	-2.56478500
H	-1.54950800	2.95848500	-3.46386100
H	-2.37280800	3.92107400	-2.22422100
H	-0.79878600	4.43961700	-2.84366900
C	1.42595400	-2.31002000	-1.10669800
C	2.62609100	-1.40972800	-1.46488100
H	2.60874100	-1.13206400	-2.52458900
H	2.61421100	-0.49790900	-0.86366200
H	3.56877100	-1.93810300	-1.27523400
C	1.52351600	-2.75400000	0.36287600
H	1.50461600	-1.91145000	1.05568800
H	0.70321400	-3.43629200	0.60983300
H	2.46731700	-3.28813400	0.52651900
C	1.46703000	-3.57970400	-1.98126800
H	0.61528900	-4.23577500	-1.77292300
H	1.46901000	-3.35060400	-3.05091700
H	2.38479300	-4.13427800	-1.75568700
C	-3.70902700	-0.54968800	3.06396200
H	-3.98169900	-1.60843700	3.09055300
H	-3.87920200	-0.13466700	4.06400000
H	-4.38034100	-0.03916000	2.36527600
C	-1.94132900	1.16752300	2.75232800
H	-0.91321700	1.40451200	2.46996400
H	-2.61717900	1.72538300	2.09793500
H	-2.08721200	1.52249300	3.77902800
C	-1.33259500	-1.09737400	3.67610300
H	-0.27301800	-0.97054900	3.43764500
H	-1.50208100	-0.72456800	4.69413400
H	-1.56269000	-2.16780200	3.67714800

TSB4Ar_Q
E_{elec} (B3LYP/BS1) = -1949.5557871 au
H_{corr} (B3LYP/BS1) = 0..706896 au
G_{corr} (B3LYP/BS1) = 0.589714 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1948.90497887 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -1950.32125948 au

0 4

Mo	-0.20240800	0.53058800	0.52257700
O	0.80119500	4.39238900	1.50069700
O	-0.71489100	1.83591600	1.72897200
N	-1.92573500	-0.52815700	0.65986600
N	0.21742200	1.20702700	-1.30939400
N	1.36187700	-0.42544600	1.31691700
S	-0.04024400	3.58524700	2.46366000
C	-2.26525800	-1.25200000	-0.52924600
C	-1.80485800	-2.56709400	-0.71691400
C	-3.07367100	-0.68085100	-1.53161700
C	-2.14054100	-3.28583700	-1.86656000
H	-1.18601800	-3.01969100	0.05054000
C	-3.41145100	-1.40160800	-2.67734000
H	-3.42696800	0.33751500	-1.40448300
C	-2.94487900	-2.70857900	-2.85064700
H	-1.77223200	-4.30119800	-1.98892900
H	-4.03808800	-0.94145400	-3.43732600
H	-3.20815200	-3.26926500	-3.74355500
C	1.05107700	0.35144100	-2.11375400
C	0.49963200	-0.72101900	-2.83455300
C	2.43945400	0.56682900	-2.19590900
C	1.31199300	-1.55484200	-3.60670900
H	-0.56893800	-0.89579700	-2.78951900
C	3.24777000	-0.26443900	-2.97104500
H	2.87815000	1.38689600	-1.63909400
C	2.68752100	-1.33167300	-3.67952100
H	0.86174600	-2.38000900	-4.15216500
H	4.31792000	-0.07946100	-3.01908400
H	3.31825700	-1.97983600	-4.28200700
C	1.31819100	-1.85908700	1.22954900
C	0.81360700	-2.64757600	2.28043200
C	1.79771600	-2.50937700	0.08055200
C	0.78343000	-4.03823500	2.17971400
H	0.43827400	-2.15888500	3.17256300
C	1.76165000	-3.90225200	-0.02060100
H	2.20151400	-1.91359000	-0.73028900
C	1.25474800	-4.67313400	1.02621300

H	0.38855500	-4.62772900	3.00343900
H	2.13586300	-4.38150400	-0.92153700
H	1.22895500	-5.75675800	0.94864800
C	-2.95634900	-0.53139100	1.76895700
C	-0.24921200	2.47876200	-1.98343700
C	2.50069700	0.16287400	2.11929600
C	-3.83684300	0.73105300	1.65660100
H	-3.21856400	1.63140000	1.70539800
H	-4.39402900	0.73648400	0.71338400
H	-4.56744300	0.76626300	2.47476700
C	-3.85595800	-1.78215800	1.69239100
H	-4.44499400	-1.81623100	0.77156400
H	-3.26799300	-2.70376500	1.75682600
H	-4.55514400	-1.76677800	2.53617100
C	-2.25419000	-0.55060900	3.13851600
H	-1.59246000	0.30865700	3.26152400
H	-3.00365200	-0.52125000	3.93870800
H	-1.67038200	-1.46878500	3.25519300
C	2.05685000	0.39022200	3.57981700
H	1.18458200	1.04851200	3.62463900
H	1.79750400	-0.55677800	4.06438400
H	2.86609100	0.85071400	4.16019600
C	2.92709900	1.49788600	1.48724800
H	3.69289300	1.97970300	2.10636900
H	3.34908500	1.33148800	0.49227700
H	2.09906400	2.20279400	1.39245300
C	3.73098100	-0.76775100	2.10739300
H	3.53600000	-1.72067500	2.60696100
H	4.06029800	-0.97858800	1.08468900
H	4.55505100	-0.27402200	2.63505500
C	-1.38507700	3.11549400	-1.16722800
H	-2.21800000	2.41773100	-1.02660000
H	-1.04277700	3.45065400	-0.18845400
H	-1.76717000	3.99092900	-1.70414900
C	0.90794000	3.49219300	-2.09576800
H	0.54924200	4.41713900	-2.56380800
H	1.29981800	3.74285000	-1.10528800
H	1.72202900	3.10477300	-2.71587600
C	-0.79365700	2.16273400	-3.39328100
H	-0.01772400	1.77027200	-4.05639900
H	-1.60733300	1.43125900	-3.34729000
H	-1.18463900	3.08218500	-3.84385200

Cartesian coordinates, electronic (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and/or single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for 3Ar-5Ar, TSB3Ar-TSB5Ar & 7Ar (doublet)

3Ar_D

E_{elec} (B3LYP/BS1) = -1949.5834277 au
H_{corr} (B3LYP/BS1) = 0.710239 au
G_{corr} (B3LYP/BS1) = 0.598858 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1948.95512713 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -1950.36153194 au

0 2

Mo	0.42080300	-0.23647900	-0.72367700
O	0.58099200	-0.70709100	-2.70561500
O	2.61877300	-2.24498700	-2.26553600
N	1.29754700	-1.12167700	0.84580500
N	0.70749100	1.73289400	-0.60577200
N	-1.48500300	-0.84292100	-0.98310200
S	2.16862000	-0.81268700	-2.34046100
C	0.29247900	-1.56274100	1.78785300
C	-0.17608000	-0.69325900	2.78769200
C	-0.20842500	-2.87717100	1.75784000
C	-1.11787400	-1.12416300	3.72513900
H	0.21204100	0.31734500	2.83395900
C	-1.15367800	-3.30290200	2.68974700
H	0.14852900	-3.55754800	0.99371700
C	-1.61298900	-2.42789100	3.67992200
H	-1.46267600	-0.43411500	4.49085200
H	-1.52890200	-4.32210800	2.64588300
H	-2.34553100	-2.76309200	4.40924600
C	-2.45854000	0.09565000	-0.49734000
C	-3.02099000	-0.05807700	0.78112200
C	-2.89721900	1.16996600	-1.29496900
C	-3.99127300	0.83174000	1.24575700
H	-2.69496600	-0.88400500	1.40210300
C	-3.86670600	2.05830500	-0.82853300
H	-2.46230100	1.30459000	-2.27925600
C	-4.41938100	1.89256500	0.44499700
H	-4.41376700	0.69178000	2.23745800
H	-4.19085000	2.88094500	-1.46097900
H	-5.17636900	2.58311600	0.80696400
C	0.57498700	2.24733400	0.73638800
C	1.70198500	2.43373200	1.55886200
C	-0.68440300	2.60658700	1.24167400
C	1.57068000	2.96138000	2.84276600

H	2.68121900	2.15471800	1.18871100
C	-0.81416500	3.12986400	2.53046200
H	-1.55923900	2.48294200	0.61609100
C	0.30977000	3.31008300	3.33695100
H	2.45532200	3.09762600	3.45955300
H	-1.80069200	3.39959800	2.89762900
H	0.20848400	3.71984700	4.33821400
C	-2.05516900	-1.96259500	-1.83674300
C	1.12759600	2.76548000	-1.64494400
C	2.71776000	-1.47105900	1.27032100
C	2.66605000	2.83805600	-1.72978900
H	2.96757500	3.55612000	-2.50202200
H	3.10238800	3.16966700	-0.78247200
H	3.09259500	1.86467900	-1.98787000
C	0.57929200	4.16052500	-1.27340200
H	0.84216600	4.86374500	-2.07122600
H	-0.51140500	4.14674200	-1.17987100
H	0.99911300	4.54315300	-0.33946300
C	0.54909700	2.40806500	-3.02499700
H	0.90939700	1.45334700	-3.40616000
H	-0.54400500	2.36210200	-2.98466000
H	0.82868000	3.18764700	-3.74268800
C	-2.36281800	-1.47375100	-3.26876700
H	-1.46042100	-1.09886700	-3.75500200
H	-2.75878500	-2.30548700	-3.86467700
H	-3.12308700	-0.68580900	-3.26436100
C	-1.07051000	-3.14488000	-1.88716700
H	-0.91675000	-3.55922900	-0.88673200
H	-1.49684300	-3.93856100	-2.51177500
H	-0.10473200	-2.87261000	-2.31076400
C	-3.36153800	-2.49091300	-1.20239900
H	-4.16060500	-1.74440400	-1.20248100
H	-3.70940600	-3.35213500	-1.78389500
H	-3.19666200	-2.82262300	-0.17187000
C	3.76285600	-0.68745900	0.45510000
H	3.90701500	-1.12038900	-0.53430700
H	3.49470800	0.36717700	0.35414300
H	4.72850400	-0.74087800	0.96996900
C	2.98309800	-2.97880200	1.07700700
H	4.02900600	-3.20175800	1.32199400
H	2.35653900	-3.58790800	1.73566000
H	2.80525800	-3.26477500	0.03677900
C	2.92582500	-1.10477900	2.75830800
H	3.96036400	-1.33457200	3.03665200
H	2.75427800	-0.03759700	2.93367200
H	2.27075600	-1.67284500	3.42311400

4Ar_D

E_{elec} (B3LYP/BS1) = -1949.5870001 au
H_{corr} (B3LYP/BS1) = 0.708966 au
G_{corr} (B3LYP/BS1) = 0.593379 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1948.93328646 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -1950.34111685 au

0 2

Mo	0.21175900	-0.04586600	-0.23164100
O	2.80829100	0.29366200	-3.06556200
O	1.97510300	-0.74965500	-0.83221400
N	-0.96964600	-1.43908200	-1.06320800
N	0.53306700	-0.19120100	1.73590800
N	0.01877900	1.83018300	-0.88329700
S	3.11520800	-0.69768800	-1.97141600
C	-2.12530200	-1.71956600	-0.26163700
C	-2.14475700	-2.80268000	0.64010000
C	-3.27548900	-0.91922100	-0.36496600
C	-3.27382600	-3.06921000	1.41309600
H	-1.26252300	-3.42819400	0.72807700
C	-4.40215900	-1.18169300	0.41867100
H	-3.28003400	-0.09606000	-1.07083000
C	-4.40741100	-2.25558200	1.30957400
H	-3.26869100	-3.91105100	2.10097700
H	-5.27875100	-0.54620100	0.32353700
H	-5.28590500	-2.46273000	1.91474900
C	-0.33139300	0.67135700	2.48899600
C	0.11842600	1.91562000	2.97577900
C	-1.65996500	0.29599200	2.75123900
C	-0.73344900	2.75163700	3.69494900
H	1.14099900	2.22134800	2.77905400
C	-2.51537700	1.14176200	3.46334900
H	-2.01350600	-0.66654600	2.39847600
C	-2.05796700	2.37079300	3.93820800
H	-0.36505500	3.70599900	4.06273400
H	-3.53948200	0.82931700	3.64963600
H	-2.72153500	3.02619100	4.49576500
C	-1.34238700	2.13163400	-1.23817500
C	-2.26634300	2.53865100	-0.25892100
C	-1.78361600	2.01798100	-2.57033600
C	-3.59093400	2.82064800	-0.60190800
H	-1.93718000	2.63252200	0.77066400
C	-3.10658900	2.29986100	-2.90896500
H	-1.07830100	1.69706400	-3.32931800
C	-4.01636600	2.70310700	-1.92594300

H	-4.28870600	3.13239000	0.17092600
H	-3.42851900	2.20390400	-3.94275000
H	-5.04649300	2.92386400	-2.19248500
C	1.57665900	-0.98188300	2.49669000
C	0.99897800	2.97147000	-1.01397900
C	-0.76190500	-2.30193400	-2.29039300
C	2.95429400	-0.30064900	2.37083500
H	3.72013300	-0.88321700	2.89817700
H	3.24839600	-0.21543500	1.32171500
H	2.93791500	0.70260400	2.81070700
C	1.64492500	-2.40755300	1.91708700
H	1.89754100	-2.39721500	0.85529700
H	2.41226400	-2.98866500	2.44284000
H	0.68457300	-2.91803500	2.04609800
C	1.20493400	-1.10127500	3.98842800
H	1.20435600	-0.13297500	4.49692900
H	0.21776300	-1.55648600	4.12061100
H	1.94228000	-1.74045800	4.48697000
C	2.34302600	2.56426600	-0.39328500
H	2.21992800	2.22818100	0.64111000
H	2.82490400	1.77470800	-0.96949600
H	3.01835500	3.42737600	-0.38975600
C	1.22179500	3.32766100	-2.49755600
H	1.96039200	4.13487300	-2.57738000
H	1.59972700	2.45991300	-3.04517800
H	0.29872700	3.68028300	-2.96873100
C	0.47351600	4.21086300	-0.25832200
H	-0.46268200	4.58445100	-0.68304600
H	0.30500400	3.98658800	0.80034200
H	1.21387600	5.01646100	-0.32441900
C	-0.27256100	-1.41428300	-3.44798000
H	0.64542000	-0.87408200	-3.21071000
H	-0.07287600	-2.02894200	-4.33407100
H	-1.04131200	-0.68017900	-3.71041200
C	0.26626000	-3.41312300	-1.99467100
H	0.43272700	-4.02802100	-2.88801700
H	1.22404200	-2.98759600	-1.68778100
H	-0.08985500	-4.07405500	-1.19678600
C	-2.08409300	-2.95581800	-2.74217300
H	-1.90351000	-3.51051600	-3.66982300
H	-2.47657700	-3.65938500	-2.00243600
H	-2.85541500	-2.20499700	-2.94301100

5Ar_D
E_{elec} (B3LYP/BS1) = -1949.5804963 au
H_{corr} (B3LYP/BS1) = 0.709603 au
G_{corr} (B3LYP/BS1) = 0.599237 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1948.94435975 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -1950.35040023 au

0 2

Mo	-0.14911200	-0.71013900	-0.65919100
O	0.14841900	-2.25691200	-1.84981500
O	-1.46110400	-0.65385700	-2.39324900
N	1.47955500	-1.14587900	0.47294200
N	0.45553500	1.10867800	-1.26883000
N	-1.66641600	-0.89068500	0.62803500
S	-0.89037800	-1.97645400	-3.12525600
C	2.35500300	-0.11536200	0.95601400
C	3.71696900	-0.04449700	0.59525700
C	1.86984300	0.86728500	1.83573300
C	4.54813200	0.95722100	1.09615400
H	4.13301800	-0.77149800	-0.08982400
C	2.70237300	1.87204300	2.33243300
H	0.83552100	0.83061700	2.14785800
C	4.04811000	1.92531500	1.96933200
H	5.59230400	0.98048000	0.79436800
H	2.29076800	2.60872400	3.01793100
H	4.69710900	2.70376300	2.36074200
C	-0.44971100	2.18802600	-0.98132900
C	-1.71542700	2.27218200	-1.59095200
C	-0.07092300	3.19879900	-0.07906900
C	-2.57050900	3.33797600	-1.30412200
H	-2.01341700	1.49274100	-2.28158600
C	-0.92416900	4.26902100	0.19191600
H	0.89171200	3.12879600	0.41364600
C	-2.17921600	4.34360200	-0.41659500
H	-3.54488900	3.38377400	-1.78413400
H	-0.60841800	5.04191700	0.88828800
H	-2.84505400	5.17525100	-0.20172100
C	-1.55254900	-0.12440900	1.84291500
C	-2.00275200	1.20371900	1.91045400
C	-1.03921200	-0.71566100	3.01239800
C	-1.94042700	1.91703700	3.11090500
H	-2.40037500	1.67622800	1.02069500
C	-0.98020700	-0.00384400	4.20819500
H	-0.68691300	-1.73972400	2.97393500
C	-1.43034600	1.31903400	4.26302100

H	-2.29168100	2.94486100	3.13665100
H	-0.58117900	-0.48219200	5.09887200
H	-1.38346000	1.87489200	5.19556900
C	1.46421500	1.40587800	-2.35864500
C	-3.02430400	-1.55924500	0.42512300
C	1.93174700	-2.57470700	0.78600900
C	0.73162400	1.86692100	-3.63870600
H	1.46289400	2.00706100	-4.44363900
H	0.00272300	1.11650300	-3.95844300
H	0.21049100	2.81713000	-3.49149200
C	2.26146000	0.13798000	-2.70478400
H	1.62200600	-0.64289800	-3.12664200
H	3.01335900	0.38836100	-3.46155700
H	2.78321100	-0.26220600	-1.83545500
C	2.44708900	2.50693500	-1.91006600
H	1.93503700	3.45768800	-1.73795800
H	2.97440100	2.22058400	-0.99642800
H	3.19026800	2.67195100	-2.69968100
C	-3.95741900	-0.62218200	-0.36472800
H	-4.13732900	0.30703100	0.18577300
H	-3.52305200	-0.38200600	-1.33687600
H	-4.92761200	-1.10943200	-0.52418300
C	-2.84507200	-2.88732600	-0.32621600
H	-3.82205800	-3.37132900	-0.43998300
H	-2.43468500	-2.74988600	-1.32666100
H	-2.19480500	-3.56770100	0.23222600
C	-3.68403000	-1.88885900	1.78162800
H	-3.05422300	-2.54354000	2.39252500
H	-3.91842500	-0.99393300	2.36374200
H	-4.62442900	-2.41578500	1.58566300
C	0.70643200	-3.50516500	0.90595300
H	0.17955700	-3.61397600	-0.04174100
H	1.04935800	-4.50038400	1.21146300
H	0.00236600	-3.14730800	1.66037700
C	2.84248200	-3.14935400	-0.32451300
H	3.01692600	-4.21576700	-0.13506400
H	2.36476700	-3.04957400	-1.30149300
H	3.82302500	-2.66788100	-0.35690200
C	2.66217300	-2.62999000	2.14638400
H	2.87380400	-3.67684500	2.39147000
H	3.61144200	-2.09046000	2.14457000
H	2.03719000	-2.21382400	2.94411200

TSB3Ar_D
E_{elec} (B3LYP/BS1) = -1949.5555570 au
H_{corr} (B3LYP/BS1) = 0.708182 au
G_{corr} (B3LYP/BS1) = 0.595382 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1948.92083684 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -1950.33519750 au

0 2

Mo	0.60556100	0.28976500	-0.40390100
O	1.57285800	1.17640000	-1.67349000
O	3.90310100	-0.09294000	-2.54216800
N	1.30082900	-1.10852800	0.84149300
N	-0.16691300	1.77167800	0.69329300
N	-0.68769800	-0.61807500	-1.57433900
S	3.48422100	1.15188000	-1.75609500
C	0.42791100	-2.22439700	1.11016200
C	-0.72531600	-2.05420000	1.89175500
C	0.70878200	-3.51670600	0.62236700
C	-1.58503600	-3.12566600	2.14998100
H	-0.94029400	-1.08179800	2.31399300
C	-0.14618800	-4.58479800	0.88885200
H	1.60427100	-3.68783900	0.03809000
C	-1.30473200	-4.39558300	1.64785600
H	-2.46940100	-2.95926300	2.75951000
H	0.09699700	-5.57054400	0.50061400
H	-1.96968400	-5.23002300	1.85266200
C	-2.06831600	-0.22359200	-1.52566700
C	-3.00853400	-1.03178300	-0.86664900
C	-2.50562900	0.96083000	-2.14138700
C	-4.35490200	-0.66567000	-0.83175500
H	-2.67142000	-1.93975900	-0.37898400
C	-3.85197200	1.32742600	-2.09744300
H	-1.78097100	1.59178700	-2.64439100
C	-4.78262500	0.51397900	-1.44545700
H	-5.07000600	-1.30434800	-0.31983500
H	-4.17311800	2.24826000	-2.57726200
H	-5.83114100	0.79757600	-1.41685600
C	-1.03642300	1.45561300	1.79047100
C	-0.51955500	1.31923000	3.09184700
C	-2.41872100	1.31382900	1.59818800
C	-1.36083200	1.03641000	4.16729700
H	0.54794000	1.43419100	3.24813200
C	-3.25810100	1.02314400	2.67629400
H	-2.82915700	1.43756800	0.60336500
C	-2.73508800	0.88111700	3.96255100

H	-0.94229700	0.93412400	5.16513300
H	-4.32559000	0.91292800	2.50531000
H	-3.39070000	0.65697600	4.79952700
C	-0.29264600	-1.46253400	-2.78129500
C	0.16839400	3.25855300	0.49835700
C	2.69082500	-1.17895800	1.46751600
C	1.66433600	3.51128900	0.75945600
H	1.89034000	4.57699600	0.63491900
H	1.93753200	3.22424700	1.78031100
H	2.29480400	2.95624600	0.06152000
C	-0.64242500	4.14073100	1.47055100
H	-0.39658300	5.18723100	1.26124000
H	-1.72080000	4.01586400	1.33684500
H	-0.40202300	3.94326700	2.51846900
C	-0.20514700	3.68638300	-0.93423000
H	0.35217100	3.11947000	-1.68230100
H	-1.27751900	3.54529700	-1.10579400
H	0.02475100	4.74927900	-1.07391400
C	-0.33323900	-0.58136000	-4.04612100
H	0.33471400	0.27888600	-3.93882500
H	0.00490600	-1.16608200	-4.90925500
H	-1.34584400	-0.22594000	-4.25995200
C	1.13073200	-2.01346100	-2.60663800
H	1.19666500	-2.65905400	-1.73054200
H	1.37932800	-2.62169100	-3.48374700
H	1.89910200	-1.23799500	-2.54743200
C	-1.25677100	-2.65460800	-2.93684400
H	-2.28358500	-2.33585900	-3.13602900
H	-0.92784200	-3.26717500	-3.78404600
H	-1.25394700	-3.28479900	-2.04136500
C	3.14434500	0.24609700	1.82725600
H	3.25140800	0.86977200	0.93701200
H	2.44459300	0.71501400	2.52531000
H	4.12814300	0.20404400	2.30863300
C	3.71008400	-1.80752100	0.49276800
H	4.71189100	-1.76670000	0.93819900
H	3.48689100	-2.86202300	0.30344300
H	3.74650200	-1.28136600	-0.46553500
C	2.64950700	-1.99137300	2.77848200
H	3.63380200	-1.93250500	3.25576900
H	1.90869000	-1.58513200	3.47581700
H	2.42191000	-3.04736300	2.61509900

TSB4Ar_D
E_{elec} (B3LYP/BS1) = -1949.5703668 au
H_{corr} (B3LYP/BS1) = 0.708321 au
G_{corr} (B3LYP/BS1) = 0.595637 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1948.92772857 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -1950.34347999 au

0 2

Mo	0.17913600	-0.08341400	-0.10199100
O	1.30786800	0.79920400	-3.63480500
O	1.74757400	-0.31144100	-0.93105100
N	-1.08244700	-1.49639200	-0.71696400
N	0.50222500	-0.24540100	1.86300700
N	-0.31326400	1.77393900	-0.54104100
S	2.44954900	0.16836800	-2.82972300
C	-2.39085700	-1.50466700	-0.11890700
C	-2.61053600	-2.23589400	1.06269400
C	-3.47728500	-0.83769300	-0.70696100
C	-3.87912800	-2.30122000	1.63853800
H	-1.77363200	-2.75442900	1.52031600
C	-4.74678300	-0.90763400	-0.12934400
H	-3.32426900	-0.26753800	-1.61542900
C	-4.95432100	-1.63661800	1.04295800
H	-4.02711900	-2.87383600	2.55044700
H	-5.57434800	-0.38441900	-0.60054800
H	-5.94414600	-1.68817300	1.48826700
C	-0.17381200	0.68518800	2.71855200
C	0.51720700	1.61382800	3.52441300
C	-1.57882800	0.70679600	2.75614500
C	-0.17321600	2.51763100	4.33057400
H	1.59986500	1.63757500	3.51508700
C	-2.26694200	1.62797300	3.54955900
H	-2.13384600	-0.01947700	2.17488000
C	-1.57023900	2.53729900	4.34480100
H	0.38793200	3.21946400	4.94229400
H	-3.35386400	1.61556200	3.55500900
H	-2.10406200	3.24729400	4.97008800
C	-1.56128800	1.98973600	-1.22913700
C	-2.69680300	2.41039800	-0.51716000
C	-1.65552300	1.80344200	-2.61892900
C	-3.89815800	2.65700700	-1.18410500
H	-2.63173600	2.53259100	0.55883500
C	-2.86490800	2.03771500	-3.27599400
H	-0.77534300	1.48355700	-3.16787000
C	-3.98778400	2.47125400	-2.56517700

H	-4.76645700	2.98641400	-0.61921800
H	-2.92366300	1.88907900	-4.35112900
H	-4.92353600	2.66246900	-3.08381900
C	1.53286700	-1.17097600	2.48222700
C	0.55162600	3.01938900	-0.38658600
C	-0.86567200	-2.52158800	-1.83733400
C	2.94780200	-0.55475700	2.42893400
H	3.68728700	-1.28982300	2.76899000
H	3.20002000	-0.26691000	1.40375600
H	3.04534800	0.32456100	3.07161200
C	1.56025300	-2.48354700	1.67845000
H	1.90904700	-2.32076300	0.65618700
H	2.25237300	-3.18899700	2.15198900
H	0.56993700	-2.94815900	1.64544200
C	1.14787400	-1.52123500	3.93350400
H	1.17198700	-0.65606600	4.59976400
H	0.14259400	-1.95500400	3.97687200
H	1.85527500	-2.26226700	4.32176600
C	1.91162900	2.64484300	0.22338100
H	1.79839400	2.15392800	1.19318600
H	2.48732400	1.99710300	-0.44146100
H	2.48878500	3.56227000	0.38376300
C	0.79731000	3.66160700	-1.76732300
H	1.50411400	4.49204300	-1.65320700
H	1.21623500	2.93616900	-2.47059900
H	-0.12409600	4.06717100	-2.19556200
C	-0.14810700	4.03249800	0.54171200
H	-1.09330700	4.38358000	0.11888000
H	-0.34156200	3.60156600	1.52848600
H	0.50062600	4.90708600	0.67060900
C	-1.05449000	-1.82317700	-3.19840400
H	-0.31120200	-1.03579700	-3.35574100
H	-0.94763900	-2.55456700	-4.00929400
H	-2.05253000	-1.37991900	-3.27807400
C	0.54307000	-3.13275700	-1.76268700
H	0.66376500	-3.84537800	-2.58650100
H	1.32628000	-2.37977200	-1.85969700
H	0.68277400	-3.67841600	-0.82415300
C	-1.87585900	-3.68213000	-1.72148600
H	-1.65986300	-4.40500900	-2.51547000
H	-1.79023700	-4.20228300	-0.76198000
H	-2.91119200	-3.35294800	-1.84219000

TSB5Ar_D
E_{elec} (B3LYP/BS1) = -1949.5636479 au
H_{corr} (B3LYP/BS1) = 0.708231 au
G_{corr} (B3LYP/BS1) = 0.598071 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1948.92356370 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -1950.33781772 au

0 2

Mo	-0.14688100	-0.71671100	-0.71435900
O	0.21477600	-2.19572400	-1.68600900
O	-1.48667000	-0.65381200	-2.36951700
N	1.43138600	-1.11649900	0.51911900
N	0.50201300	1.06668300	-1.34522000
N	-1.68940500	-0.86314000	0.55220600
S	-1.04868900	-1.89934500	-3.30866000
C	2.27525300	-0.05638500	1.00393200
C	3.57607700	0.14558300	0.50033800
C	1.83602200	0.79533900	2.02943400
C	4.39755800	1.15287000	1.00605800
H	3.94810500	-0.48345500	-0.29811100
C	2.65984900	1.80489400	2.53381000
H	0.84991000	0.65073100	2.44727100
C	3.94574800	1.99169500	2.02785000
H	5.39588500	1.28157300	0.59515400
H	2.28841600	2.44033500	3.33396000
H	4.58824500	2.77350700	2.42344900
C	-0.30617300	2.18568100	-0.93775700
C	-1.59823500	2.36459800	-1.46605000
C	0.19287000	3.13321600	-0.02804600
C	-2.36321600	3.47349500	-1.09946100
H	-1.98648000	1.62368200	-2.15535200
C	-0.57696500	4.23969000	0.33203200
H	1.17896700	2.98937700	0.39696200
C	-1.85546000	4.41679500	-0.20268700
H	-3.35837000	3.59870000	-1.51841800
H	-0.17504400	4.96431600	1.03551200
H	-2.45134900	5.28117700	0.07813900
C	-1.59185200	-0.14208200	1.79622200
C	-2.00980700	1.19334500	1.89167800
C	-1.14314600	-0.78540100	2.96503300
C	-1.97548400	1.86662300	3.11656100
H	-2.36575900	1.70263000	1.00475200
C	-1.11556100	-0.11549300	4.18599900
H	-0.81848300	-1.81739200	2.90828900

C	-1.52974100	1.21798800	4.26748200
H	-2.30130300	2.90205700	3.16264700
H	-0.76836700	-0.63499000	5.07540500
H	-1.50678300	1.74132200	5.21953200
C	1.39423700	1.33116400	-2.54139500
C	-3.02856100	-1.57681100	0.34209800
C	1.92708000	-2.51609400	0.88429600
C	0.54420700	1.75076600	-3.76108600
H	1.20065600	1.86404700	-4.63185900
H	-0.20702100	0.99037100	-3.98843300
H	0.03989900	2.70745300	-3.59703000
C	2.17257500	0.05875300	-2.91164400
H	1.51173900	-0.72894900	-3.28126900
H	2.88329600	0.29843800	-3.71016100
H	2.73848900	-0.32796400	-2.06234700
C	2.40127600	2.45306100	-2.21205100
H	1.89977400	3.40279600	-2.00673700
H	3.02086300	2.19028700	-1.35042200
H	3.05807300	2.60616300	-3.07632800
C	-3.96749100	-0.65425100	-0.45934500
H	-4.16017100	0.27380100	0.09019200
H	-3.52976800	-0.41323900	-1.42911400
H	-4.93109300	-1.15338500	-0.62140900
C	-2.81519900	-2.90717000	-0.39443000
H	-3.78313300	-3.40674800	-0.51862400
H	-2.38635900	-2.77540800	-1.38702700
H	-2.16495400	-3.57203900	0.18330000
C	-3.70879900	-1.90926300	1.68830000
H	-3.09212000	-2.56441500	2.31118200
H	-3.95967300	-1.01685700	2.26724800
H	-4.64267900	-2.43908100	1.47087900
C	0.75177700	-3.51347800	0.95861700
H	0.30243800	-3.69102100	-0.01758900
H	1.12733700	-4.47065100	1.33853000
H	-0.02576000	-3.16531500	1.64249500
C	2.92855300	-3.04289100	-0.16904700
H	3.14003100	-4.10161900	0.02529500
H	2.50574600	-2.95791200	-1.17300400
H	3.88380300	-2.51258100	-0.13255500
C	2.59539300	-2.50721900	2.27723900
H	2.87833200	-3.53272700	2.53989600
H	3.49882600	-1.89393200	2.31013200
H	1.90511400	-2.13895500	3.04412100

7Ar_D
E_{elec} (B3LYP/BS1) = -1476.23712354 au
H_{corr} (B3LYP/BS1) = 0.701601 au
G_{corr} (B3LYP/BS1) = 0.593740 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1475.59339407 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -1476.92747399 au

0 2

Mo	-0.54323300	2.15043100	4.84280400
O	-1.43759300	3.61211200	5.01269000
N	-1.46258100	0.55701300	5.66307400
N	1.22475900	2.61803400	5.67110000
N	-0.18207700	1.77980400	2.89491800
C	-2.61785500	1.73925700	2.40473600
H	-2.87298800	2.36001900	3.26898900
H	-2.67685200	0.68656500	2.69579100
H	-3.37993400	1.92465200	1.63910800
C	1.87703900	2.10842000	1.51820500
H	1.45779500	2.99179100	1.05289300
C	-1.22397600	2.08386500	1.83889100
C	1.12801600	1.39279500	2.47634900
C	1.55280200	1.94513300	6.89417900
C	-0.81822600	-0.72134900	5.50618500
C	-1.07877200	-1.51446900	4.37313300
H	-1.76138000	-1.14263200	3.61681800
C	3.75847300	0.59655900	1.76223000
H	4.76411500	0.29156800	1.48664400
C	0.82850500	2.19230800	8.07512800
H	0.01690300	2.91390200	8.04894900
C	2.93291000	0.36775300	8.13729300
C	3.16594700	1.71038900	1.16404000
C	1.73685900	0.26512900	3.05878300
H	1.17856400	-0.32582600	3.77420900
C	-2.77706700	0.51166600	6.41538500
C	-3.37440300	1.91760500	6.57191000
H	-2.70362900	2.58942800	7.11512100
H	-4.30858200	1.83999900	7.13897500
H	-3.60167800	2.38258200	5.60975000
C	3.03351700	-0.12002300	2.71507800
C	2.60530100	1.01364100	6.94365600
H	3.14964800	0.79031600	6.03274300
C	0.08345700	-1.20953400	6.46633500
H	0.29453400	-0.61253400	7.34454900
C	-1.01729700	1.20523300	0.58794400
H	-0.99938800	0.14345800	0.85808600

H	-0.09147800	1.43231500	0.05563800
H	-1.84992300	1.36678400	-0.10587200
C	2.07691600	3.83604000	5.37129800
C	0.70404000	-2.44893900	6.29613000
C	3.52862100	3.42094000	5.05251800
H	3.55977000	2.71834200	4.21423400
H	4.01846700	2.96135500	5.91569600
H	4.11180200	4.30880500	4.77903100
C	-0.46169700	-2.75444800	4.20780100
C	0.43460100	-3.22744400	5.16928500
H	0.91869400	-4.19163500	5.03969000
C	2.20441700	0.62035500	9.30172400
H	2.45718100	0.11309000	10.22882100
C	1.51294200	4.60126700	4.16296600
H	1.49933800	3.97897000	3.26642400
H	2.15818200	5.46334300	3.95824700
H	0.50344100	4.97168200	4.35695600
C	-1.23359200	3.58108600	1.45801900
H	-1.37388600	4.19888500	2.35041500
H	-2.05967900	3.78684700	0.76623600
H	-0.30952800	3.89384000	0.96456700
C	-3.80007500	-0.36950600	5.66671200
H	-3.45312900	-1.40171900	5.56665500
H	-4.00238800	0.02756500	4.66637100
H	-4.74581300	-0.38851600	6.22069100
C	-2.55419300	-0.06702000	7.83092500
H	-2.20642700	-1.10315200	7.79938800
H	-3.49907700	-0.04939400	8.38621800
H	-1.81940300	0.52700700	8.38389000
C	1.14549600	1.53203900	9.26316000
C	2.07015000	4.79516400	6.58101600
H	2.52302400	4.34216900	7.46779000
H	1.04699500	5.09830700	6.82936200
H	2.64224800	5.69828700	6.33821700
H	3.71262800	2.28594000	0.42107600
H	3.46700400	-0.99883700	3.18592400
H	-0.67726900	-3.34767800	3.32293500
H	1.40115800	-2.80279900	7.05114400
H	0.57116400	1.73927300	10.16267100
H	3.75337900	-0.34540900	8.15222900

Cartesian coordinates, electronic (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and/or single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for INT-SO & TSBINT-SO (quintet/triplet/singlet)

INT-SO_Q_T
E_{elec} (B3LYP/BS1) = -945.6781571 au
H_{corr} (B3LYP/BS1) = 0.176135 au
G_{corr} (B3LYP/BS1) = 0.107696 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -945.56446607 au

0 5

Mo	0.18857900	0.13919500	0.47873200
N	-0.76747100	-1.47984800	0.03004600
N	0.80191800	1.37816300	-0.92750300
N	1.59462800	-0.28012300	1.79312400
H	-1.79741000	-1.54286200	0.08335000
H	-0.35548100	-2.28629200	-0.43713400
H	0.41762800	2.30588100	-1.09574400
H	1.31974000	1.06654100	-1.74687200
H	2.38686500	0.33921800	1.95014100
H	1.45470400	-0.88332900	2.60136900
S	-1.62463200	1.60081500	1.10175900
O	-2.24454500	0.78134300	2.48535200
Mo	-3.89464900	0.23033400	1.56740800
N	-4.88140000	-0.97812000	2.83949700
N	-5.23817800	1.63390300	1.37115500
N	-3.82593200	-1.21557100	0.17575800
H	-5.00536900	-0.69885600	3.81146500
H	-5.68603200	-1.53012800	2.54638500
H	-5.15083600	2.44219500	0.75937500
H	-6.14039700	1.62174400	1.83915200
H	-3.86923500	-0.98769300	-0.81639500
H	-4.31178900	-2.09553000	0.34385300

INT-SO_T

E_{elec} (B3LYP/BS1) = -945.6816788 au

H_{corr} (B3LYP/BS1) = 0.177301 au

G_{corr} (B3LYP/BS1) = 0.110902 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -945.57193608 au

0 3

Mo	0.14884100	0.12520400	0.50711300
N	-0.80159400	-1.50790000	0.08210400
N	0.63971800	1.42685200	-0.89178900
N	1.66620700	-0.30305700	1.68901200
H	-1.81576500	-1.59795800	0.23799700
H	-0.42632300	-2.28034100	-0.46550500
H	0.20590400	2.33876900	-1.02049100
H	1.11416000	1.15023400	-1.74928600
H	2.45532600	0.33019600	1.79874000
H	1.60074000	-0.92501000	2.49248100
S	-1.61457900	1.53844600	1.34947900
O	-2.22320800	0.53499300	2.60984800
Mo	-3.91660000	0.25120300	1.67135400
N	-4.96955800	-0.87948700	2.83336600
N	-5.14699600	1.70377200	1.23971400
N	-3.88010200	-1.15526600	0.28337700
H	-5.44366600	-0.59370900	3.69064700
H	-5.07712600	-1.89077900	2.70479000
H	-4.82027500	2.60655800	0.90250200
H	-6.15837500	1.62845900	1.14999600
H	-3.66919500	-0.96873500	-0.69695200
H	-4.49682800	-1.97146600	0.33577800

INT-SO_S

E_{elec} (B3LYP/BS1) = -945.6953953 au

H_{corr} (B3LYP/BS1) = 0.178406 au

G_{corr} (B3LYP/BS1) = 0.115677 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -945.59040351 au

0 1

Mo	0.07459200	0.18124400	0.68149700
N	-0.72519000	-1.52334500	0.24914100
N	0.18888300	1.41678600	-0.82793800
N	1.82211800	-0.05664300	1.49857300
H	-1.72732900	-1.73264300	0.32068500
H	-0.22707700	-2.23504800	-0.28704100
H	-0.54386000	2.04597400	-1.14957800
H	0.84931900	1.24647400	-1.58794800
H	2.46151400	0.71320700	1.69243700
H	2.06530200	-0.87299600	2.05757400
S	-1.39383700	1.17489800	2.02623900
O	-2.36726200	0.00960600	2.96031000
Mo	-3.85047100	0.11798400	1.74406700
N	-5.32062600	-0.79255900	2.60079500
N	-4.69240200	1.78984700	1.17753800
N	-3.84653100	-1.24166800	0.30786500
H	-5.87258300	-0.44542800	3.38441500
H	-5.64336000	-1.72720400	2.33344600
H	-4.16475400	2.65252900	1.07048700
H	-5.65199500	1.90512400	0.85836000
H	-3.51404600	-1.07921100	-0.64105000
H	-4.54969900	-1.98594800	0.28440000

TSBINT-SO_Q_T
E_{elec} (B3LYP/BS1) = -945.6694940 au
H_{corr} (B3LYP/BS1) = 0.175007 au
G_{corr} (B3LYP/BS1) = 0.107248 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -945.55643821 au

0 5

Mo	-2.18419500	0.13095800	-0.08441700
N	-1.38787400	1.78583900	-0.71067800
N	-3.31264600	-0.92170600	-1.30063200
N	-3.12693200	0.46337000	1.60773000
H	-0.38982000	1.84480900	-0.95143100
H	-1.91206000	2.59314100	-1.04278700
H	-3.00615100	-1.79285200	-1.73032500
H	-4.08732400	-0.52479300	-1.82857800
H	-3.83529800	-0.17179500	1.96950000
H	-2.74496400	1.03184500	2.36120900
S	-0.33430200	-1.44216900	-0.26083400
O	0.61281100	-0.36999700	1.13485900
Mo	2.00661500	-0.02019400	-0.01439100
N	3.46007500	1.16816700	0.65054400
N	3.23842700	-1.53154800	-0.22301200
N	1.56459100	1.23446600	-1.50922600
H	4.11894300	0.85474800	1.36003800
H	3.34571700	2.17801500	0.70708500
H	2.94695200	-2.45301200	-0.53881600
H	4.25121200	-1.44619500	-0.20330600
H	1.10284500	0.87032300	-2.34199500
H	2.24492400	1.94136500	-1.78492500

TSBINT-SO_T
E_{elec} (B3LYP/BS1) = -945.6793883 au
H_{corr} (B3LYP/BS1) = 0.175713 au
G_{corr} (B3LYP/BS1) = 0.110015 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -945.56676919 au

0 3

Mo	-2.21493500	0.11071500	-0.04078500
N	-1.37110100	1.72920800	-0.69165800
N	-3.13632700	-1.12355100	-1.27547600
N	-3.38827600	0.56534600	1.47957500
H	-0.35197500	1.79343600	-0.81624400
H	-1.86215600	2.49545900	-1.14947100
H	-2.77611300	-2.01936400	-1.59415100
H	-3.86001100	-0.79771700	-1.91433400
H	-4.05884100	-0.10458400	1.85191500
H	-3.12438200	1.22943500	2.20511900
S	-0.33587700	-1.27302000	0.31870400
O	0.77606800	-0.24960100	1.37243800
Mo	2.09064100	-0.03435900	0.04711100
N	3.49893500	1.12999800	0.69934600
N	3.08826300	-1.60059700	-0.55877800
N	1.66420200	1.34933000	-1.30365300
H	4.10349800	0.94498900	1.49751800
H	3.73073600	2.03571400	0.28405800
H	2.65263000	-2.51838400	-0.61234600
H	4.02150400	-1.60958000	-0.96177300
H	1.24989900	1.12526800	-2.20693900
H	2.17115800	2.23536900	-1.37336200

TSBINT-SO_S
E_{elec} (B3LYP/BS1) = -945.6924496 au
H_{corr} (B3LYP/BS1) = 0.177129 au
G_{corr} (B3LYP/BS1) = 0.115540 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -945.59506167 au

0 1

Mo	-1.68085700	-0.01775700	0.03597700
N	-1.52099200	1.71654300	0.87694800
N	-1.27171100	-0.18341500	-1.87031000
N	-3.47877500	-0.65344500	0.48412700
H	-0.72888900	1.97398900	1.46483500
H	-2.07651100	2.52830800	0.60932200
H	-0.34143600	-0.30210100	-2.26438100
H	-1.91323100	0.18009500	-2.57561700
H	-3.90154200	-1.45102300	0.00988200
H	-3.93598800	-0.49708600	1.38011000
S	-0.07631000	-0.92567600	1.22240200
O	1.07126800	0.44005600	2.01933800
Mo	1.93891800	0.37506200	0.35249900
N	3.66949100	1.22578400	0.60330800
N	2.50917300	-1.25616200	-0.59421700
N	1.48440700	1.84503000	-0.86376900
H	4.44489700	0.84107900	1.13973500
H	3.90270400	2.16396900	0.27032600
H	1.99131800	-2.12922300	-0.58728100
H	3.28967600	-1.29261500	-1.24550100
H	2.14466400	2.59038700	-1.09284700
H	0.63253700	1.94699500	-1.40657400

Cartesian coordinates, electronic (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for 9 (quintet/triplet/singlet)

9Ar_Q_T
E_{elec} (B3LYP/BS1) = -3350.5707271 au
H_{corr} (B3LYP/BS1) = 1.407657 au
G_{corr} (B3LYP/BS1) = 1.209027 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -3349.29115339 au

0 5

Mo	-3.12247600	0.09795900	-0.06878900
O	-1.17634800	0.20337900	-0.56883300
O	1.18250500	0.32297300	0.50476400
N	-3.41761800	-0.60937300	1.79092800
N	-3.78709900	1.97455000	-0.39530300
N	-3.61990100	-1.26322700	-1.46092500
S	0.01023900	1.28409600	-0.16241400
C	-4.57431100	-1.45915400	1.90445300
C	-5.85441000	-0.91279800	2.10193600
C	-4.45604300	-2.86009600	1.82790600
C	-6.97655400	-1.73750800	2.21456800
H	-5.96424000	0.16378400	2.16507800
C	-5.57678100	-3.68237400	1.94117400
H	-3.47487600	-3.29555000	1.67234300
C	-6.84448800	-3.12436300	2.13499000
H	-7.95530600	-1.28896900	2.36416400
H	-5.46001500	-4.76138000	1.87742900
H	-7.71730200	-3.76578900	2.22332700
C	-4.91610000	-1.05156100	-2.04265400
C	-6.06705300	-1.58781400	-1.43889500
C	-5.07634500	-0.30234500	-3.22472700
C	-7.33197200	-1.37687100	-1.99220900
H	-5.96037700	-2.17207700	-0.53253300
C	-6.34013300	-0.09479400	-3.77769500
H	-4.19933300	0.12342500	-3.69971700
C	-7.47584900	-0.63022100	-3.16260700
H	-8.20539500	-1.80083900	-1.50335600
H	-6.43811000	0.48872800	-4.68984200
H	-8.46015700	-0.46735700	-3.59353000
C	-4.99182600	2.25369600	0.33706600
C	-4.95127800	2.91672100	1.57912400
C	-6.24718100	1.87505700	-0.17154600
C	-6.12397000	3.19431100	2.28202700
H	-3.98902800	3.20433600	1.99049600

C	-7.41959200	2.14976600	0.53586600
H	-6.29544900	1.36702100	-1.12844800
C	-7.36498600	2.81129400	1.76381800
H	-6.06798200	3.70758900	3.23877900
H	-8.37701400	1.84537200	0.12087800
H	-8.27756200	3.02761500	2.31279200
C	-2.81342600	-2.39913500	-2.03950400
C	-3.28960600	3.10381900	-1.27066000
C	-2.70716500	-0.33398400	3.09095800
C	-2.42159200	4.07183000	-0.43962300
H	-2.01484900	4.86736900	-1.07657700
H	-3.01226200	4.54885500	0.34946200
H	-1.58562200	3.54428300	0.02929300
C	-4.46793300	3.89516100	-1.88043800
H	-4.07020900	4.66771400	-2.54854600
H	-5.12256900	3.24321400	-2.46845700
H	-5.07391900	4.39292500	-1.11842100
C	-2.47175900	2.54110900	-2.44563400
H	-1.60564400	1.96470200	-2.12098000
H	-3.09645700	1.89402300	-3.06863900
H	-2.11154400	3.36725600	-3.06991900
C	-2.14850600	-1.95683500	-3.36002200
H	-1.53160500	-1.06872700	-3.19446100
H	-1.50728900	-2.75608200	-3.75251100
H	-2.89705600	-1.72917400	-4.12598400
C	-1.72102500	-2.82366000	-1.04271300
H	-2.16295900	-3.13379600	-0.09053500
H	-1.16880300	-3.67817500	-1.45127300
H	-1.01138600	-2.01693500	-0.85231200
C	-3.71240100	-3.62530400	-2.30495900
H	-4.48333900	-3.41994100	-3.05322600
H	-3.09555200	-4.45108200	-2.67835100
H	-4.20651700	-3.95786200	-1.38569800
C	-1.60861300	0.70356900	2.84697000
H	-0.83761600	0.32386200	2.17520300
H	-2.01620700	1.62613300	2.41871500
H	-1.12468500	0.96166400	3.79601900
C	-2.05672600	-1.62468400	3.63185600
H	-1.49186400	-1.40509100	4.54595400
H	-2.80594100	-2.38271100	3.88074600
H	-1.36386900	-2.04499600	2.89551400
C	-3.68313600	0.22178300	4.15062200
H	-3.13036000	0.45826500	5.06755100
H	-4.16670600	1.13773700	3.79641200
H	-4.46345500	-0.49987500	4.40884800
Mo	3.12612700	0.08611600	0.04732600

N	3.38760100	-1.10129100	-1.55320000
N	3.81240800	1.96965000	-0.16770100
N	3.61463700	-0.83480200	1.76600900
C	4.52260100	-1.97918300	-1.43613800
C	2.65772800	-1.18773200	-2.86993900
C	5.00501400	2.01723200	-0.96945000
C	3.35174900	3.30337900	0.37671000
C	4.92788900	-0.50308500	2.24303100
C	2.78185000	-1.71613400	2.66437200
C	5.80888400	-1.54781000	-1.80348000
C	4.37605200	-3.29479600	-0.95678400
C	1.57705800	-0.10381900	-2.92083000
C	1.98228600	-2.56707700	-3.01933100
C	3.62492200	-0.96778200	-4.05344200
C	4.94383700	2.32239600	-2.34306200
C	6.26633000	1.76233000	-0.40182100
C	2.51054900	4.04564600	-0.68340000
C	4.55606700	4.18920900	0.76529200
C	2.51578900	3.09665900	1.65121200
C	6.05201600	-1.21796200	1.79382600
C	5.13352300	0.54297000	3.16409700
C	2.08524900	-0.85996200	3.74311100
C	1.71509300	-2.44777400	1.83050400
C	3.66048300	-2.78486000	3.34761000
C	6.91026500	-2.39987000	-1.69161500
H	5.93783100	-0.53888200	-2.17733000
C	5.47595000	-4.14502200	-0.84575600
H	3.38927600	-3.63894300	-0.66719800
H	0.79957700	-0.26587100	-2.17283800
H	2.00165800	0.89454700	-2.76742400
H	1.09456500	-0.11171800	-3.90521400
H	1.40656600	-2.60366600	-3.95210100
H	2.71805800	-3.37658900	-3.05212800
H	1.29557000	-2.75183000	-2.18688400
H	3.06132500	-0.98873100	-4.99375100
H	4.12485200	0.00297900	-3.97533400
H	4.39199000	-1.74551700	-4.10828400
C	6.10292000	2.37890200	-3.11725500
H	3.97533100	2.50563000	-2.79699200
C	7.42510500	1.81479800	-1.17990600
H	6.33019700	1.52531900	0.65461100
H	2.13738100	4.99580900	-0.28096900
H	3.10922900	4.27504900	-1.57098300
H	1.65188100	3.44239700	-0.99427200
H	4.18586100	5.12112600	1.20760700
H	5.19151400	3.69144600	1.50523100

H	5.17468600	4.45236100	-0.09716300
H	1.61989700	2.49998300	1.47930700
H	3.11058000	2.60129100	2.42458300
H	2.19754600	4.07068500	2.04094000
C	7.33495800	-0.89233300	2.23978200
H	5.90975200	-2.03268000	1.09342500
C	6.41491500	0.86470900	3.61151900
H	4.27829500	1.10805900	3.51740100
H	1.48087500	-0.07901600	3.27337800
H	1.42749800	-1.48264200	4.36256000
H	2.81612000	-0.38935400	4.40906100
H	2.18321100	-3.08103400	1.07010700
H	1.12013000	-3.09440300	2.48634000
H	1.03875900	-1.74752700	1.33763000
H	4.40779000	-2.34360200	4.01344100
H	3.02337300	-3.44420400	3.94866600
H	4.18269300	-3.39933000	2.60625400
C	6.75033200	-3.70085500	-1.21276800
H	7.89476200	-2.04046900	-1.97986600
H	5.33798500	-5.15613700	-0.47085800
C	7.35047500	2.12501300	-2.53878700
H	6.03131100	2.61742100	-4.17552000
H	8.38797700	1.61339100	-0.71748000
C	7.52389300	0.14960800	3.14900500
H	8.18686900	-1.45930800	1.87324200
H	6.54768200	1.67816200	4.32059300
H	7.60702900	-4.36389800	-1.12604300
H	8.25286300	2.16883000	-3.14274700
H	8.52210800	0.40202200	3.49674200

9Ar_T
E_{elec} (B3LYP/BS1) = -3350.5711901 au
H_{corr} (B3LYP/BS1) = 1.408061 au
G_{corr} (B3LYP/BS1) = 1.211504 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -3349.29532201 au

0 3

Mo	3.05775700	0.23937300	0.42453400
O	1.12203100	0.31427000	0.73467300
O	-1.04679900	0.17038900	-0.75597600
N	3.17353700	-1.12053900	-1.02652100
N	3.57483200	2.15275800	0.17674000
N	4.14455900	-0.38814800	1.96762300
S	0.11252900	1.23420000	-0.27213100
C	2.96020900	-2.44820000	-0.51835500
C	3.95155100	-3.44673800	-0.62057200
C	1.74345900	-2.79140400	0.09614800
C	3.73354300	-4.73035800	-0.12569500
H	4.89224800	-3.21076900	-1.10701700
C	1.53422000	-4.07720200	0.60585700
H	0.95947500	-2.04494800	0.16104300
C	2.52372500	-5.05309500	0.49776500
H	4.51332600	-5.48163100	-0.22365800
H	0.58492800	-4.31295300	1.08032400
H	2.35704200	-6.05323500	0.88816900
C	5.57131500	-0.30243700	1.77946100
C	6.25953300	-1.25194400	1.00727700
C	6.31760800	0.74754300	2.34920100
C	7.63805300	-1.15393300	0.80255300
H	5.69973400	-2.07443200	0.58100400
C	7.69554900	0.83975100	2.15525900
H	5.80391900	1.49575000	2.94181400
C	8.36330700	-0.10886900	1.37522000
H	8.14507000	-1.90272600	0.19896000
H	8.24741400	1.65992000	2.60764700
H	9.43613600	-0.03387800	1.21966600
C	4.38727700	2.54590900	-0.93953800
C	3.83819200	3.20720400	-2.05490500
C	5.77258900	2.30091500	-0.93621100
C	4.64409300	3.60520200	-3.12279100
H	2.77014400	3.39192400	-2.08840100
C	6.57518700	2.69698600	-2.00724800
H	6.21695600	1.80336300	-0.08196400
C	6.01736500	3.35406900	-3.10574000
H	4.19215800	4.10981600	-3.97322300

H	7.64258700	2.49292100	-1.97656500
H	6.64345900	3.66562700	-3.93744600
C	3.70736200	-1.01848800	3.27114300
C	3.23788900	3.29299600	1.12293900
C	3.35074500	-0.99466000	-2.52784700
C	2.23662600	4.28080300	0.48286200
H	1.94072200	5.03329700	1.22409200
H	2.67322900	4.81177900	-0.36699200
H	1.33213800	3.76392700	0.14692900
C	4.51148400	4.07462600	1.51148100
H	4.25470200	4.85903700	2.23327500
H	5.25541100	3.41790300	1.97143400
H	4.97401200	4.55519500	0.64493700
C	2.60071600	2.73634700	2.40651400
H	1.65571700	2.22427200	2.20555200
H	3.27509500	2.03933900	2.90939800
H	2.39144200	3.56152600	3.09668300
C	4.32208100	-0.30970800	4.49910400
H	4.04159500	0.74836300	4.53651900
H	3.94829900	-0.78513700	5.41330100
H	5.41301100	-0.38050500	4.51384100
C	2.17987400	-0.95789200	3.40026000
H	1.68134200	-1.48789700	2.58726500
H	1.88651100	-1.43301100	4.34395700
H	1.81036700	0.07034800	3.40840100
C	4.14873900	-2.49851400	3.28900800
H	5.23766300	-2.59152400	3.22486500
H	3.82822200	-2.97385400	4.22420200
H	3.70469100	-3.04732800	2.45410200
C	2.47019200	0.17074900	-3.00512400
H	1.41259600	-0.05174500	-2.83523300
H	2.71487900	1.09043200	-2.47631900
H	2.62288900	0.34922800	-4.07667900
C	2.87360600	-2.25273200	-3.28551800
H	2.89252700	-2.03361200	-4.35915600
H	3.50741500	-3.12656000	-3.11605000
H	1.84652000	-2.51757200	-3.01415500
C	4.82827100	-0.72672900	-2.86518400
H	4.95440300	-0.59002500	-3.94640600
H	5.18593300	0.17401500	-2.36270500
H	5.46319000	-1.56563400	-2.55813800
Mo	-3.01676900	-0.00374400	-0.35822700
N	-3.23658800	-1.11663700	1.29747900
N	-3.80315600	1.83867800	-0.18591200
N	-3.40718500	-0.95042000	-2.09338000
C	-4.24994200	-2.13072300	1.18617600

C	-2.54969800	-1.04071800	2.63764800
C	-5.01906700	1.84429300	0.58234900
C	-3.38603700	3.17489500	-0.75537500
C	-4.75329900	-0.76098000	-2.55027700
C	-2.48051600	-1.70402600	-3.02390800
C	-5.59451000	-1.84191200	1.47954800
C	-3.92389400	-3.43815400	0.77953900
C	-1.65359600	0.20337300	2.67694600
C	-1.67654100	-2.29160600	2.86722100
C	-3.58648100	-0.93422200	3.77737400
C	-5.02344500	2.22166100	1.93947500
C	-6.24121300	1.47282600	-0.00548900
C	-2.57414300	3.96553200	0.29209700
C	-4.61642400	4.00764900	-1.17468400
C	-2.53219200	2.96021800	-2.01621500
C	-5.78816000	-1.58727500	-2.07927100
C	-5.08063900	0.24691300	-3.47933700
C	-1.66953500	-0.70796500	-3.87816000
C	-1.52273000	-2.57496600	-2.19227300
C	-3.27120100	-2.64394400	-3.95772500
C	-6.57823100	-2.82733100	1.36992100
H	-5.86214900	-0.83777000	1.78968800
C	-4.90799400	-4.42056500	0.66827500
H	-2.89091100	-3.66928600	0.54173400
H	-0.80176500	0.11232200	2.00222400
H	-2.21716900	1.10654500	2.41943600
H	-1.25405800	0.33556300	3.68934700
H	-1.13691600	-2.20543600	3.81801500
H	-2.28083800	-3.20344000	2.90943400
H	-0.93767500	-2.39617900	2.06589900
H	-3.06315200	-0.83920600	4.73611600
H	-4.22389000	-0.05394100	3.64662800
H	-4.22780500	-1.81828700	3.83444200
C	-6.20678000	2.22934600	2.67759600
H	-4.08733100	2.49912000	2.41210100
C	-7.42405900	1.47382900	0.73781100
H	-6.25755700	1.18831900	-1.05162900
H	-2.23084200	4.91907800	-0.12881900
H	-3.18324500	4.19470200	1.17247700
H	-1.69785100	3.39367000	0.61261400
H	-4.27657400	4.94295900	-1.63404600
H	-5.22728500	3.47112300	-1.90837100
H	-5.25181400	4.26572200	-0.32284800
H	-1.62901000	2.38159000	-1.81884100
H	-3.10604800	2.43858600	-2.78800500
H	-2.22130300	3.93037000	-2.42090300

C	-7.10494900	-1.40334000	-2.50816700
H	-5.54796600	-2.37693100	-1.37650600
C	-6.39405600	0.42380900	-3.91318800
H	-4.29360800	0.89253400	-3.85421600
H	-1.08964800	-0.04229100	-3.23458600
H	-0.97740400	-1.24346200	-4.54062200
H	-2.33036500	-0.10250200	-4.50819500
H	-2.08302100	-3.32526400	-1.62447700
H	-0.82805000	-3.10336200	-2.85633600
H	-0.93403600	-1.96929200	-1.50186700
H	-3.92823000	-2.09867400	-4.64159500
H	-2.56173800	-3.21952300	-4.56327700
H	-3.88308900	-3.35229900	-3.38917400
C	-6.24097800	-4.11975600	0.96427100
H	-7.61115500	-2.57939000	1.60067700
H	-4.63333300	-5.42268800	0.34855100
C	-7.41420900	1.85283400	2.08072500
H	-6.18496100	2.52540800	3.72345300
H	-8.35453500	1.17979400	0.25904300
C	-7.41503600	-0.39863700	-3.42571000
H	-7.88689400	-2.05366000	-2.12458200
H	-6.62206800	1.20760600	-4.63140700
H	-7.00685900	-4.88596400	0.87846700
H	-8.33504100	1.85724100	2.65775000
H	-8.43873300	-0.25804600	-3.76231600

9Ar_S

E_{elec} (B3LYP/BS1) = -3350.5657423 au
H_{corr} (B3LYP/BS1) = 1.408572 au
G_{corr} (B3LYP/BS1) = 1.213641 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -3349.29283870 au

0 1

Mo	-2.96290800	-0.40230900	-0.26908600
O	-1.01625600	-0.19714700	-0.48700900
O	1.14028800	0.12172900	1.01626200
N	-3.74777000	-1.01427700	1.46902600
N	-3.51011000	1.41982500	-0.80540200
N	-3.38462600	-1.79724100	-1.64561100
S	-0.05829000	0.99545900	0.21246000
C	-5.17748200	-1.16618200	1.55283900
C	-6.00158800	-0.11996700	2.00001100
C	-5.78782200	-2.38338100	1.19482500
C	-7.38602900	-0.28406000	2.07973000
H	-5.54919900	0.82130600	2.28486400
C	-7.17073900	-2.54788300	1.27943800
H	-5.16533700	-3.19492000	0.83178600
C	-7.97769400	-1.49687500	1.72144300
H	-8.00159200	0.54235000	2.42596600
H	-7.61721500	-3.49672100	0.99302800
H	-9.05522800	-1.62257300	1.78558900
C	-4.46138100	-1.53315400	-2.54739100
C	-5.73660300	-1.20472000	-2.04830600
C	-4.30732800	-1.54958000	-3.95159100
C	-6.79919800	-0.90221700	-2.90195500
H	-5.90324000	-1.21136300	-0.97901800
C	-5.37399100	-1.25961000	-4.80136100
H	-3.34179800	-1.77729500	-4.38561100
C	-6.62988800	-0.93122400	-4.28629300
H	-7.76833700	-0.65924600	-2.47320100
H	-5.21490700	-1.28267400	-5.87678200
H	-7.45851200	-0.70546100	-4.95163600
C	-4.08882300	2.23603500	0.22708700
C	-3.30341600	2.69775600	1.29819300
C	-5.44906900	2.59375400	0.19572500
C	-3.86152500	3.48610800	2.30631200
H	-2.24995600	2.43609900	1.32791700
C	-5.99632400	3.40508900	1.19050300
H	-6.08003600	2.21077100	-0.59760200
C	-5.20819600	3.85310200	2.25318500
H	-3.23491400	3.82716400	3.12669500
H	-7.04902500	3.67247900	1.14219900

H	-5.63781600	4.47955100	3.03017500
C	-2.58193000	-3.06106000	-1.86452600
C	-3.26458200	2.14092600	-2.12305200
C	-3.02037900	-1.42017300	2.73626100
C	-2.60448400	3.50961900	-1.85096100
H	-2.37319200	3.99516300	-2.80617000
H	-3.25793000	4.17854400	-1.28386100
H	-1.66705300	3.39025300	-1.29628400
C	-4.57769100	2.35524600	-2.90440400
H	-4.34938800	2.77107800	-3.89328900
H	-5.11098600	1.41180900	-3.04565500
H	-5.23992200	3.06461600	-2.40050800
C	-2.30008400	1.32069400	-2.99527300
H	-1.32972700	1.19079700	-2.51151500
H	-2.70672700	0.33640700	-3.23129800
H	-2.14260900	1.84979600	-3.94209000
C	-1.35645700	-2.78958400	-2.76628900
H	-0.78206200	-1.94697700	-2.37084500
H	-0.70388700	-3.67120400	-2.79308300
H	-1.63816400	-2.56230200	-3.79806900
C	-2.05990500	-3.53444100	-0.49829900
H	-2.88623000	-3.76021800	0.18074900
H	-1.45802100	-4.44167200	-0.62368000
H	-1.41459000	-2.78275400	-0.03502200
C	-3.44334800	-4.20249900	-2.44262700
H	-3.79403400	-3.99910600	-3.45659900
H	-2.84982400	-5.12361900	-2.47264100
H	-4.32175700	-4.38386200	-1.81265000
C	-1.50999500	-1.21756100	2.57479500
H	-1.08569400	-1.82581200	1.77362400
H	-1.25982700	-0.17289100	2.37523600
H	-1.00807700	-1.50772700	3.50478500
C	-3.28827000	-2.89201300	3.11874400
H	-2.75572100	-3.13106900	4.04689200
H	-4.35129300	-3.08388700	3.28929500
H	-2.93265100	-3.57777100	2.34373800
C	-3.48516300	-0.51778600	3.90301100
H	-2.90647000	-0.75630000	4.80333600
H	-3.32737500	0.53850700	3.66229000
H	-4.54278500	-0.66488600	4.13894500
Mo	3.02868600	0.33336000	0.51354700
N	3.14597800	-0.80379100	-1.11715000
N	3.30558600	2.30939500	0.51895100
N	4.32144600	-0.36831800	1.85194900
C	3.11795700	-2.20305600	-0.78635800
C	3.16221600	-0.46374300	-2.59614100

C	3.94613100	2.94705600	-0.59572600
C	2.94637500	3.25869500	1.64927700
C	5.70409700	-0.07751100	1.56684300
C	4.08335800	-1.22329200	3.07723300
C	4.19579900	-3.05839200	-1.09693100
C	1.99909600	-2.76086800	-0.14519400
C	2.11477600	0.63528800	-2.83542300
C	2.75845300	-1.66298500	-3.48076700
C	4.56161000	0.02508300	-3.00963600
C	3.21292900	3.67762600	-1.55024300
C	5.34289600	2.87814600	-0.74896200
C	1.76938100	4.17932000	1.25593000
C	4.15474800	4.14389500	2.02320300
C	2.53120300	2.45766600	2.89346600
C	6.41408800	-0.80568500	0.59895100
C	6.38103400	0.96261100	2.23341500
C	4.70333500	-0.60848000	4.35250300
C	2.57684800	-1.39589800	3.31258000
C	4.71297800	-2.61545300	2.85096300
C	4.15510600	-4.41238300	-0.77247300
H	5.06119800	-2.65454700	-1.61214800
C	1.96863800	-4.11754500	0.19384900
H	1.15018600	-2.12269700	0.07225100
H	1.11423600	0.27277000	-2.57967400
H	2.32440600	1.51875300	-2.23420000
H	2.11846700	0.93984800	-3.88929600
H	2.66092600	-1.30910600	-4.51328500
H	3.49529000	-2.46965200	-3.47661100
H	1.79329100	-2.07927000	-3.17480100
H	4.56630600	0.31885500	-4.06667500
H	4.86602500	0.88784400	-2.41389300
H	5.31047500	-0.76440600	-2.87866500
C	3.85394800	4.31252100	-2.61529300
H	2.13327600	3.73011200	-1.46320500
C	5.98035500	3.51157600	-1.81694700
H	5.92479000	2.33005900	-0.01676700
H	1.46831100	4.78135600	2.12212000
H	2.04321600	4.87115600	0.45524600
H	0.90118400	3.59671000	0.93099300
H	3.89213700	4.78291100	2.87463900
H	5.01860400	3.53541700	2.30601600
H	4.45402100	4.79394300	1.19658200
H	1.63856400	1.85271000	2.71199300
H	3.33758300	1.79803400	3.22132000
H	2.30453600	3.14907200	3.71298400
C	7.74558900	-0.50503600	0.30132100

H	5.91075500	-1.61907800	0.09237600
C	7.71350300	1.25621300	1.94534500
H	5.84909300	1.54542100	2.97662100
H	4.28820600	0.38215000	4.56673600
H	4.47837300	-1.25449900	5.20901200
H	5.79106300	-0.52245700	4.28326200
H	2.08991300	-1.89326900	2.47191500
H	2.42743700	-2.01494700	4.20525600
H	2.07500300	-0.43877400	3.47312200
H	5.79640700	-2.54621400	2.70903900
H	4.53153900	-3.25425300	3.72397000
H	4.27936600	-3.10151200	1.97279200
C	3.04265400	-4.95015500	-0.11687300
H	4.99734300	-5.05023200	-1.02888500
H	1.09225400	-4.52147300	0.69449700
C	5.24094700	4.23501800	-2.75497900
H	3.26264400	4.86623400	-3.34041600
H	7.06124300	3.44104900	-1.90986000
C	8.40297100	0.52595600	0.97300000
H	8.27020400	-1.08551000	-0.45361800
H	8.21145600	2.06374300	2.47623000
H	3.01515600	-6.00519500	0.14129500
H	5.73837500	4.73132000	-3.58384400
H	9.43971200	0.75807800	0.74497700

Cartesian coordinates, electronic (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for 9 & TSB9 (quintet/triplet/singlet)

9_Q_T

E_{elec} (B3LYP/BS1) = -1020.8913257 au
H_{corr} (B3LYP/BS1) = 0.181397 au
G_{corr} (B3LYP/BS1) = 0.111536 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1020.77734599 au

0 5

Mo	-2.38284700	0.30781800	0.13745500
O	-0.97881200	1.70445700	-0.34702100
O	0.71337700	0.79247000	1.45537000
N	-3.27640400	-0.23716800	1.79585100
N	-3.67034800	1.34861600	-0.91840700
N	-1.45014400	-1.23083100	-0.59442900
S	0.33345400	2.11253900	0.53065100
Mo	2.14314700	0.32936000	0.09765300
N	1.49356200	-0.48588500	-1.59063800
N	3.80160200	1.36154100	0.05221100
N	2.87227500	-1.33929500	0.95637800
H	4.68120200	0.98949700	0.40094200
H	3.91082000	2.31187500	-0.29257200
H	3.48713500	-2.02033200	0.51644700
H	2.41035500	-1.75648800	1.76113000
H	1.86071500	-1.37263100	-1.93082600
H	1.16027400	0.07835300	-2.37071000
H	-4.02744800	0.29776600	2.22821400
H	-2.86353200	-0.87161800	2.47724000
H	-0.49344200	-1.12900000	-0.95718100
H	-1.89004400	-2.09155500	-0.91369500
H	-3.34090900	2.15291900	-1.45080400
H	-4.52102600	0.97093500	-1.32978500

9_T

E_{elec} (B3LYP/BS1) = -1020.8990713 au
H_{corr} (B3LYP/BS1) = 0.182503 au
G_{corr} (B3LYP/BS1) = 0.114969 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1020.78618695 au

0 3

Mo	-2.26614500	0.16158100	0.00561200
O	-0.94760800	-1.33415800	0.41870400
O	0.68748600	-0.28580500	-1.35270000
N	-3.06916100	0.83621900	-1.65176000
N	-3.63252300	-0.89290700	0.94103300
N	-1.34111900	1.62358700	0.89783100
S	0.42679200	-1.63099100	-0.42079900
Mo	2.12052600	0.09581800	0.02038600
N	1.55820100	0.64858200	1.82840100
N	3.76628000	-0.95073500	0.01115600
N	2.77371300	1.78192200	-0.71296200
H	4.69199700	-0.53369500	0.11401400
H	3.82473600	-1.95921600	0.13735500
H	2.31804300	2.68642000	-0.57541000
H	3.40570900	1.85130800	-1.51374500
H	2.05549100	1.37393500	2.34760100
H	1.12927800	-0.00147600	2.48711600
H	-3.81595900	0.35214900	-2.14672400
H	-2.59765000	1.48492300	-2.27980800
H	-0.40582400	1.47186000	1.29453100
H	-1.78797500	2.45319900	1.28293500
H	-3.35885300	-1.75321600	1.41391000
H	-4.47843100	-0.50804900	1.35517900

9_S

E_{elec} (B3LYP/BS1) = -1020.89806744 au
H_{corr} (B3LYP/BS1) = 0.182731 au
G_{corr} (B3LYP/BS1) = 0.115793 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1020.78771004 au

0 1

Mo	-2.11516800	0.41168000	0.02156100
O	-0.97034200	1.98276400	0.24820100
O	0.70686100	0.57158100	1.73304200
N	-3.05860400	0.04740900	1.65826600
N	-3.50837100	0.87219400	-1.25295000
N	-1.30508200	-1.28292300	-0.46765900
S	0.49787000	2.05482300	1.04759400
Mo	2.00133100	0.29176300	0.19988500
N	1.38515300	0.18173600	-1.67164700
N	3.74506100	1.14724700	0.34504700
N	2.54372900	-1.53424300	0.60362900
H	3.91068000	2.15158900	0.36920400
H	4.62119400	0.65594400	0.16224100
H	1.98263200	-2.36257400	0.39479200
H	3.24590400	-1.77951800	1.30564100
H	1.84986100	-0.42045300	-2.35266100
H	0.99457600	0.99018000	-2.15519800
H	-3.84135600	0.59910700	2.01438000
H	-2.67318800	-0.53692700	2.40294800
H	-0.53786200	-1.30848200	-1.14274700
H	-1.72320400	-2.20528100	-0.34107600
H	-3.32631000	1.20903600	-2.19962300
H	-4.45240100	0.48669100	-1.20939600

TSB9_Q_T
E_{elec} (B3LYP/BS1) = -1020.8761892 au
H_{corr} (B3LYP/BS1) = 0.178880 au
G_{corr} (B3LYP/BS1) = 0.108575 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1020.75725876 au

0 5

Mo	-1.92384500	-0.10519500	0.09782000
O	-1.21414400	1.38094300	-0.82776900
O	0.36561500	0.54031300	0.94043200
N	-2.38021600	0.28551000	1.97631800
N	-3.77996100	-0.40017300	-0.48200200
N	-1.24223600	-1.81606000	-0.59256100
S	0.40313600	1.89190800	-0.06856800
Mo	2.06974700	-0.13637700	0.02287600
N	1.77223800	-1.10893100	-1.65871100
N	3.77201000	0.79703300	0.23941100
N	2.46167000	-1.68528400	1.23056300
H	4.50991500	0.45540100	0.84990800
H	4.03623000	1.67051600	-0.20946300
H	3.18484600	-2.38467300	1.07472400
H	1.74307800	-2.05821000	1.84765200
H	2.13387500	-2.04505100	-1.82866100
H	1.54828500	-0.64674200	-2.53827300
H	-3.21236300	-0.07513300	2.43585500
H	-1.65879500	0.52366400	2.65332000
H	-0.27419200	-1.92499800	-0.89846600
H	-1.74872100	-2.69754000	-0.58541000
H	-4.00579600	-0.86690400	-1.35810400
H	-4.53871900	0.22415900	-0.21356000

TSB9_T

E_{elec} (B3LYP/BS1) = -1020.8888333 au
H_{corr} (B3LYP/BS1) = 0.180250 au
G_{corr} (B3LYP/BS1) = 0.113726 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1020.77558196 au

0 3

Mo	-1.83920400	-0.06314200	0.03205000
O	-0.98525800	-1.68149900	0.55890400
O	0.38823300	-0.31934500	-1.02034800
N	-2.39099100	-0.00808200	-1.86333900
N	-3.68014500	-0.04268300	0.75788800
N	-1.26001700	1.45270800	1.15901400
S	0.65073100	-1.81245700	-0.27025000
Mo	2.10446600	0.10004800	-0.00099700
N	1.89337600	0.59839900	1.87274400
N	3.77972900	-0.82236900	-0.38463600
N	2.43705900	1.84132700	-0.81689600
H	4.67508100	-0.33452000	-0.40961100
H	3.92831600	-1.82717800	-0.32344700
H	1.94223200	2.69678700	-0.55670000
H	2.81572900	1.95327500	-1.75928800
H	2.39675300	1.38179600	2.29056500
H	1.57583300	-0.04110600	2.59941800
H	-3.27706800	0.38714300	-2.16739400
H	-1.70305000	0.01582100	-2.61306400
H	-0.28890800	1.60033600	1.42994200
H	-1.86652500	2.20334600	1.47783000
H	-4.39790000	-0.68142600	0.41937800
H	-3.86318800	0.18976700	1.73202900

TSB9_S

E_{elec} (B3LYP/BS1) = -1020.90005760 au
H_{corr} (B3LYP/BS1) = 0.182145 au
G_{corr} (B3LYP/BS1) = 0.120792 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1020.79140526 au

0 1

Mo	-1.70698400	-0.11388100	-0.09213500
O	-1.20654700	-1.74755500	0.69886400
O	0.29342600	-0.82683900	-1.06681600
N	-2.38584500	-0.08491000	-1.91840900
N	-3.39363000	0.04782300	0.84952500
N	-0.51053500	1.39511100	0.51658600
S	0.53687600	-2.06272100	0.04613400
Mo	1.61280400	0.21130500	0.16347800
N	1.83145300	0.32410300	2.12003500
N	3.29575400	-0.51356800	-0.52387500
N	2.16930700	1.95064000	-0.52865200
H	4.03175700	0.08324800	-0.90781100
H	3.60835900	-1.48226700	-0.53375000
H	1.68824100	2.84197200	-0.40246500
H	2.98944000	2.09293800	-1.12246400
H	2.66563300	0.75125100	2.51822000
H	1.47323000	-0.39635200	2.74005200
H	-3.29705700	-0.47114800	-2.16573000
H	-1.74623100	-0.15589100	-2.70921000
H	-0.51586300	2.27975500	0.00718400
H	-0.45357800	1.59711000	1.51550700
H	-4.14367300	0.70593300	0.63088000
H	-3.64968900	-0.51910100	1.65834100

Cartesian coordinates, electronic (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for 13 & 13Ar (doublet)

13_D

E_{elec} (B3LYP/BS1) = -709.5449030 au
H_{corr} (B3LYP/BS1) = 0.091390 au
G_{corr} (B3LYP/BS1) = 0.045306 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -709.49084915 au

0 2

O	1.01716500	0.00045700	-1.34214500
S	2.11281100	0.00037400	0.04216200
Mo	-0.30719500	0.00000100	0.02503900
N	-0.60154200	1.64373800	1.02466300
N	-0.59965500	-1.64408200	1.02467100
N	-1.91380700	-0.00069500	-1.10336400
H	-1.51075100	1.99791500	1.31353300
H	0.16297500	2.15892700	1.45267500
H	-2.27282800	0.83147200	-1.57167700
H	-2.27170700	-0.83327500	-1.57180100
H	-1.50839800	-1.99906100	1.31400900
H	0.16560500	-2.15840200	1.45239400

13Ar_D

E_{elec} (B3LYP/BS1) = -1874.37363962 au
H_{corr} (B3LYP/BS1) = 0.705105 au
G_{corr} (B3LYP/BS1) = 0.595699 au
SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -1873.73609234 au

0 2

Mo	0.42682200	-0.19934000	-0.80652400
O	0.36782700	-0.61644100	-2.72571700
N	1.31018900	-1.17265000	0.74306600
N	0.64816400	1.74753800	-0.49926600
N	-1.51932800	-0.71308800	-0.80606200
S	2.07692700	-0.71380700	-2.50446600
C	0.37901500	-1.64083000	1.74066300
C	-0.24108900	-0.72973000	2.61173200
C	0.08225900	-3.00897000	1.90863900
C	-1.14922200	-1.15950800	3.58257200
H	0.00560900	0.32069000	2.53645100
C	-0.81222100	-3.43826400	2.88803900
H	0.55680800	-3.74347200	1.26925700
C	-1.44346400	-2.51509900	3.72629600
H	-1.61179600	-0.42588600	4.23798600
H	-1.01843400	-4.50053400	2.99292200
H	-2.14345100	-2.85132000	4.48627600
C	-2.50857300	0.32076800	-0.68646400
C	-3.27150200	0.42765900	0.48897200
C	-2.74432600	1.23569800	-1.72648100
C	-4.24876900	1.41666900	0.61439900
H	-3.07857800	-0.26136400	1.30386700
C	-3.70896400	2.23537000	-1.59005700
H	-2.16150300	1.15306300	-2.63772300
C	-4.46932800	2.32780400	-0.42100800
H	-4.83072400	1.48076900	1.53038600
H	-3.87217600	2.93739500	-2.40380400
H	-5.22522300	3.10175300	-0.31933200
C	0.41533900	2.24326500	0.83514800
C	1.46710300	2.35693900	1.76150200
C	-0.86291300	2.67530100	1.21948400
C	1.24171300	2.87115600	3.03809100
H	2.45992400	2.03113500	1.47795800
C	-1.08764400	3.18360600	2.50057300
H	-1.67519900	2.62095500	0.50678300
C	-0.03941000	3.28223200	3.41645900
H	2.06886700	2.94677700	3.73916800
H	-2.08757400	3.50818700	2.77590300
H	-0.21532600	3.67912700	4.41254900

C	-2.06443000	-2.02583400	-1.34995500
C	1.19172500	2.80239400	-1.47145400
C	2.75421800	-1.60769900	0.96052100
C	2.73186700	2.81408300	-1.43394000
H	3.11406300	3.56790400	-2.13290100
H	3.10422600	3.06904600	-0.43666800
H	3.13142700	1.84142400	-1.72811900
C	0.67270300	4.20503200	-1.08480900
H	1.02917300	4.91879600	-1.83539100
H	-0.42117500	4.24174600	-1.07792500
H	1.03644000	4.53738200	-0.10929200
C	0.69987200	2.52502900	-2.90169900
H	1.02661400	1.55825100	-3.28203800
H	-0.39273400	2.56837900	-2.94688400
H	1.09610700	3.30032000	-3.56755500
C	-2.70607300	-1.81499300	-2.73740200
H	-1.97561500	-1.40338000	-3.43987700
H	-3.05041600	-2.78046600	-3.12703900
H	-3.57160500	-1.14783800	-2.69105000
C	-0.93678200	-3.06415600	-1.49635200
H	-0.40307400	-3.20865700	-0.55606100
H	-1.37974600	-4.02765100	-1.77334700
H	-0.22716000	-2.78462000	-2.27649500
C	-3.11708000	-2.59423100	-0.37409600
H	-3.99326900	-1.94563300	-0.29113500
H	-3.46017300	-3.56667000	-0.74637700
H	-2.69116800	-2.73998100	0.62353400
C	3.72231400	-0.50971600	0.48263700
H	3.60074500	-0.26943900	-0.57382900
H	3.58155900	0.40825000	1.05915200
H	4.75484500	-0.84502800	0.63258700
C	3.06701200	-2.92046600	0.20891900
H	4.13143500	-3.16512900	0.31313000
H	2.50012000	-3.76377900	0.61381700
H	2.83820500	-2.82434600	-0.85535600
C	3.04293800	-1.80407300	2.46703200
H	4.11223200	-2.00531700	2.59696500
H	2.79476400	-0.90305800	3.03822400
H	2.49217300	-2.64293200	2.89816000

Cartesian coordinates, electronic (E_{elec}), thermal corrections to enthalpies (H_{corr}) and Gibbs (G_{corr}) energies and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for TSB9Ar (singlet)

TSB9Ar_S
E_{elec} (B3LYP/BS1) = -3350.5586049 au
H_{corr} (B3LYP/BS1) = 1.407380 au
G_{corr} (B3LYP/BS1) = 1.212954 au

SPE (M06/BS2//B3LYP/BS1, Solvent = Et_2O) = -3349.28040390 au
SPE (B3LYP-D3BJ/BS2//B3LYP/BS1, Solvent = Et_2O) = -3351.99631934 au

0 1

Mo	-2.96906700	-0.53885100	-0.34525400
O	-1.14784400	-0.43078200	-0.46125600
O	1.19489200	0.22449700	1.22347000
N	-3.71764000	-1.18668600	1.40340400
N	-3.49563300	1.27602500	-0.92639100
N	-3.43646300	-1.87676200	-1.76644600
S	-0.06385900	1.00582400	0.42181100
C	-5.15048600	-1.29154800	1.50973200
C	-5.93084600	-0.23193900	2.00021000
C	-5.80527600	-2.48086800	1.13597700
C	-7.31661800	-0.35979600	2.11517200
H	-5.44444700	0.69136900	2.29039900
C	-7.18947300	-2.60824100	1.25482100
H	-5.21619500	-3.30107400	0.73859300
C	-7.95269200	-1.54638800	1.74609800
H	-7.89778500	0.47623700	2.49513200
H	-7.67070600	-3.53659500	0.95790600
H	-9.03114400	-1.64315600	1.83854400
C	-4.52929100	-1.54499100	-2.62751000
C	-5.78874200	-1.22637900	-2.08626800
C	-4.39555300	-1.47519900	-4.03185800
C	-6.85625200	-0.84345100	-2.90134200
H	-5.94036500	-1.30410300	-1.01729900
C	-5.46871300	-1.11121000	-4.84373700
H	-3.44152800	-1.69695100	-4.49382900
C	-6.70809300	-0.78642300	-4.28702000
H	-7.81380000	-0.60979400	-2.44239100
H	-5.32768300	-1.07107300	-5.92110400
H	-7.54128700	-0.50021500	-4.92268800
C	-4.24794400	2.05177000	0.02295200
C	-3.61554400	2.60412100	1.15149800
C	-5.62320900	2.28024600	-0.15437600

C	-4.33864400	3.36456400	2.07192200
H	-2.55261000	2.43288800	1.29530800
C	-6.33763900	3.05897000	0.75739000
H	-6.12909400	1.82713900	-0.99953600
C	-5.70124900	3.60459800	1.87427200
H	-3.83093600	3.77980700	2.93880800
H	-7.40000300	3.22666800	0.59932600
H	-6.26029400	4.20787200	2.58443900
C	-2.63940900	-3.12558300	-2.07950800
C	-3.06904200	2.04121800	-2.17035700
C	-2.98548500	-1.66856200	2.64283400
C	-2.33564300	3.33732100	-1.76593100
H	-1.99954100	3.86006600	-2.66895000
H	-2.98137200	4.01910100	-1.20511500
H	-1.45263600	3.11556500	-1.15642000
C	-4.29494000	2.39893300	-3.03688800
H	-3.95374400	2.87640800	-3.96340800
H	-4.86430000	1.50412500	-3.30399300
H	-4.96025400	3.10450900	-2.53186800
C	-2.10699800	1.18954900	-3.01254400
H	-1.19693400	0.94534700	-2.46247200
H	-2.57843500	0.26245000	-3.34380000
H	-1.82375600	1.75715500	-3.90618300
C	-1.40647200	-2.79816900	-2.94918400
H	-0.81341600	-2.01093500	-2.47527100
H	-0.77469400	-3.68832700	-3.05777700
H	-1.67979300	-2.46707200	-3.95520100
C	-2.13572100	-3.71692600	-0.75171400
H	-2.97180700	-3.96435100	-0.09103600
H	-1.56580100	-4.63274200	-0.94507000
H	-1.46985500	-3.02128200	-0.23641500
C	-3.51163000	-4.20595400	-2.75299600
H	-3.84242700	-3.92683400	-3.75534200
H	-2.93113900	-5.13142600	-2.83964900
H	-4.40246300	-4.41863100	-2.15107700
C	-1.46879700	-1.55770200	2.45831500
H	-1.10278300	-2.18832000	1.64488500
H	-1.15613400	-0.53073300	2.26182600
H	-0.97310300	-1.88675700	3.37837400
C	-3.33226400	-3.13394100	2.98425300
H	-2.77427700	-3.43947900	3.87709000
H	-4.39625600	-3.26846600	3.19673200
H	-3.05373000	-3.80835900	2.16817600
C	-3.37567500	-0.77332600	3.84152700
H	-2.80637100	-1.07804800	4.72741300
H	-3.14683300	0.27658100	3.63102500

H	-4.43876600	-0.85476600	4.08464700
Mo	3.06148100	0.44653100	0.65525000
N	3.15285600	-0.74676000	-0.94070000
N	3.30303400	2.42545300	0.60550300
N	4.40436000	-0.20374500	1.96936500
C	3.11833200	-2.13404500	-0.56570400
C	3.17729400	-0.45229200	-2.42823600
C	3.88616800	3.05679500	-0.54298100
C	2.96072200	3.38864100	1.73032400
C	5.77048000	0.10474600	1.62961600
C	4.22104400	-1.03724600	3.21805600
C	4.18778100	-3.00763200	-0.85488300
C	1.99951700	-2.66364700	0.09981800
C	2.13732400	0.64483400	-2.70308000
C	2.76943300	-1.67482300	-3.27875600
C	4.58063900	0.01678300	-2.85170700
C	3.10152100	3.75344300	-1.48209500
C	5.27772300	3.01628300	-0.74688600
C	1.75308700	4.27746500	1.35768800
C	4.16315800	4.30258000	2.04973000
C	2.59829400	2.60321100	3.00083300
C	6.45745700	-0.62675800	0.64754900
C	6.45268900	1.16851000	2.25256000
C	4.87720400	-0.38838200	4.45800200
C	2.72586100	-1.22331200	3.50972100
C	4.86110000	-2.42572600	2.99863800
C	4.13886700	-4.35058000	-0.48821700
H	5.05385300	-2.62803900	-1.38699600
C	1.96111000	-4.00860600	0.48160700
H	1.15705000	-2.01289400	0.30356900
H	1.13624600	0.29778000	-2.42983000
H	2.35492000	1.54665600	-2.13289000
H	2.13938800	0.91304800	-3.76688700
H	2.67778800	-1.35097300	-4.32166500
H	3.50063300	-2.48610100	-3.24846400
H	1.80045100	-2.07584500	-2.96425200
H	4.58867100	0.28599300	-3.91529500
H	4.88916900	0.89159200	-2.27569600
H	5.32445500	-0.77387300	-2.70102900
C	3.68853900	4.38410000	-2.58023400
H	2.02472100	3.78147200	-1.35686300
C	5.86068600	3.64457200	-1.84860000
H	5.89878700	2.49479300	-0.02716600
H	1.46587800	4.88737700	2.22324800
H	1.98841600	4.96149400	0.53824600
H	0.89051600	3.66755800	1.06906700

H	3.91528300	4.95144400	2.89816700
H	5.04763400	3.71598900	2.31483100
H	4.42324700	4.94357400	1.20288500
H	1.71266700	1.97871100	2.85498900
H	3.42669900	1.96636400	3.31846300
H	2.38086000	3.30616900	3.81309500
C	7.77147400	-0.30820400	0.29572200
H	5.95003700	-1.45586200	0.17160900
C	7.76796200	1.48036700	1.91021200
H	5.93786100	1.75534200	3.00460300
H	4.45695700	0.60134100	4.66662900
H	4.69144400	-1.01929300	5.33496200
H	5.96053800	-0.29013100	4.34806900
H	2.21414600	-1.73772200	2.69423500
H	2.61558600	-1.83067200	4.41607100
H	2.21987200	-0.26911100	3.67483700
H	5.93674100	-2.34482100	2.81061200
H	4.72492700	-3.04601100	3.89297400
H	4.39950000	-2.93863800	2.15055800
C	3.02665500	-4.85919000	0.19037400
H	4.97514400	-5.00225500	-0.72904800
H	1.08496900	-4.38957300	1.00053900
C	5.07082000	4.33499300	-2.77020000
H	3.05860800	4.91180300	-3.29218200
H	6.93878400	3.59679300	-1.98053800
C	8.43446100	0.74534700	0.92548000
H	8.27790400	-0.89170400	-0.46925700
H	8.27029300	2.30594100	2.40824200
H	2.99288100	-5.90539400	0.48173500
H	5.52590200	4.82794100	-3.62504600
H	9.45770400	0.99166800	0.65519700

Cartesian coordinates, electronic energies (E_{elec}) and single-point energies (SPE) in Solvent = diethyl ether (Et_2O) for Minimum Energy Crossing Points (MECP) at 2M, 4M, 5M, INT-SO-M1, INT-SO-M2, 9-M1, 9-M2, 9Ar-M1 & 9Ar-M2

2M

E_{elec} (B3LYP/BS1, quartet) = -784.6927850 au
E_{elec} (B3LYP/BS1, doublet) = -784.6927922 au
SPE (M06/BS2//B3LYP/BS1, doublet, Solvent = Et_2O) = -784.65801273 au

Mo	-0.6558340	-0.0832368	-0.0300758
O	1.9830144	-1.1672954	0.2159518
O	2.3994819	1.3657112	-0.0524135
N	-0.6364832	-1.6431444	-1.1919072
N	-2.0674314	-0.1990810	1.3283126
N	-0.5147020	1.7122429	-0.7684389
H	0.2324173	-2.1493101	-1.3561843
H	-1.3438341	-1.8766823	-1.8858572
H	-2.3787010	-1.0610257	1.7713071
H	-2.4908637	0.6092914	1.7774855
H	-1.2053066	2.1328959	-1.3881037
H	0.3909851	2.1797341	-0.8467106
S	1.7613125	0.2509491	0.7203664

4M

E_{elec} (B3LYP/BS1, quartet) = -784.7242569 au
E_{elec} (B3LYP/BS1, doublet) = -784.7242916 au
SPE (M06/BS2//B3LYP/BS1, doublet, Solvent = Et_2O) = -784.67261000 au

Mo	-0.7490100	-0.0561412	0.0480003
O	2.5845010	-0.6834159	-0.8981188
O	0.9748718	0.6178837	0.6435615
N	-2.0594090	-0.8782682	1.2509803
N	-1.4233466	1.6776675	-0.5558396
N	-0.1971599	-1.3483312	-1.2728868
H	-2.0379606	-1.8639275	1.5084767
H	-2.6162397	-0.3563294	1.9262341
H	-2.2882859	1.8067224	-1.0778723
H	-0.8022910	2.4730436	-0.6996854
H	0.7999310	-1.3719680	-1.5190446
H	-0.7881124	-1.8369544	-1.9433419
S	2.5266674	0.2498094	0.2965449

5M

E_{elec} (B3LYP/BS1, quartet) = -784.7368130 au
E_{elec} (B3LYP/BS1, doublet) = -784.7368280 au
SPE (M06/BS2//B3LYP/BS1, doublet, Solvent = Et_2O) = -784.68298734 au

Mo	0.5221319	-0.0255911	0.0380295
O	-1.0944523	1.2997149	-0.0867303
O	-1.5249892	-1.1003862	-0.0409997
N	1.1715962	-1.0218522	-1.5040857
N	1.9140338	1.3922490	0.0076862
N	0.8554004	-0.8408634	1.7719976
H	0.7576167	-1.8949398	-1.8223028
H	1.9908736	-0.7702521	-2.0503206
H	1.6786914	2.3743244	0.1309494
H	2.9196466	1.2715011	-0.0846344
H	0.3397756	-1.6491772	2.1136703
H	1.6589502	-0.6273197	2.3566165
S	-2.3047515	0.2467833	-0.1188675

INT-SO-M1

E_{elec} (B3LYP/BS1, quintet) = -945.6760741 au

E_{elec} (B3LYP/BS1, triplet) = -945.6761020 au

SPE (M06/BS2//B3LYP/BS1, triplet, Solvent = Et_2O) = -945.56442839 au

Mo	0.17018920	0.13593960	0.49230030
N	-0.78318170	-1.48933680	0.05475370
N	0.77799230	1.35318200	-0.93087520
N	1.63859120	-0.23263250	1.74699970
H	-1.81569130	-1.53931620	0.06590430
H	-0.36830670	-2.27927480	-0.43934750
H	0.27385000	2.17067180	-1.26790430
H	1.48682310	1.08382480	-1.61173700
H	2.35445880	0.45226100	1.98205240
H	1.54903050	-0.91656410	2.49665900
S	-1.54353690	1.58857090	1.23002470
O	-2.26846220	0.73313460	2.54488610
Mo	-3.89674000	0.22151980	1.58173060
N	-4.90730090	-0.98456900	2.83204580
N	-5.22493330	1.63718770	1.36877130
N	-3.83794800	-1.20269060	0.16470520
H	-5.02425330	-0.70500880	3.80546140
H	-5.73404290	-1.49768210	2.52934500
H	-5.11420640	2.45618090	0.77558360
H	-6.13615430	1.63089090	1.81934350
H	-3.92156650	-0.96219610	-0.82205360
H	-4.30390460	-2.09311300	0.33562420

INT-SO-M2

E_{elec} (B3LYP/BS1, triplet) = -945.6878943 au

E_{elec} (B3LYP/BS1, singlet) = -945.6879015 au

SPE (M06/BS2//B3LYP/BS1, singlet, Solvent = Et_2O) = -945.58025513 au

Mo	0.15123250	0.15653250	0.61544580
N	-0.75254710	-1.48956560	0.18963240
N	0.51640900	1.26894730	-0.94897050
N	1.80358380	-0.11130680	1.60010810
H	-1.77988450	-1.59108210	0.16309830
H	-0.27564680	-2.29352080	-0.22022220
H	-0.12184510	1.93436470	-1.37986550
H	1.23024010	0.99385000	-1.62520280
H	2.45059450	0.64470610	1.82136130
H	1.96372260	-0.91164860	2.20981530
S	-1.34003440	1.37122700	1.72053170
O	-2.35523470	0.38169640	2.83092330
Mo	-3.90323620	0.18803450	1.71676200
N	-5.30015320	-0.87224010	2.60267960
N	-4.97416270	1.80930030	1.44021060
N	-3.79746550	-1.18039420	0.24204300
H	-5.79754700	-0.58520910	3.44180350
H	-5.64889690	-1.76525600	2.25967050
H	-4.60870180	2.65334150	1.00397870
H	-5.98518030	1.85594990	1.53262580
H	-3.71525090	-0.88353470	-0.72979370
H	-4.38928900	-2.01321210	0.26763850

9-M1

E_{elec} (B3LYP/BS1, quintet) = -1020.8891931 au
E_{elec} (B3LYP/BS1, triplet) = -1020.8891802 au
SPE (M06/BS2//B3LYP/BS1, triplet, Solvent = Et_2O) = -1020.77420672 au

Mo	-2.74312450	0.22754150	0.41204010
O	-0.96710230	1.15627750	0.04863310
O	0.85638510	-0.36831410	1.17134690
N	-4.27017550	0.70855280	1.55033880
N	-3.21256300	0.57130380	-1.46098980
N	-1.97816010	-1.43234800	1.08064770
S	0.24130330	1.17542860	1.14960820
Mo	2.33640220	0.20082740	-0.06996010
N	1.83902530	0.47299940	-1.94903350
N	3.80751420	1.18635980	0.78348070
N	3.50672460	-1.35204210	-0.55527490
H	4.77511160	0.90782730	0.62950320
H	3.76531180	2.15589410	1.09077080
H	3.25438290	-2.01645380	-1.28441470
H	4.14338440	-1.79262320	0.10586250
H	2.37482200	0.06675520	-2.71324640
H	1.27532670	1.25350200	-2.27825460
H	-4.92719990	1.44880150	1.31155350
H	-4.31245080	0.51377100	2.54875860
H	-0.96072550	-1.52058240	1.15662950
H	-2.43145070	-2.34357960	1.06066060
H	-2.49857090	0.95662280	-2.07872310
H	-3.90120880	0.04681920	-1.99645720

9-M2

E_{elec} (B3LYP/BS1, triplet) = -1020.8909153 au
E_{elec} (B3LYP/BS1, singlet) = -1020.8909486 au
SPE (M06/BS2//B3LYP/BS1, singlet, Solvent = Et_2O) = -1020.77996177 au

Mo	-2.74312450	0.22754150	0.41204010
O	-0.96710230	1.15627750	0.04863310
O	0.85638510	-0.36831410	1.17134690
N	-4.27017550	0.70855280	1.55033880
N	-3.21256300	0.57130380	-1.46098980
N	-1.97816010	-1.43234800	1.08064770
S	0.24130330	1.17542860	1.14960820
Mo	2.33640220	0.20082740	-0.06996010
N	1.83902530	0.47299940	-1.94903350
N	3.80751420	1.18635980	0.78348070
N	3.50672460	-1.35204210	-0.55527490
H	4.77511160	0.90782730	0.62950320
H	3.76531180	2.15589410	1.09077080
H	3.25438290	-2.01645380	-1.28441470
H	4.14338440	-1.79262320	0.10586250
H	2.37482200	0.06675520	-2.71324640
H	1.27532670	1.25350200	-2.27825460
H	-4.92719990	1.44880150	1.31155350
H	-4.31245080	0.51377100	2.54875860
H	-0.96072550	-1.52058240	1.15662950
H	-2.43145070	-2.34357960	1.06066060
H	-2.49857090	0.95662280	-2.07872310
H	-3.90120880	0.04681920	-1.99645720

9Ar-M1

E_{elec} (B3LYP/BS1, quintet) = -3350.5573186 au

E_{elec} (B3LYP/BS1, triplet) = -3350.5573239 au

SPE (M06/BS2//B3LYP/BS1, triplet, Solvent = Et_2O) = -3349.27947465 au

Mo	-3.10330920	0.05373050	0.00697430
O	-1.15292670	-0.18017550	-0.18081700
O	1.26846680	0.30458090	0.65506660
N	-3.55940390	-0.66547480	1.82300170
N	-3.63160110	1.91556040	-0.49162400
N	-3.75907440	-1.14680570	-1.43526170
S	-0.04250940	1.08671960	0.05007790
C	-4.52750930	-1.72233850	1.90549350
C	-5.88339570	-1.41457890	2.12331670
C	-4.16212040	-3.07432330	1.79968010
C	-6.83900950	-2.42475500	2.24098080
H	-6.18153930	-0.37373830	2.18365630
C	-5.12310500	-4.08367130	1.89565830
H	-3.11772490	-3.32330500	1.64137450
C	-6.46453570	-3.76472960	2.12419860
H	-7.87948650	-2.15934690	2.41107560
H	-4.81991770	-5.12340890	1.80148610
H	-7.20923460	-4.55187720	2.21049270
C	-5.13250770	-1.03250180	-1.85253580
C	-6.15095230	-1.76352050	-1.22248790
C	-5.48390690	-0.20013220	-2.93213510
C	-7.47904020	-1.64463850	-1.64104260
H	-5.89590500	-2.43346430	-0.41168920
C	-6.80784370	-0.09154100	-3.35685850
H	-4.70927970	0.36736350	-3.43615890
C	-7.81557670	-0.80969990	-2.70703650
H	-8.25127900	-2.21615990	-1.13274470
H	-7.05315690	0.55680240	-4.19409990
H	-8.84784850	-0.72378580	-3.03465910
C	-4.74033150	2.34996530	0.32176910
C	-4.56776740	3.22322380	1.41464820
C	-6.04585120	1.90594830	0.03634950
C	-5.65258420	3.61691020	2.19817920
H	-3.57410660	3.58309020	1.65659960
C	-7.12825540	2.29321380	0.83016770
H	-6.20968490	1.26788150	-0.82392430
C	-6.93966420	3.14968960	1.91566010
H	-5.48996740	4.28800220	3.03768700
H	-8.12361510	1.93174870	0.58474480
H	-7.78280710	3.45599900	2.52908800
C	-2.91880930	-2.09481020	-2.29726080

C	-3.15948370	2.92080600	-1.51691110
C	-3.06258410	-0.16561020	3.15996520
C	-2.35167220	4.05306760	-0.84495190
H	-1.92439420	4.71306320	-1.60988030
H	-2.97914350	4.67108450	-0.19591530
H	-1.52849710	3.64472670	-0.24940820
C	-4.35660880	3.54075290	-2.26958630
H	-3.98819240	4.22000000	-3.04770290
H	-4.96382930	2.76735410	-2.75078920
H	-5.00441030	4.11703140	-1.60282590
C	-2.26364990	2.21581300	-2.54305920
H	-1.36772660	1.79010670	-2.08350880
H	-2.80385970	1.41658230	-3.05541570
H	-1.93123380	2.93680730	-3.29871830
C	-2.14730490	-1.33394130	-3.39061740
H	-1.47351410	-0.59709070	-2.94912880
H	-1.54470750	-2.03496590	-3.98176150
H	-2.82836680	-0.82479140	-4.08148970
C	-1.92718620	-2.85439370	-1.39649170
H	-2.46782660	-3.42090440	-0.63165460
H	-1.35332460	-3.56632770	-2.00224180
H	-1.22576280	-2.17703640	-0.90736150
C	-3.81502560	-3.15646390	-2.97521930
H	-4.51805120	-2.72418700	-3.69228890
H	-3.16979420	-3.85529170	-3.51970910
H	-4.38543900	-3.73189870	-2.23902330
C	-2.02344240	0.93460530	2.91586530
H	-1.13575200	0.54545780	2.41385210
H	-2.43521500	1.75273560	2.31562780
H	-1.70021400	1.36305560	3.87143820
C	-2.36888310	-1.32366040	3.90945320
H	-1.94111020	-0.95290270	4.84876850
H	-3.06883180	-2.12805130	4.15541360
H	-1.55592470	-1.74183610	3.30616290
C	-4.19503640	0.40038320	4.04113720
H	-3.76895080	0.78701370	4.97530300
H	-4.71621060	1.22097010	3.53914760
H	-4.92568280	-0.36850030	4.30677970
Mo	3.18940970	0.06833160	0.10499360
N	3.41626150	-1.08211580	-1.52445620
N	3.85571730	1.95448750	-0.11903410
N	3.66893380	-0.86727170	1.81635330
C	4.54182290	-1.97555600	-1.44120270
C	2.66125950	-1.12772720	-2.82686010
C	5.05650810	2.00791230	-0.90636030
C	3.34779720	3.28425220	0.39096900

C	4.98948860	-0.55758770	2.28343950
C	2.81443440	-1.72260200	2.72093270
C	5.83070020	-1.54795980	-1.80682940
C	4.38304600	-3.30073490	-0.99397540
C	1.63367580	0.00744630	-2.84572340
C	1.91678160	-2.47165800	-2.96965260
C	3.61614490	-0.94408740	-4.02602500
C	5.01105980	2.31093650	-2.28146810
C	6.31157850	1.76020860	-0.32246330
C	2.39164790	3.91493660	-0.64260370
C	4.51331850	4.26408940	0.64899280
C	2.61436200	3.08524720	1.72854710
C	6.09830680	-1.28594140	1.81768780
C	5.21889910	0.47993400	3.20855280
C	2.07408990	-0.83779300	3.74574760
C	1.78856660	-2.50085300	1.87699570
C	3.68090610	-2.75583840	3.47076290
C	6.92300190	-2.41488840	-1.72145020
H	5.97057940	-0.53127640	-2.15647900
C	5.47453990	-4.16512500	-0.91014670
H	3.39460680	-3.63916310	-0.70320950
H	0.87854950	-0.11872680	-2.06860080
H	2.11200680	0.98344720	-2.70629720
H	1.11403980	0.02275930	-3.81068040
H	1.32953790	-2.47904730	-3.89594460
H	2.61279300	-3.31510650	-3.01074320
H	1.23056170	-2.62455470	-2.13031700
H	3.03287040	-0.91683040	-4.95390440
H	4.17225330	-0.00466110	-3.94381740
H	4.33688480	-1.76264920	-4.10912780
C	6.17889210	2.37061990	-3.04171450
H	4.04802380	2.48987460	-2.74868450
C	7.47966140	1.81359860	-1.08733900
H	6.36396060	1.52961100	0.73628450
H	1.99101730	4.86538690	-0.26805170
H	2.91240960	4.12291740	-1.58331430
H	1.55008620	3.24881860	-0.85631990
H	4.11198170	5.19126830	1.07379690
H	5.23353390	3.84958750	1.36221500
H	5.05014790	4.52210750	-0.26842300
H	1.76647400	2.40500250	1.64159940
H	3.29937780	2.68367100	2.48165060
H	2.23999170	4.04975430	2.09108050
C	7.39044250	-0.98073980	2.25167000
H	5.93729760	-2.09462590	1.11362420
C	6.50933010	0.78053090	3.64464340

H	4.37512170	1.05599390	3.57251980
H	1.47091390	-0.08537490	3.23082930
H	1.40946360	-1.44757650	4.37086390
H	2.78085110	-0.33196860	4.41227590
H	2.29852670	-3.16484710	1.17144950
H	1.16861100	-3.12164060	2.53509190
H	1.12875820	-1.83192950	1.32237390
H	4.40206600	-2.28393230	4.14447090
H	3.02859730	-3.39763700	4.07412440
H	4.23209450	-3.39373230	2.77123170
C	6.75113080	-3.72515150	-1.27391080
H	7.91089750	-2.06009110	-2.00448800
H	5.32931430	-5.18321720	-0.55815820
C	7.42015250	2.12011140	-2.44775000
H	6.12056920	2.60729810	-4.10098390
H	8.43810350	1.61634880	-0.61470250
C	7.60295270	0.05244910	3.16548640
H	8.23150800	-1.55472720	1.87183400
H	6.66291750	1.58869630	4.35521430
H	7.60110570	-4.39909210	-1.20627800
H	8.32921980	2.16537740	-3.04077820
H	8.60819120	0.28987810	3.50266100

9Ar-M2

E_{elec} (B3LYP/BS1, triplet) = -3350.5567403 au

E_{elec} (B3LYP/BS1, singlet) = -3350.5567395 au

SPE (M06/BS2//B3LYP/BS1, singlet, Solvent = Et_2O) = -3349.28256712 au

Mo	3.12741580	0.22411600	0.44481710
O	1.20215400	0.26487510	0.82761600
O	-1.02627910	-0.25259850	-0.40536090
N	3.21279030	-1.13233050	-1.00791430
N	3.60600950	2.14586880	0.19249860
N	4.22337360	-0.40240960	1.97954400
S	0.07206570	1.00642150	-0.16744660
C	2.98235360	-2.46114770	-0.50319320
C	3.96965130	-3.46414990	-0.59015110
C	1.75127440	-2.79576780	0.08597090
C	3.73359970	-4.74768140	-0.10264320
H	4.92046310	-3.23321240	-1.05960540
C	1.52441040	-4.08107620	0.58854400
H	0.97065570	-2.04532480	0.13807680
C	2.51007620	-5.06275960	0.49735810
H	4.50949920	-5.50440470	-0.18807240
H	0.56446130	-4.31149010	1.04408650
H	2.32946260	-6.06254580	0.88246820
C	5.64850290	-0.31390420	1.78538640
C	6.33563960	-1.26342000	1.01233850
C	6.39407520	0.74072690	2.34729850
C	7.71324030	-1.16347210	0.80290210
H	5.77561470	-2.08769150	0.58939100
C	7.77126860	0.83493120	2.14879070
H	5.87997320	1.49126000	2.93697480
C	8.43860320	-0.11577690	1.37093130
H	8.21948690	-1.91290750	0.19948710
H	8.32272910	1.65815280	2.59610690
H	9.51094260	-0.04003040	1.21263390
C	4.41766380	2.54423740	-0.92338420
C	3.86883890	3.20769570	-2.03787090
C	5.80355290	2.30095140	-0.91967420
C	4.67476080	3.60729620	-3.10503700
H	2.80100460	3.39326800	-2.07297750
C	6.60623900	2.69884990	-1.99034190
H	6.24885590	1.80515490	-0.06442590
C	6.04806370	3.35636570	-3.08829310
H	4.22293490	4.11250440	-3.95516540
H	7.67390340	2.49632430	-1.95946620
H	6.67387330	3.66884850	-3.91988720
C	3.79105020	-1.03387330	3.28514000

C	3.25822270	3.28229210	1.13922070
C	3.37980730	-1.00476480	-2.51107890
C	2.22371420	4.23686370	0.50291160
H	1.90845270	4.98436840	1.24114470
H	2.63943390	4.77574510	-0.35242980
H	1.33385930	3.68948400	0.17399370
C	4.51933950	4.09412790	1.50576680
H	4.25598230	4.87347330	2.23066560
H	5.28406500	3.45393350	1.95573330
H	4.95850090	4.58398530	0.63237340
C	2.65448400	2.72008120	2.43637710
H	1.72039760	2.18240180	2.25330870
H	3.35432690	2.04497010	2.93510100
H	2.43506880	3.54619730	3.12233860
C	4.40299590	-0.31838530	4.51022420
H	4.11403040	0.73756980	4.54492220
H	4.03443910	-0.79381140	5.42658150
H	5.49447290	-0.38059680	4.52336750
C	2.26341290	-0.98316810	3.41560250
H	1.76830570	-1.50974990	2.59799190
H	1.97284800	-1.46557890	4.35631710
H	1.88804910	0.04274520	3.43009140
C	4.23847320	-2.51216310	3.30499360
H	5.32763220	-2.60336400	3.24109630
H	3.91938920	-2.98606970	4.24137680
H	3.79509940	-3.06515280	2.47212030
C	2.51191540	0.17203850	-2.98405460
H	1.45291400	-0.03168850	-2.80062230
H	2.78145710	1.09047030	-2.46522010
H	2.65530340	0.34179690	-4.05826980
C	2.88396260	-2.25640880	-3.26623020
H	2.90866560	-2.03982670	-4.34024070
H	3.50385720	-3.13919940	-3.09261490
H	1.85242460	-2.50474130	-2.99605890
C	4.85722130	-0.75087190	-2.86039550
H	4.97483600	-0.62203910	-3.94361400
H	5.22541870	0.15169730	-2.36838850
H	5.48825730	-1.59224840	-2.55315840
Mo	-2.97638030	-0.07699530	-0.30737540
N	-3.32072090	-1.11223580	1.35407700
N	-3.72265590	1.76653810	-0.26814550
N	-3.57273310	-0.85681760	-2.05385590
C	-4.21395780	-2.22530680	1.20008100
C	-2.75744350	-0.92324330	2.74399870
C	-4.94036720	1.83400290	0.50844860
C	-3.28245580	3.08145070	-0.87015570

C	-4.94010250	-0.75321180	-2.46815600
C	-2.61955780	-1.46884200	-3.08447560
C	-5.58334490	-2.05157910	1.47521750
C	-3.77269330	-3.49178730	0.77992860
C	-1.88328130	0.34024160	2.77718910
C	-1.85879450	-2.13404180	3.08039640
C	-3.86203050	-0.80220630	3.81283710
C	-4.94610450	2.28381290	1.84356610
C	-6.16724180	1.44159750	-0.05509140
C	-2.48883760	3.89587920	0.17325450
C	-4.49059990	3.91093640	-1.35381950
C	-2.38925740	2.80821670	-2.08767110
C	-5.91695400	-1.65047400	-2.01256300
C	-5.33281210	0.25635050	-3.36939980
C	-1.75325120	-0.39742650	-3.77122790
C	-1.71462080	-2.50300030	-2.38385150
C	-3.40480600	-2.23945350	-4.16917980
C	-6.48163440	-3.10904070	1.33602130
H	-5.93398320	-1.07242640	1.78354550
C	-4.67745180	-4.54502730	0.62561120
H	-2.71888770	-3.63899980	0.56758560
H	-0.96852420	0.21499250	2.19550230
H	-2.42015860	1.21571000	2.40196660
H	-1.58544580	0.55065000	3.81105510
H	-1.37493530	-1.98187520	4.05279400
H	-2.43347850	-3.06399720	3.13397480
H	-1.07354680	-2.24886440	2.32548030
H	-3.39846160	-0.65834270	4.79640490
H	-4.51557430	0.05196330	3.61336090
H	-4.47712440	-1.70478990	3.86606530
C	-6.12545880	2.31386040	2.58738990
H	-4.01639550	2.59549850	2.30487130
C	-7.34668430	1.46560330	0.69380900
H	-6.19457820	1.12593930	-1.09005150
H	-2.09305410	4.81409130	-0.27839550
H	-3.12302990	4.19186010	1.01463530
H	-1.64743750	3.30973260	0.55660900
H	-4.13254430	4.82694040	-1.83795910
H	-5.08753210	3.35105050	-2.08166040
H	-5.14579430	4.20416290	-0.52884570
H	-1.50154630	2.22515330	-1.82978840
H	-2.93770440	2.26735250	-2.86371390
H	-2.04250220	3.75701580	-2.51344410
C	-7.24494850	-1.53311640	-2.43276010
H	-5.62709790	-2.44385840	-1.33381260
C	-6.65428960	0.36345120	-3.80003000

H	-4.58627510	0.95864310	-3.72652540
H	-1.14584180	0.14402060	-3.04221010
H	-1.07313840	-0.86605050	-4.49369620
H	-2.37262230	0.32311990	-4.31632190
H	-2.32403800	-3.28358440	-1.91576830
H	-1.05661310	-2.98160290	-3.12004420
H	-1.08666670	-2.03886190	-1.62254120
H	-4.02988920	-1.59078710	-4.78770580
H	-2.68242600	-2.73675890	-4.82656700
H	-4.04396450	-3.01080450	-3.72816450
C	-6.03426950	-4.36080550	0.90628850
H	-7.53452780	-2.94853120	1.55307990
H	-4.31928540	-5.51494040	0.29036510
C	-7.33349870	1.89763850	2.01945030
H	-6.09875200	2.65777980	3.61847180
H	-8.27648950	1.14899270	0.22821930
C	-7.62091140	-0.52987030	-3.32758920
H	-7.98501440	-2.23898030	-2.06423940
H	-6.92990590	1.14740520	-4.50137260
H	-6.73491610	-5.18318990	0.79069670
H	-8.25034630	1.91718840	2.60245860
H	-8.65234310	-0.44560060	-3.65905800