

# Mechanistic insights of BHT-Mg-catalyzed ethylene phosphate's coordination ring-opening polymerization: DFT modeling and experimental data

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## SUPPORTING INFORMATION

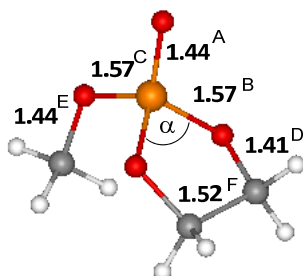
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## S1. DFT calculations

### S1.1. Rationale for the functional and basis set used for DFT calculations

To confirm the applicability of the B3PW91/DGTZVP functional/basis combination for the modeling of reactions with cyclic ethylene phosphate, we calculated the optimized molecular structure of MeOEP using a number of functional/basis pairs implemented in the Gaussian 09 program package [1]. The calculated values of the bond lengths and endocyclic angle O–P–O for MeOEP and relative deviations of these parameters from the X-ray data (Figure S1) [2]  $\Delta X (\%) = |X_{X\text{-Ray}} - X_{\text{DFT}}| \cdot 100$  are provided in Table S1. As a criterion for the rating, we used the results of the multiplication of the total relative deviations  $\Sigma \Delta$  and the computation time (Table S2). We found that B3PW91/DGTZVP set that was used in the earlier DFT modeling of  $\epsilon$ -caprolactone and rac-lactide ROP [3] is suitable for the modeling of cyclic phosphate polymerization.

Clearly, our calculations performed for the gas phase are rough approximations. However, the complexity of molecular models makes it impossible to perform calculations using standard algorithms that take into account the influence of the solvent (IEFPCM, etc.) but dramatically increase the calculation time.



**Figure S1.** Molecular structure of MeOEP and geometry parameters analyzed in DFT calculations

**Table S1** Structural parameters of the MeOEP molecule calculated by DFT using different functional/basis sets, and deviations  $\Delta_X$  from the X-Ray data [2].

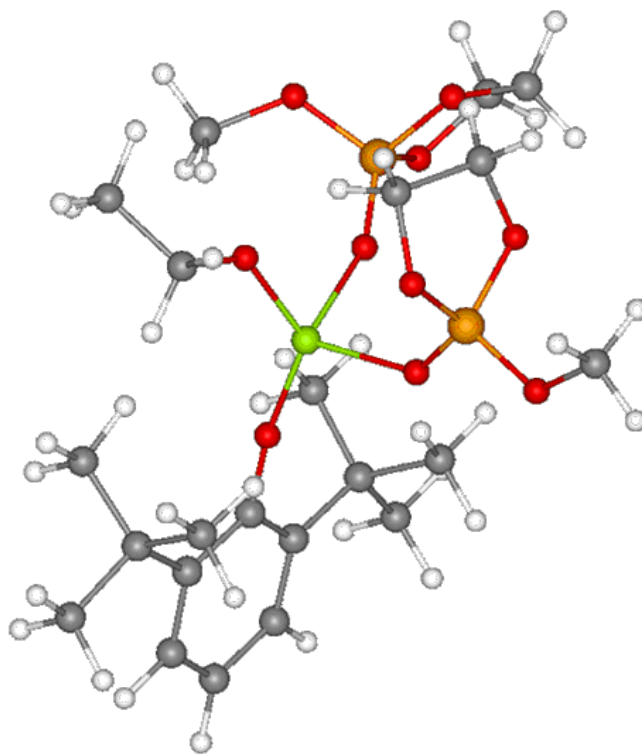
| Functional | Basis       | A     | $\Delta_A, \%$ | B     | $\Delta_B, \%$ | C     | $\Delta_C, \%$ | D     | $\Delta_D, \%$ | E     | $\Delta_E, \%$ | F     | $\Delta_F, \%$ | $\alpha$ | $\Delta_\alpha, \%$ |
|------------|-------------|-------|----------------|-------|----------------|-------|----------------|-------|----------------|-------|----------------|-------|----------------|----------|---------------------|
| X-Ray data |             | 1.440 | $\Delta_A, \%$ | 1.570 | 0              | 1.570 | 0              | 1.410 | 0              | 1.440 | 0              | 1.520 | 0              | 99.10    | 0                   |
| B3LYP      | 6-31g       | 1.574 | 9.31           | 1.759 | 12.04          | 1.706 | 8.66           | 1.480 | 4.96           | 1.474 | 2.36           | 1.536 | 1.05           | 92.99    | 6.17                |
| B3LYP      | 6-31g(d)    | 1.469 | 2.01           | 1.638 | 4.33           | 1.600 | 1.91           | 1.439 | 2.06           | 1.436 | 0.28           | 1.537 | 1.12           | 96.00    | 3.13                |
| B3LYP      | 6-31g(d,p)  | 1.469 | 2.01           | 1.637 | 4.27           | 1.600 | 1.91           | 1.439 | 2.06           | 1.436 | 0.28           | 1.537 | 1.12           | 96.00    | 3.13                |
| B3LYP      | 6-311g      | 1.554 | 7.92           | 1.746 | 11.21          | 1.681 | 7.07           | 1.477 | 4.75           | 1.468 | 1.94           | 1.535 | 0.99           | 92.66    | 6.50                |
| B3LYP      | 6-311g(d)   | 1.463 | 1.60           | 1.634 | 4.08           | 1.593 | 1.46           | 1.440 | 2.13           | 1.435 | 0.35           | 1.536 | 1.05           | 95.68    | 3.45                |
| B3LYP      | 6-311g(d,p) | 1.463 | 1.60           | 1.634 | 4.08           | 1.593 | 1.46           | 1.440 | 2.13           | 1.437 | 0.21           | 1.537 | 1.12           | 95.69    | 3.44                |
| B3LYP      | DGTZVP      | 1.469 | 2.01           | 1.636 | 4.20           | 1.597 | 1.72           | 1.444 | 2.41           | 1.443 | 0.21           | 1.539 | 1.25           | 96.04    | 3.09                |
| B3LYP      | LanL2DZ     | 1.568 | 8.89           | 1.747 | 11.27          | 1.689 | 7.58           | 1.479 | 4.89           | 1.472 | 2.22           | 1.553 | 2.17           | 92.99    | 6.17                |
| B3PW91     | 6-31g       | 1.571 | 9.10           | 1.755 | 11.78          | 1.701 | 8.34           | 1.471 | 4.33           | 1.466 | 1.81           | 1.531 | 0.72           | 92.98    | 6.18                |
| B3PW91     | 6-31g(d)    | 1.467 | 1.88           | 1.633 | 4.01           | 1.596 | 1.66           | 1.432 | 1.56           | 1.429 | 0.76           | 1.531 | 0.72           | 96.05    | 3.08                |
| B3PW91     | 6-31g(d,p)  | 1.467 | 1.88           | 1.634 | 4.08           | 1.596 | 1.66           | 1.432 | 1.56           | 1.429 | 0.76           | 1.531 | 0.72           | 96.05    | 3.08                |
| B3PW91     | 6-311g      | 1.549 | 7.57           | 1.742 | 10.96          | 1.676 | 6.75           | 1.468 | 4.11           | 1.459 | 1.32           | 1.529 | 0.59           | 92.73    | 6.43                |
| B3PW91     | 6-311g(d)   | 1.460 | 1.39           | 1.630 | 3.82           | 1.589 | 1.21           | 1.432 | 1.56           | 1.428 | 0.83           | 1.530 | 0.66           | 95.79    | 3.34                |
| B3PW91     | 6-311g(d,p) | 1.460 | 1.39           | 1.629 | 3.76           | 1.589 | 1.21           | 1.433 | 1.63           | 1.430 | 0.69           | 1.530 | 0.66           | 95.80    | 3.33                |
| B3PW91     | DGTZVP      | 1.466 | 1.81           | 1.630 | 3.82           | 1.593 | 1.46           | 1.436 | 1.84           | 1.435 | 0.35           | 1.532 | 0.79           | 96.09    | 3.04                |
| B3PW91     | LanL2DZ     | 1.567 | 8.82           | 1.745 | 11.15          | 1.688 | 7.52           | 1.472 | 4.40           | 1.465 | -1.74          | 1.547 | 1.78           | 92.96    | 6.20                |
| BPW86      | 6-31g(d)    | 1.483 | 2.99           | 1.657 | 5.54           | 1.618 | 3.06           | 1.448 | 2.70           | 1.445 | 0.35           | 1.539 | 1.25           | 96.35    | 2.77                |
| BPW86      | 6-31g(d,p)  | 1.483 | 2.99           | 1.657 | 5.54           | 1.618 | 3.06           | 1.448 | 2.70           | 1.446 | 0.42           | 1.538 | 1.18           | 96.35    | 2.77                |
| BPW86      | 6-311g(d)   | 1.476 | 2.50           | 1.654 | 5.35           | 1.610 | 2.55           | 1.449 | 2.77           | 1.445 | 0.35           | 1.537 | 1.12           | 96.01    | 3.12                |
| BPW86      | DGTZVP      | 1.482 | 2.92           | 1.622 | 3.31           | 1.614 | 2.80           | 1.453 | 3.05           | 1.452 | 0.83           | 1.540 | 1.32           | 96.32    | 2.81                |
| CAM-B3LYP  | 6-31g(d)    | 1.462 | 1.53           | 1.625 | 3.50           | 1.589 | 1.21           | 1.431 | 1.49           | 1.427 | 0.90           | 1.531 | 0.72           | 95.85    | 3.28                |
| CAM-B3LYP  | 6-31g(d,p)  | 1.462 | 1.53           | 1.624 | 3.44           | 1.589 | 1.21           | 1.431 | 1.49           | 1.428 | 0.83           | 1.530 | 0.66           | 95.85    | 3.28                |
| CAM-B3LYP  | 6-311g(d)   | 1.455 | 1.04           | 1.623 | 3.38           | 1.582 | 0.76           | 1.431 | 1.49           | 1.426 | 0.97           | 1.530 | 0.66           | 95.50    | 3.63                |
| CAM-B3LYP  | DGTZVP      | 1.461 | 1.46           | 1.624 | 3.44           | 1.586 | 1.02           | 1.435 | 1.77           | 1.433 | 0.49           | 1.533 | 0.86           | 95.89    | 3.24                |
| LSDA       | 6-31g(d,p)  | 1.469 | 2.01           | 1.631 | 3.89           | 1.594 | 1.53           | 1.422 | 0.85           | 1.417 | 1.60           | 1.516 | 0.26           | 96.01    | 3.12                |
| MPW1PW91   | 6-31g(d)    | 1.464 | 1.67           | 1.628 | 3.69           | 1.592 | 1.40           | 1.429 | 1.35           | 1.425 | 1.04           | 1.529 | 0.59           | 96.03    | 3.10                |
| MPW1PW91   | 6-31g(d,p)  | 1.464 | 1.67           | 1.629 | 3.76           | 1.592 | 1.40           | 1.429 | 1.35           | 1.426 | 0.97           | 1.529 | 0.59           | 96.03    | 3.10                |
| MPW1PW91   | 6-311g(d)   | 1.457 | 1.18           | 1.625 | 3.50           | 1.584 | 0.89           | 1.428 | 1.28           | 1.424 | 1.11           | 1.527 | 0.46           | 95.79    | 3.34                |
| MPW1PW91   | DGTZVP      | 1.462 | 1.53           | 1.625 | 3.50           | 1.588 | 1.15           | 1.432 | 1.56           | 1.431 | 0.62           | 1.530 | 0.66           | 96.08    | 3.05                |
| PBEPBE     | 6-31g(d)    | 1.483 | 2.99           | 1.656 | 5.48           | 1.618 | 3.06           | 1.445 | 2.48           | 1.442 | 0.14           | 1.537 | 1.12           | 96.41    | 2.71                |
| PBEPBE     | 6-31g(d,p)  | 1.483 | 2.99           | 1.657 | 5.54           | 1.618 | 3.06           | 1.445 | 2.48           | 1.443 | 0.21           | 1.536 | 1.05           | 96.40    | 2.72                |
| PBEPBE     | 6-311g(d)   | 1.477 | 2.57           | 1.653 | 5.29           | 1.610 | 2.55           | 1.446 | 2.55           | 1.441 | 0.07           | 1.534 | 0.92           | 96.09    | 3.04                |
| PBEPBE     | DGTZVP      | 1.482 | 2.92           | 1.655 | 5.41           | 1.615 | 2.87           | 1.450 | 2.84           | 1.448 | 0.56           | 1.538 | 1.18           | 96.40    | 2.72                |
| WB97XD     | 6-31g(d,p)  | 1.462 | 1.53           | 1.626 | 3.57           | 1.592 | 1.40           | 1.428 | 1.28           | 1.426 | 0.97           | 1.532 | 0.79           | 96.09    | 3.04                |

**Table S2** Efficiency rating for the functional/basis sets used for the MeOEP molecule calculations

| Functional | Basis       | Time | Deviation<br>$\Sigma\Delta^a$ | T· $\Sigma\Delta$ | Range |
|------------|-------------|------|-------------------------------|-------------------|-------|
| B3LYP      | 6-31g       | 238  | 44.55                         | 10603             | 12    |
| B3LYP      | 6-31g(d)    | 656  | 14.84                         | 9733              | 7     |
| B3LYP      | 6-31g(d,p)  | 851  | 14.77                         | 12572             | 21    |
| B3LYP      | 6-311g      | 477  | 40.38                         | 19261             | 34    |
| B3LYP      | 6-311g(d)   | 1042 | 14.12                         | 14710             | 27    |
| B3LYP      | 6-311g(d,p) | 1336 | 14.03                         | 18749             | 33    |
| B3LYP      | DGTZVP      | 727  | 14.89                         | 10829             | 14    |
| B3LYP      | LanL2DZ     | 236  | 43.19                         | 10194             | 10    |
| B3PW91     | 6-31g       | 234  | 42.26                         | 9888              | 9     |
| B3PW91     | 6-31g(d)    | 641  | 13.67                         | 8762              | 3     |
| B3PW91     | 6-31g(d,p)  | 826  | 13.73                         | 11343             | 16    |
| B3PW91     | 6-311g      | 471  | 37.73                         | 17771             | 32    |
| B3PW91     | 6-311g(d)   | 1054 | 12.81                         | 13504             | 23    |
| B3PW91     | 6-311g(d,p) | 1354 | 12.67                         | 17156             | 30    |
| B3PW91     | DGTZVP      | 730  | 13.11                         | 9570              | 6     |
| B3PW91     | LanL2DZ     | 236  | 38.11                         | 8995              | 5     |
| BPW86      | 6-31g(d)    | 592  | 18.65                         | 11042             | 15    |
| BPW86      | 6-31g(d,p)  | 745  | 18.66                         | 13899             | 24    |
| BPW86      | 6-311g(d)   | 915  | 17.75                         | 16239             | 29    |
| BPW86      | DGTZVP      | 669  | 17.04                         | 11397             | 17    |
| CAM-B3LYP  | 6-31g(d)    | 856  | 12.64                         | 10817             | 13    |
| CAM-B3LYP  | 6-31g(d,p)  | 1122 | 12.44                         | 13955             | 25    |
| CAM-B3LYP  | 6-311g(d)   | 1470 | 11.93                         | 17543             | 31    |
| CAM-B3LYP  | DGTZVP      | 1007 | 12.27                         | 12356             | 19    |
| LSDA       | 6-31g(d,p)  | 370  | 13.26                         | 4905              | 1     |
| MPW1PW91   | 6-31g(d)    | 646  | 12.84                         | 8296              | 2     |
| MPW1PW91   | 6-31g(d,p)  | 819  | 12.84                         | 10512             | 11    |
| MPW1PW91   | 6-311g(d)   | 1051 | 11.76                         | 12364             | 20    |
| MPW1PW91   | DGTZVP      | 734  | 12.07                         | 8858              | 4     |
| PBEPBE     | 6-31g(d)    | 549  | 17.98                         | 9868              | 8     |
| PBEPBE     | 6-31g(d,p)  | 745  | 18.05                         | 13449             | 20    |
| PBEPBE     | 6-311g(d)   | 916  | 16.98                         | 15558             | 28    |
| PBEPBE     | DGTZVP      | 664  | 18.50                         | 12283             | 18    |
| WB97XD     | 6-31g(d,p)  | 1144 | 12.57                         | 14382             | 26    |

## S1.2. Molecular structures, energies and cartesian coordinates for mononuclear mechanism

### MI-1\_endo



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1639202.4 (Joules/Mol)      |
|                                              | 391.77877 (Kcal/Mol)        |
| Zero-point correction=                       | 0.624339 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.666862                    |
| Thermal correction to Enthalpy=              | 0.667806                    |
| Thermal correction to Gibbs Free Energy=     | 0.544211                    |
| Sum of electronic and zero-point Energies=   | -2496.477872                |
| Sum of electronic and thermal Energies=      | -2496.435350                |
| Sum of electronic and thermal Enthalpies=    | -2496.434406                |
| Sum of electronic and thermal Free Energies= | -2496.558000                |

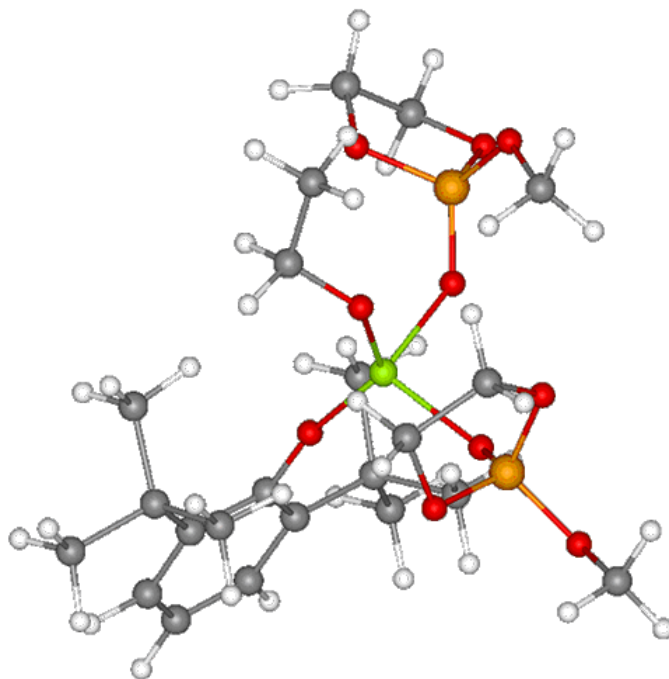
| cartesian |             |             |             |    |             |                         |
|-----------|-------------|-------------|-------------|----|-------------|-------------------------|
| 12        | 0.31897891  | -0.36698934 | -0.23176536 | 1  | -0.15942112 | 2.78511071 2.59413481   |
| 8         | 1.21027887  | -1.28258932 | -1.64466524 | 1  | -0.44542113 | 1.16211069 1.94253469   |
| 8         | -1.45792115 | 0.16491066  | 0.00173464  | 1  | -0.10942110 | -2.77738929 -2.23686528 |
| 6         | 0.93297887  | -2.44438934 | -2.37146521 | 8  | 1.06997883  | -1.24288940 1.47293472  |
| 1         | 1.55657887  | -3.28908944 | -2.01646519 | 15 | 2.33447886  | -1.95838928 1.77233458  |
| 6         | 1.18927884  | -2.26758933 | -3.86756516 | 8  | 3.66187906  | -1.04538941 1.68703461  |
| 6         | -2.71292090 | 0.36491066  | 0.38123465  | 8  | 2.80927896  | -3.11948943 0.77323467  |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -3.73152089 | -0.58588934 | 0.04803464  | 6  | 4.56017876  | -1.53788936 | 0.66223466  |
| 6 | -5.04042149 | -0.34608933 | 0.47643465  | 6  | 3.74227905  | -2.52698946 | -0.17356536 |
| 1 | -5.82442141 | -1.05678940 | 0.23703465  | 1  | 5.40737867  | -2.01428938 | 1.16423464  |
| 6 | -5.38372135 | 0.78601068  | 1.20743465  | 1  | 4.89957857  | -0.68208933 | 0.07833464  |
| 6 | -4.39532137 | 1.71571064  | 1.51173472  | 1  | 3.15317893  | -2.02558947 | -0.95106536 |
| 1 | -4.68042135 | 2.59901071  | 2.07393456  | 1  | 4.34537888  | -3.33718944 | -0.58296537 |
| 6 | -3.06582093 | 1.54401064  | 1.11593461  | 8  | 2.23447895  | -2.59668946 | 3.21213460  |
| 6 | -3.41502094 | -1.84928942 | -0.77276534 | 6  | 3.32567906  | -3.34958935 | 3.77583480  |
| 6 | -2.01992106 | 2.61901069  | 1.46373463  | 1  | 3.54777908  | -4.21918917 | 3.15373468  |
| 6 | -2.43972111 | -2.76088929 | -0.00076535 | 1  | 4.20857906  | -2.71438932 | 3.88233471  |
| 1 | -1.52432120 | -2.23948932 | 0.28313464  | 1  | 2.98517895  | -3.67318940 | 4.75803471  |
| 1 | -2.16582108 | -3.63648939 | -0.60256535 | 8  | 1.54927886  | 1.28391063  | -0.24156535 |
| 1 | -2.90582108 | -3.11848927 | 0.92413461  | 15 | 2.60097909  | 2.16661072  | -0.79446536 |
| 6 | -2.83732104 | -1.45928931 | -2.14856529 | 8  | 4.11397886  | 1.91961062  | -0.29406536 |
| 1 | -1.92552125 | -0.86828929 | -2.05336523 | 8  | 2.45587897  | 3.68991065  | -0.29756537 |
| 1 | -3.56662107 | -0.86168933 | -2.70726538 | 6  | 4.54307890  | 3.00601053  | 0.55483460  |
| 1 | -2.61362100 | -2.35578942 | -2.74036527 | 6  | 3.73827887  | 4.21851063  | 0.08633465  |
| 6 | -4.66812134 | -2.69808936 | -1.05396533 | 1  | 5.61737871  | 3.13151073  | 0.41713464  |
| 1 | -5.42012119 | -2.14688945 | -1.62876534 | 1  | 4.32517862  | 2.74491072  | 1.59393454  |
| 1 | -5.13762140 | -3.06498933 | -0.13496536 | 1  | 3.57387900  | 4.94951057  | 0.87823462  |
| 1 | -4.38282108 | -3.57548928 | -1.64586544 | 1  | 4.19667864  | 4.70381069  | -0.78036535 |
| 6 | -2.62882113 | 3.81311059  | 2.21933460  | 8  | 2.73627901  | 2.15111065  | -2.36316538 |
| 1 | -3.06262112 | 3.51921058  | 3.18133473  | 6  | 1.69967890  | 1.58291066  | -3.22036529 |
| 1 | -3.40132093 | 4.32461071  | 1.63493466  | 1  | 1.46397889  | 0.56691068  | -2.88976526 |
| 1 | -1.83992112 | 4.54521084  | 2.42833471  | 1  | 0.81927890  | 2.22791052  | -3.20066524 |
| 6 | -1.40152109 | 3.18801069  | 0.17043464  | 1  | 2.13577890  | 1.57621062  | -4.21806526 |
| 1 | -0.96112108 | 2.39701056  | -0.43646538 | 1  | 1.01327884  | -3.20258927 | -4.41386509 |
| 1 | -0.62262106 | 3.92401052  | 0.40623465  | 1  | 0.52627885  | -1.50218940 | -4.28616524 |
| 1 | -2.17252111 | 3.68771052  | -0.42716539 | 1  | 2.22527885  | -1.95618939 | -4.04696512 |
| 6 | -0.93022108 | 2.03241062  | 2.38343477  | 1  | -6.41002131 | 0.94501066  | 1.53013468  |
| 1 | -1.36792111 | 1.71971059  | 3.33803463  |    |             |             |             |

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## MI-1\_exo



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1638160.6 (Joules/Mol)      |
|                                              | 391.52977 (Kcal/Mol)        |
| Zero-point correction=                       | 0.623942 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.666703                    |
| Thermal correction to Enthalpy=              | 0.667647                    |
| Thermal correction to Gibbs Free Energy=     | 0.543208                    |
| Sum of electronic and zero-point Energies=   | -2496.480479                |
| Sum of electronic and thermal Energies=      | -2496.437719                |
| Sum of electronic and thermal Enthalpies=    | -2496.436775                |
| Sum of electronic and thermal Free Energies= | -2496.561213                |

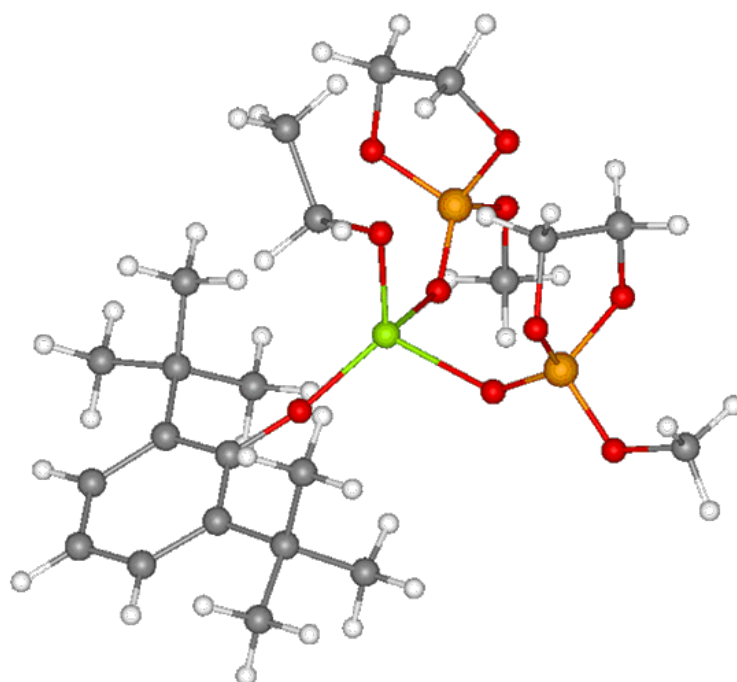
|    |             |             |             | cartesian |             |             |             |
|----|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 12 | 0.61740255  | 0.17141742  | 0.16157193  | 1         | -1.30479741 | 1.32141745  | 3.73557210  |
| 8  | 1.97870255  | 0.01081741  | -1.17392814 | 1         | -0.86489737 | 0.18811741  | 2.44897199  |
| 8  | -1.24289739 | -0.05588260 | 0.07257193  | 6         | 3.28400254  | 0.73591739  | -3.09402800 |
| 6  | 1.97560263  | 0.14851740  | -2.56452799 | 8         | 1.49490261  | -0.99968261 | 1.59577191  |
| 1  | 1.14980257  | 0.79141742  | -2.91522789 | 15        | 2.53400254  | -2.05778265 | 1.54237187  |
| 1  | 1.81180263  | -0.82768261 | -3.06222796 | 8         | 4.00910282  | -1.57008255 | 1.12457192  |
| 6  | -2.49749756 | -0.47388262 | 0.17457193  | 8         | 2.36990237  | -3.22068262 | 0.45137194  |
| 6  | -3.02579761 | -1.42018259 | -0.76382810 | 6         | 4.43480253  | -2.19108272 | -0.11222808 |
| 6  | -4.34529734 | -1.85518253 | -0.60912806 | 6         | 3.20340252  | -2.90098262 | -0.69282806 |
| 1  | -4.75969744 | -2.57748270 | -1.30472803 | 1         | 5.24590254  | -2.88268256 | 0.13177192  |
| 6  | -5.16269732 | -1.39028251 | 0.41517192  | 1         | 4.79240227  | -1.40458250 | -0.77622807 |
| 6  | -4.65569735 | -0.44968259 | 1.30527186  | 1         | 2.64110255  | -2.23288274 | -1.34672809 |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1 | -5.30979776 | -0.08498260 | 2.09047198  | 1  | 3.44850254  | -3.84148264 | -1.18622804 |
| 6 | -3.34659743 | 0.03191741  | 1.21347189  | 8  | 2.61410236  | -2.75338268 | 2.95797205  |
| 6 | -2.18149757 | -1.95198262 | -1.93662798 | 6  | 3.54550242  | -3.82268262 | 3.21027207  |
| 6 | -2.85389757 | 1.09531748  | 2.21207190  | 1  | 3.34680247  | -4.66408253 | 2.54297209  |
| 6 | -0.96769738 | -2.74448276 | -1.41382813 | 1  | 4.57180262  | -3.46718264 | 3.08917212  |
| 1 | -0.33879742 | -2.13978267 | -0.76012808 | 1  | 3.37930250  | -4.12248278 | 4.24377203  |
| 1 | -0.35119745 | -3.10078263 | -2.24932790 | 8  | 1.04790258  | 2.03171730  | 0.89767194  |
| 1 | -1.29819739 | -3.61648273 | -0.83902812 | 15 | 1.60740256  | 3.27651739  | 0.30687195  |
| 6 | -1.72569740 | -0.78298259 | -2.83272791 | 8  | 1.17740262  | 4.65801716  | 1.00037193  |
| 1 | -1.16219735 | -0.04118259 | -2.26632786 | 8  | 1.06320262  | 3.59051728  | -1.17422807 |
| 1 | -2.59599757 | -0.28248259 | -3.27202797 | 6  | 0.23190257  | 5.35401726  | 0.15877193  |
| 1 | -1.09559739 | -1.14838254 | -3.65332794 | 6  | 0.60440254  | 4.95481730  | -1.26962805 |
| 6 | -2.96929741 | -2.91578269 | -2.84172797 | 1  | 0.34820256  | 6.42151737  | 0.34637195  |
| 1 | -3.84809732 | -2.43918276 | -3.28882790 | 1  | -0.77799737 | 5.03231716  | 0.42517191  |
| 1 | -3.29869747 | -3.81328273 | -2.30702806 | 1  | -0.24739745 | 4.97201729  | -1.94962800 |
| 1 | -2.32319760 | -3.24528265 | -3.66382790 | 1  | 1.41660261  | 5.56841755  | -1.66952813 |
| 6 | -3.94919729 | 1.52651751  | 3.20407200  | 8  | 3.18310237  | 3.33451724  | 0.31357193  |
| 1 | -4.29589748 | 0.69521743  | 3.82727194  | 6  | 3.97180247  | 2.13351727  | 0.55597192  |
| 1 | -4.81779766 | 1.96471751  | 2.70027208  | 1  | 3.93100238  | 1.88961744  | 1.61837196  |
| 1 | -3.54259753 | 2.28911734  | 3.87847209  | 1  | 3.59490252  | 1.30451751  | -0.04792808 |
| 6 | -2.42649746 | 2.36861730  | 1.45257187  | 1  | 4.98750257  | 2.40101743  | 0.26737192  |
| 1 | -1.65039742 | 2.14671731  | 0.71997190  | 1  | 3.27290249  | 0.80491740  | -4.18892813 |
| 1 | -2.04479742 | 3.12081742  | 2.15557194  | 1  | 3.44890237  | 1.74171746  | -2.69252801 |
| 1 | -3.28709745 | 2.79721737  | 0.92557192  | 1  | 4.13880253  | 0.11251741  | -2.80412793 |
| 6 | -1.69089746 | 0.54651743  | 3.06167197  | 1  | -6.18459749 | -1.74908257 | 0.51297194  |
| 1 | -2.03389764 | -0.29438260 | 3.67447209  |    |             |             |             |

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## MI-1\_front



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1638508.7 (Joules/Mol)      |
|                                              | 391.61299 (Kcal/Mol)        |
| Zero-point correction=                       | 0.624075 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.666802                    |
| Thermal correction to Enthalpy=              | 0.667746                    |
| Thermal correction to Gibbs Free Energy=     | 0.543363                    |
| Sum of electronic and zero-point Energies=   | -2496.482337                |
| Sum of electronic and thermal Energies=      | -2496.439610                |
| Sum of electronic and thermal Enthalpies=    | -2496.438666                |
| Sum of electronic and thermal Free Energies= | -2496.563049                |

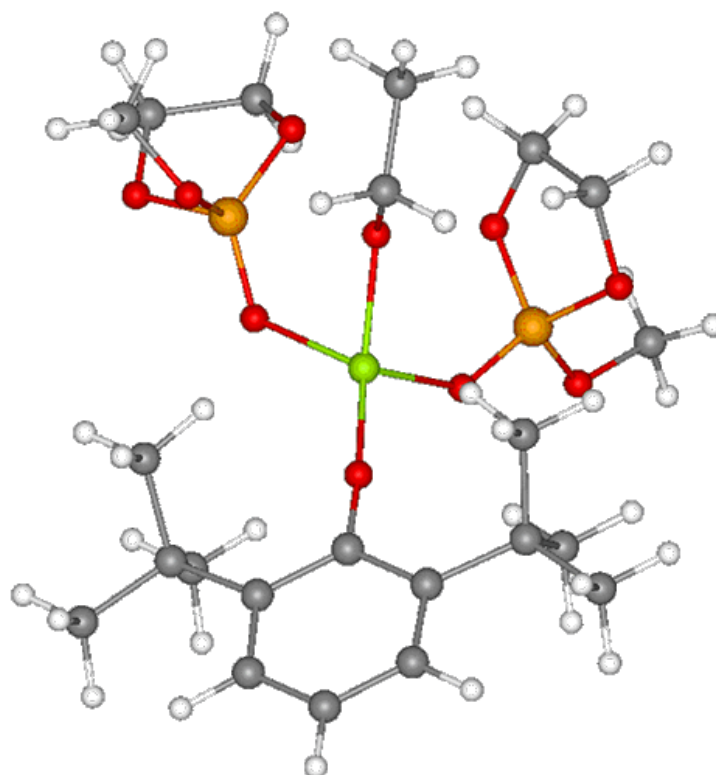
| cartesian |             |             |             |    |             |             |             |  |  |  |  |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|--|--|
| 12        | -0.52917743 | 0.00792127  | 0.16738404  | 1  | 1.68022275  | -3.40807867 | 1.84568405  |  |  |  |  |
| 8         | -1.43587732 | -0.24947873 | -1.51161599 | 1  | 1.31212258  | -1.66827869 | 1.84758401  |  |  |  |  |
| 8         | 1.31352258  | 0.19312127  | 0.42098403  | 6  | -1.15727735 | -1.01647878 | -3.81221604 |  |  |  |  |
| 6         | -0.84607744 | 0.03982127  | -2.75321603 | 8  | -1.58137751 | 1.51832128  | 1.07628405  |  |  |  |  |
| 1         | 0.25112259  | 0.12962127  | -2.67591596 | 15 | -2.80577731 | 2.28942132  | 0.75298405  |  |  |  |  |
| 1         | -1.19337738 | 1.01952136  | -3.13511610 | 8  | -4.18007755 | 1.45572126  | 0.86318403  |  |  |  |  |
| 6         | 2.62882257  | 0.31722128  | 0.31058404  | 8  | -2.99417734 | 2.81842136  | -0.74931592 |  |  |  |  |
| 6         | 3.22912264  | 1.61592126  | 0.22348404  | 6  | -4.85557747 | 1.40142131  | -0.41561592 |  |  |  |  |
| 6         | 4.61802244  | 1.70382130  | 0.09138405  | 6  | -3.82557726 | 1.85512125  | -1.45501590 |  |  |  |  |
| 1         | 5.09242249  | 2.67682123  | 0.01758404  | 1  | -5.72247744 | 2.06642127  | -0.36381596 |  |  |  |  |
| 6         | 5.43122244  | 0.57612127  | 0.05378404  | 1  | -5.18217754 | 0.37382126  | -0.57601595 |  |  |  |  |

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|   |            |             |             |    |             |             |             |
|---|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 4.84572268 | -0.68057877 | 0.16128404  | 1  | -3.17967725 | 1.02852130  | -1.77421594 |
| 1 | 5.49522257 | -1.54957867 | 0.14188404  | 1  | -4.27437735 | 2.37472129  | -2.30151606 |
| 6 | 3.46412277 | -0.84707874 | 0.29348403  | 8  | -2.88707733 | 3.54532123  | 1.70528400  |
| 6 | 2.38442278 | 2.90202141  | 0.28738403  | 6  | -3.99377728 | 4.46532106  | 1.63928401  |
| 6 | 2.87322259 | -2.26267862 | 0.42378405  | 1  | -4.04727745 | 4.92462111  | 0.64978403  |
| 6 | 1.62362266 | 2.97142124  | 1.62698400  | 1  | -4.92777729 | 3.95122123  | 1.87888408  |
| 1 | 0.98022264 | 2.10472131  | 1.77468407  | 1  | -3.79027724 | 5.22712135  | 2.39018393  |
| 1 | 1.00012255 | 3.87362123  | 1.66828406  | 8  | -1.37697744 | -1.48107874 | 1.29268408  |
| 1 | 2.33322263 | 3.01402140  | 2.46118402  | 15 | -2.24707747 | -2.64217877 | 0.95518404  |
| 6 | 1.40642262 | 2.96712136  | -0.90241599 | 8  | -1.56587744 | -3.68957877 | -0.05011596 |
| 1 | 0.74412256 | 2.10162139  | -0.93481588 | 8  | -3.60367727 | -2.38427877 | 0.14868404  |
| 1 | 1.95782256 | 2.99492121  | -1.84881604 | 6  | -2.45377731 | -3.99117875 | -1.14921594 |
| 1 | 0.78622264 | 3.87052131  | -0.84481597 | 6  | -3.41227722 | -2.80387878 | -1.23121595 |
| 6 | 3.24492264 | 4.17582130  | 0.20738405  | 1  | -2.96717739 | -4.93137884 | -0.92791593 |
| 1 | 3.79742289 | 4.24922132  | -0.73571593 | 1  | -1.84497738 | -4.09547853 | -2.04691601 |
| 1 | 3.96132278 | 4.24282122  | 1.03308403  | 1  | -2.96707726 | -1.96287870 | -1.77031589 |
| 1 | 2.59202266 | 5.05412149  | 0.27138406  | 1  | -4.39197731 | -3.07617879 | -1.62511599 |
| 6 | 3.95622253 | -3.35647869 | 0.42508405  | 8  | -2.74217725 | -3.39807868 | 2.25328398  |
| 1 | 4.65722275 | -3.24587870 | 1.25948405  | 6  | -2.00097752 | -3.32107878 | 3.49508405  |
| 1 | 4.53122282 | -3.37537861 | -0.50691593 | 1  | -1.17677736 | -4.03607893 | 3.47078395  |
| 1 | 3.47662258 | -4.33687878 | 0.52958405  | 1  | -1.62157750 | -2.31087875 | 3.65028405  |
| 6 | 1.94812274 | -2.57297873 | -0.77001595 | 1  | -2.70867729 | -3.58957863 | 4.27788401  |
| 1 | 1.14782262 | -1.83897865 | -0.87331593 | 1  | -0.69327736 | -0.76147878 | -4.77271605 |
| 1 | 1.48992252 | -3.56327868 | -0.65651596 | 1  | -0.77367741 | -1.99517870 | -3.50261617 |
| 1 | 2.52112269 | -2.56827879 | -1.70401597 | 1  | -2.23897743 | -1.10307872 | -3.97521615 |
| 6 | 2.11282277 | -2.40247869 | 1.75848401  | 1  | 6.50922251  | 0.67612123  | -0.04971595 |
| 1 | 2.79912257 | -2.25717878 | 2.60038400  |    |             |             |             |

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# MTS-12\_endo



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1638572.4 (Joules/Mol)      |
|                                              | 391.62820 (Kcal/Mol)        |
| Zero-point correction=                       | 0.624099 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.665768                    |
| Thermal correction to Enthalpy=              | 0.666712                    |
| Thermal correction to Gibbs Free Energy=     | 0.546409                    |
| Sum of electronic and zero-point Energies=   | -2496.471257                |
| Sum of electronic and thermal Energies=      | -2496.429588                |
| Sum of electronic and thermal Enthalpies=    | -2496.428643                |
| Sum of electronic and thermal Free Energies= | -2496.548947                |

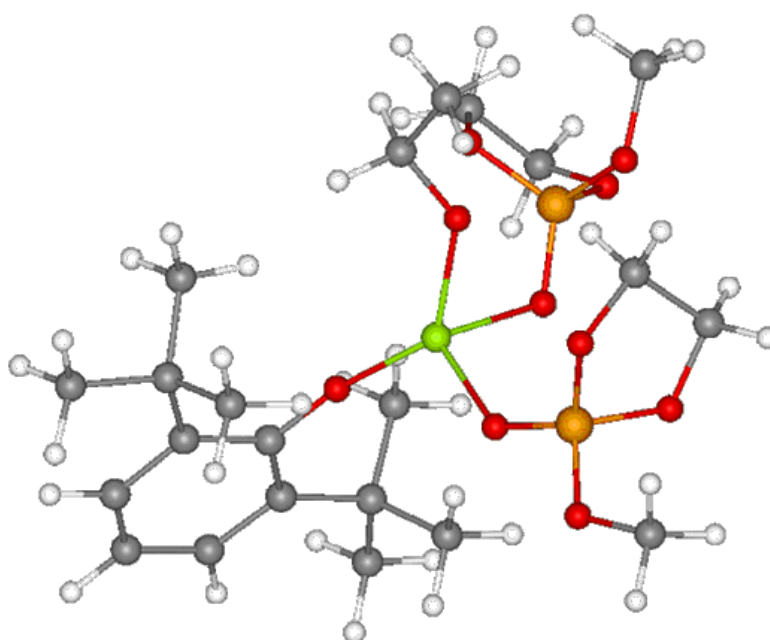
|    |             |             |             | cartesian |             |             |             |
|----|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 12 | -0.25081635 | 0.02683736  | 0.32960403  | 1         | 1.35618365  | -2.64716268 | 3.08470392  |
| 8  | -1.52621639 | -0.16206264 | -1.12849593 | 1         | 1.32848358  | -1.01256263 | 2.40320396  |
| 8  | 1.60698366  | 0.03993736  | 0.30200404  | 1         | -0.76461637 | -1.26256263 | -2.71009612 |
| 6  | -1.30801642 | -0.32546264 | -2.50649595 | 8         | -0.93981636 | 1.63263738  | 1.38370407  |
| 1  | -0.66601634 | 0.48403734  | -2.89309597 | 15        | -2.08391643 | 2.56693721  | 1.25010407  |
| 6  | -2.60671616 | -0.33836266 | -3.31109595 | 8         | -3.52091622 | 1.88633740  | 1.02140403  |
| 6  | 2.92938375  | -0.05596264 | 0.27830404  | 8         | -2.09711623 | 3.53363729  | -0.03069597 |
| 6  | 3.71418357  | 1.00333738  | -0.28129596 | 6         | -4.01401615 | 2.13943720  | -0.31709599 |

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|   |            |             |             |    |             |             |             |
|---|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 5.10478354 | 0.86433738  | -0.30759597 | 6  | -2.90841627 | 2.91223717  | -1.05859590 |
| 1 | 5.71788359 | 1.65333736  | -0.73089600 | 1  | -4.93581629 | 2.71783733  | -0.21539597 |
| 6 | 5.74398327 | -0.26256266 | 0.19870403  | 1  | -4.20431662 | 1.17563736  | -0.78809601 |
| 6 | 4.97708368 | -1.28026259 | 0.75610399  | 1  | -2.27751637 | 2.23343730  | -1.63349593 |
| 1 | 5.49148369 | -2.14846277 | 1.15510404  | 1  | -3.29831624 | 3.71193719  | -1.68799591 |
| 6 | 3.58198380 | -1.21186256 | 0.81560403  | 8  | -2.15451622 | 3.48263717  | 2.53120399  |
| 6 | 3.05798364 | 2.28263736  | -0.83249599 | 6  | -3.16901636 | 4.49723721  | 2.67000389  |
| 6 | 2.78248382 | -2.36256266 | 1.45330405  | 1  | -3.06481624 | 5.24543715  | 1.88170409  |
| 6 | 2.28848362 | 3.00673723  | 0.29120404  | 1  | -4.16291618 | 4.04433727  | 2.64380383  |
| 1 | 1.54288363 | 2.36073732  | 0.75470400  | 1  | -2.99721622 | 4.95523739  | 3.64260387  |
| 1 | 1.78288352 | 3.89843726  | -0.10229598 | 8  | -1.39131641 | -1.43046260 | 1.15760410  |
| 1 | 2.98198366 | 3.33193731  | 1.07470405  | 15 | -2.39631629 | -2.05166268 | 0.23770402  |
| 6 | 2.11768365 | 1.94313741  | -2.00629616 | 8  | -3.77421618 | -1.29346263 | -0.17349596 |
| 1 | 1.35918367 | 1.21573734  | -1.71469593 | 8  | -3.13701630 | -3.23096275 | 1.11110401  |
| 1 | 2.68598366 | 1.51283741  | -2.83849597 | 6  | -4.83851671 | -1.66246259 | 0.72650403  |
| 1 | 1.61558366 | 2.84823728  | -2.37229609 | 6  | -4.55781651 | -3.11196280 | 1.11210406  |
| 6 | 4.08898354 | 3.28703737  | -1.37719595 | 1  | -5.77991629 | -1.53666258 | 0.18980403  |
| 1 | 4.66908360 | 2.87603736  | -2.21059608 | 1  | -4.81161642 | -0.99506259 | 1.59270406  |
| 1 | 4.78738356 | 3.62413716  | -0.60399598 | 1  | -4.92751646 | -3.35836267 | 2.10970402  |
| 1 | 3.56368375 | 4.17363739  | -1.75119591 | 1  | -4.98431635 | -3.81336284 | 0.38550401  |
| 6 | 3.68998384 | -3.48646283 | 1.98460412  | 8  | -1.77681637 | -2.85396266 | -0.98499602 |
| 1 | 4.37608337 | -3.13356280 | 2.76200390  | 6  | -2.47001624 | -3.95116282 | -1.59889591 |
| 1 | 4.28108358 | -3.95426273 | 1.18980408  | 1  | -2.62281632 | -4.75726271 | -0.87779599 |
| 1 | 3.06668377 | -4.27006292 | 2.43070388  | 1  | -3.42651629 | -3.62086272 | -2.01459599 |
| 6 | 1.85568368 | -3.01546264 | 0.40800405  | 1  | -1.82461643 | -4.29146290 | -2.40779614 |
| 1 | 1.18638361 | -2.29286265 | -0.05919598 | 1  | -2.40281630 | -0.49466267 | -4.37719584 |
| 1 | 1.24358356 | -3.79876280 | 0.87140399  | 1  | -3.27191615 | -1.13626266 | -2.96619606 |
| 1 | 2.45108366 | -3.47446275 | -0.38939601 | 1  | -3.14931631 | 0.60893738  | -3.21059608 |
| 6 | 1.97858369 | -1.84756267 | 2.66520405  | 1  | 6.82798338  | -0.34396264 | 0.16480403  |
| 1 | 2.66058373 | -1.49966264 | 3.44910407  |    |             |             |             |

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# MTS-12\_exo



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1639406.3 (Joules/Mol)      |
|                                              | 391.82751 (Kcal/Mol)        |
| Zero-point correction=                       | 0.624417 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.665903                    |
| Thermal correction to Enthalpy=              | 0.666847                    |
| Thermal correction to Gibbs Free Energy=     | 0.547305                    |
| Sum of electronic and zero-point Energies=   | -2496.473564                |
| Sum of electronic and thermal Energies=      | -2496.432077                |
| Sum of electronic and thermal Enthalpies=    | -2496.431133                |
| Sum of electronic and thermal Free Energies= | -2496.550676                |

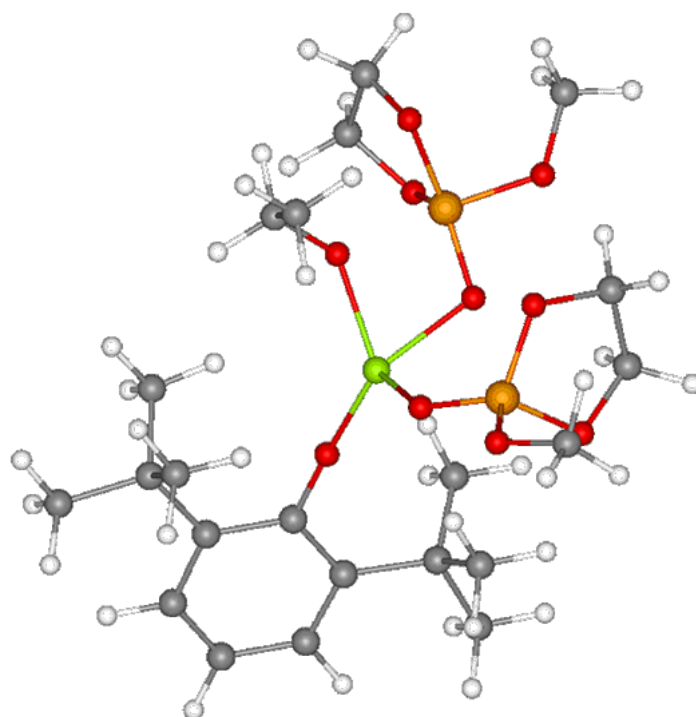
|    |             |             |             | cartesian |             |             |             |
|----|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 12 | 0.41053650  | -0.26081076 | 0.00927469  | 1         | -0.99606347 | 0.42068923  | 3.92087483  |
| 8  | 1.70083654  | 0.20168923  | -1.33782530 | 1         | -0.92176342 | -0.48121077 | 2.39757466  |
| 8  | -1.44706345 | -0.08801077 | 0.07387469  | 1         | 1.42073655  | 1.32478929  | -3.04362535 |
| 6  | 1.65293658  | 0.29098922  | -2.73432517 | 8         | 1.01333654  | -2.01641083 | 0.84527469  |
| 1  | 0.84523654  | -0.33471078 | -3.14752531 | 15        | 2.32193661  | -2.67321086 | 1.09177470  |
| 6  | 2.96323657  | -0.13601077 | -3.39512539 | 8         | 3.31803656  | -1.86601079 | 2.06067467  |
| 6  | -2.75746346 | -0.23241076 | 0.21807469  | 8         | 3.31543660  | -2.83241081 | -0.15822530 |
| 6  | -3.53666353 | -0.83991075 | -0.81902528 | 6         | 4.49573660  | -1.42741072 | 1.34067476  |
| 6  | -4.91456366 | -0.97861075 | -0.62862527 | 6         | 4.20833635  | -1.68381071 | -0.14432532 |
| 1  | -5.52156353 | -1.43981075 | -1.40082526 | 1         | 5.34263659  | -2.01081085 | 1.71227467  |
| 6  | -5.54876328 | -0.53931075 | 0.52877468  | 1         | 4.64263630  | -0.36821079 | 1.55047476  |
| 6  | -4.78966331 | 0.06338924  | 1.52637470  | 1         | 3.69033647  | -0.84441078 | -0.61892533 |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1 | -5.30016327 | 0.40738922  | 2.42017484  | 1  | 5.09973669  | -1.96281075 | -0.70622528 |
| 6 | -3.40726352 | 0.23388924  | 1.40677476  | 8  | 2.07273650  | -4.11221075 | 1.68447471  |
| 6 | -2.88956356 | -1.32431078 | -2.12922525 | 6  | 3.17173648  | -4.96501112 | 2.06267476  |
| 6 | -2.61666346 | 0.91208923  | 2.54017472  | 1  | 3.79483652  | -5.18691111 | 1.19377470  |
| 6 | -1.86916351 | -2.44581079 | -1.84572530 | 1  | 3.76103663  | -4.49251080 | 2.85187483  |
| 1 | -1.11956346 | -2.14651084 | -1.11232531 | 1  | 2.71853662  | -5.88081121 | 2.43847466  |
| 1 | -1.35426342 | -2.74311066 | -2.76802516 | 8  | 1.47173655  | 1.11868930  | 1.12057471  |
| 1 | -2.37706351 | -3.32891083 | -1.44272530 | 15 | 2.18853641  | 2.15588927  | 0.32037470  |
| 6 | -2.22156358 | -0.13981077 | -2.85652518 | 8  | 2.39523649  | 3.51798916  | 1.19717467  |
| 1 | -1.47936344 | 0.35518926  | -2.22922540 | 8  | 1.42913651  | 2.86898923  | -0.91042531 |
| 1 | -2.97606349 | 0.60538924  | -3.13312531 | 6  | 1.36103654  | 4.45328903  | 0.85837471  |
| 1 | -1.73136353 | -0.47991079 | -3.77752519 | 6  | 1.14133656  | 4.25988913  | -0.64302528 |
| 6 | -3.91676331 | -1.91561079 | -3.11122537 | 1  | 1.71523654  | 5.45428896  | 1.10787475  |
| 1 | -4.67496347 | -1.18321073 | -3.40802526 | 1  | 0.46003652  | 4.22528887  | 1.43537474  |
| 1 | -4.42716360 | -2.79301071 | -2.69992518 | 1  | 0.11253650  | 4.44938898  | -0.95112526 |
| 1 | -3.39906335 | -2.23751068 | -4.02232552 | 1  | 1.82723653  | 4.86548901  | -1.24212527 |
| 6 | -3.52086353 | 1.37238920  | 3.69767475  | 8  | 3.69383645  | 1.76108921  | -0.00962530 |
| 1 | -4.03886366 | 0.53598922  | 4.17897463  | 6  | 4.52263641  | 2.66868925  | -0.75712526 |
| 1 | -4.27116346 | 2.10148931  | 3.37317467  | 1  | 4.10643625  | 2.82318926  | -1.75512528 |
| 1 | -2.90396357 | 1.85578930  | 4.46417427  | 1  | 4.62253666  | 3.61878920  | -0.22612530 |
| 6 | -1.91006351 | 2.17748928  | 2.01087475  | 1  | 5.49823666  | 2.19028926  | -0.83912528 |
| 1 | -1.26306343 | 1.94288921  | 1.16517472  | 1  | 2.90783644  | -0.02351077 | -4.48502541 |
| 1 | -1.30366349 | 2.63438916  | 2.80407476  | 1  | 3.80183649  | 0.47188926  | -3.03512526 |
| 1 | -2.65376353 | 2.91258931  | 1.68147469  | 1  | 3.18493652  | -1.18611073 | -3.17512536 |
| 6 | -1.59826350 | -0.07291076 | 3.14817476  | 1  | -6.62266350 | -0.66091073 | 0.64997470  |
| 1 | -2.12096357 | -0.91671073 | 3.61177468  |    |             |             |             |

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## MTS-12\_front



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1641309.6 (Joules/Mol)      |
|                                              | 392.28241 (Kcal/Mol)        |
| Zero-point correction=                       | 0.625142 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.665915                    |
| Thermal correction to Enthalpy=              | 0.666859                    |
| Thermal correction to Gibbs Free Energy=     | 0.548622                    |
| Sum of electronic and zero-point Energies=   | -2496.456592                |
| Sum of electronic and thermal Energies=      | -2496.415818                |
| Sum of electronic and thermal Enthalpies=    | -2496.414874                |
| Sum of electronic and thermal Free Energies= | -2496.533112                |

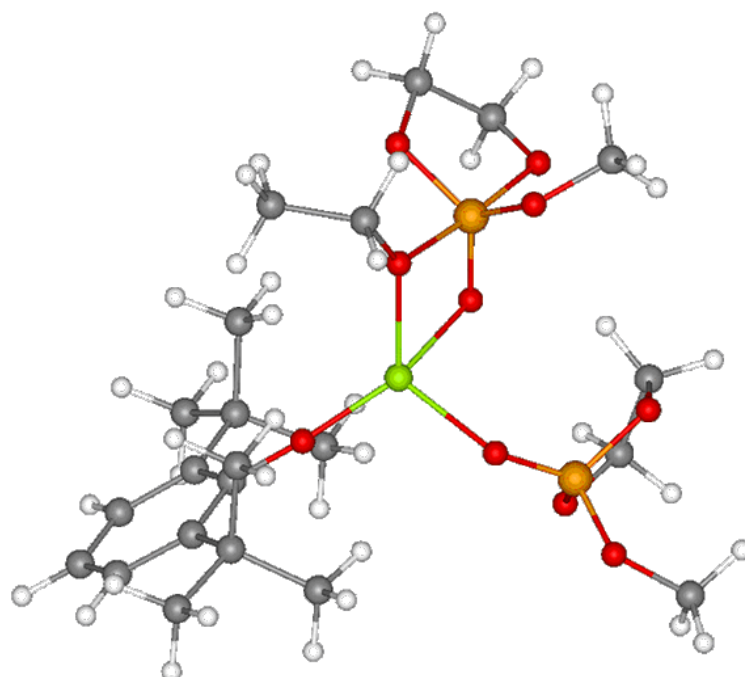
| cartesian |             |             |             |    |             |             |             |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 12        | 0.28057578  | -0.00476795 | 0.28229997  | 1  | -0.82382417 | 3.17853189  | -2.21530008 |
| 8         | 1.32387578  | -1.65776789 | 0.63599998  | 1  | -0.99442422 | 2.25653195  | -0.70680004 |
| 8         | -1.53742421 | 0.03223205  | -0.04360004 | 1  | 2.01597571  | -3.32716799 | 1.65969992  |
| 6         | 1.51877582  | -2.37086797 | 1.85219991  | 8  | 0.92287576  | 1.57533205  | 1.38509989  |
| 1         | 0.52227581  | -2.61106801 | 2.24339986  | 15 | 2.02647567  | 2.55643201  | 1.19919991  |
| 6         | 2.31157565  | -1.58666790 | 2.88800001  | 8  | 2.02627587  | 3.42923188  | -0.14310004 |
| 6         | -2.84522414 | 0.16013205  | -0.22680004 | 8  | 3.49847579  | 1.93723202  | 1.07019997  |
| 6         | -3.76002407 | -0.49466795 | 0.65739995  | 6  | 3.00727582  | 2.89513183  | -1.07230008 |
| 6         | -5.13142395 | -0.33806795 | 0.43629998  | 6  | 4.10847569  | 2.26533198  | -0.20520005 |
| 1         | -5.84352398 | -0.82436794 | 1.09479988  | 1  | 3.36867571  | 3.73193192  | -1.67010009 |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -5.62612438 | 0.42813206  | -0.61370003 | 1  | 2.52267575  | 2.14543200  | -1.69770014 |
| 6 | -4.73052406 | 1.05693197  | -1.47250009 | 1  | 4.47497559  | 1.34013212  | -0.64910001 |
| 1 | -5.13332415 | 1.64823210  | -2.28830004 | 1  | 4.93157578  | 2.95523190  | -0.00110004 |
| 6 | -3.34622407 | 0.94663209  | -1.31220007 | 8  | 1.98877585  | 3.56083202  | 2.41709995  |
| 6 | -3.26192427 | -1.36726797 | 1.82439995  | 6  | 2.94407582  | 4.63403177  | 2.52600002  |
| 6 | -2.39762425 | 1.66363204  | -2.29070020 | 1  | 3.95787573  | 4.23273182  | 2.59759998  |
| 6 | -2.43482423 | -0.52486795 | 2.81699991  | 1  | 2.85387588  | 5.30913210  | 1.67209995  |
| 1 | -1.60982418 | -0.00416796 | 2.32830000  | 1  | 2.69197583  | 5.16263199  | 3.44379997  |
| 1 | -2.02632427 | -1.15816796 | 3.61500001  | 8  | 1.85487580  | -0.00056796 | -0.94450003 |
| 1 | -3.06512427 | 0.23913205  | 3.28499985  | 15 | 2.59367585  | -1.34866798 | -0.89140004 |
| 6 | -2.43442416 | -2.55146813 | 1.28379989  | 8  | 1.91077578  | -2.45726800 | -1.86000013 |
| 1 | -1.57872415 | -2.21636796 | 0.69589996  | 8  | 3.57617593  | -2.41376805 | -0.04440004 |
| 1 | -3.05462408 | -3.18216801 | 0.63720000  | 6  | 2.02197576  | -3.76036811 | -1.27710009 |
| 1 | -2.07202411 | -3.17536807 | 2.11159992  | 6  | 3.33627582  | -3.75696802 | -0.48280004 |
| 6 | -4.41762400 | -1.97896802 | 2.63629985  | 8  | 3.86817575  | -0.74226797 | -1.77150011 |
| 1 | -5.04702425 | -2.63816810 | 2.02909994  | 6  | 4.91687584  | -1.56606793 | -2.26570010 |
| 1 | -5.05652428 | -1.21396792 | 3.08999991  | 1  | 5.52437592  | -1.97726786 | -1.45410013 |
| 1 | -4.00402403 | -2.58356810 | 3.45179987  | 1  | 4.52297592  | -2.37936807 | -2.88610005 |
| 6 | -3.15592408 | 2.43633199  | -3.38450003 | 1  | 5.54037571  | -0.92736793 | -2.89569998 |
| 1 | -3.79852438 | 3.22073197  | -2.97040009 | 1  | 2.40847588  | -2.17096806 | 3.81040001  |
| 1 | -3.77172422 | 1.77693200  | -4.00540018 | 1  | 3.31487584  | -1.36006796 | 2.51749992  |
| 1 | -2.43172407 | 2.92443204  | -4.04680014 | 1  | 1.81107581  | -0.64586794 | 3.13769984  |
| 6 | -1.50192416 | 0.64293206  | -3.02220011 | 1  | -6.69832420 | 0.53223205  | -0.76280004 |
| 1 | -0.91962421 | 0.03363204  | -2.33080006 | 1  | 3.29207587  | -4.41516829 | 0.38959998  |
| 1 | -0.80622423 | 1.15713203  | -3.69740009 | 1  | 4.17817593  | -4.06546783 | -1.11310005 |
| 1 | -2.11532426 | -0.03586796 | -3.62490010 | 1  | 2.03567576  | -4.48976803 | -2.08899999 |
| 6 | -1.54332423 | 2.70293188  | -1.53700006 | 1  | 1.15307581  | -3.93376827 | -0.63750005 |
| 1 | -2.18202424 | 3.48863196  | -1.11820006 |    |             |             |             |

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## MI-2



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1643868.5 (Joules/Mol)      |
|                                              | 392.89400 (Kcal/Mol)        |
| Zero-point correction=                       | 0.626116 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.667507                    |
| Thermal correction to Enthalpy=              | 0.668451                    |
| Thermal correction to Gibbs Free Energy=     | 0.549132                    |
| Sum of electronic and zero-point Energies=   | -2496.488615                |
| Sum of electronic and thermal Energies=      | -2496.447225                |
| Sum of electronic and thermal Enthalpies=    | -2496.446280                |
| Sum of electronic and thermal Free Energies= | -2496.565600                |

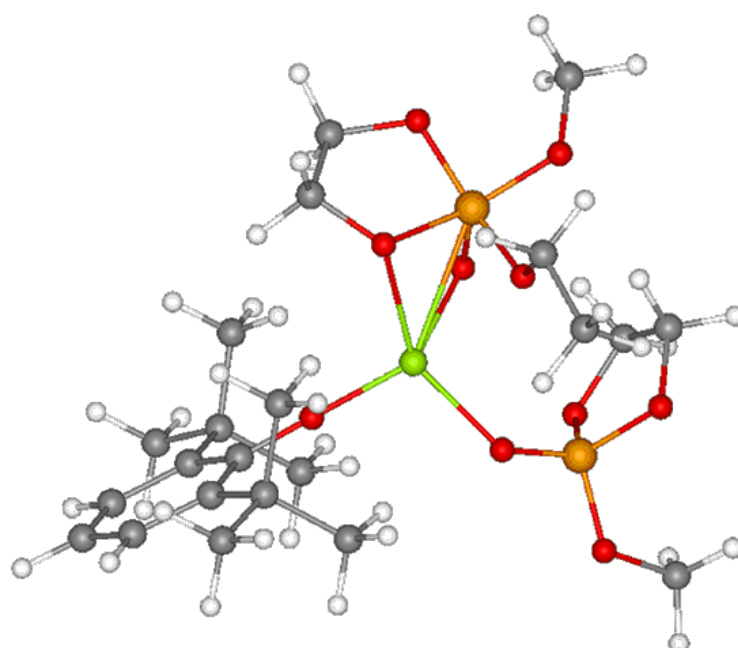
|    |             |             |             | cartesian |             |             |             |
|----|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 12 | 0.40965077  | 0.16324402  | 0.40965867  | 1         | -0.26054922 | -0.64395601 | -3.51344132 |
| 8  | 1.38165081  | -1.14505601 | 1.59255862  | 1         | -0.62824929 | 0.37664402  | -2.10824132 |
| 8  | -1.41184926 | 0.10424402  | 0.11315867  | 1         | 2.22695065  | -2.21815610 | 3.13935876  |
| 6  | 1.26205075  | -1.77715588 | 2.87625861  | 8         | 1.00705075  | 2.09214401  | 0.63155866  |
| 6  | 0.16595076  | -2.82685614 | 2.87855864  | 15        | 1.86575079  | 2.98484397  | -0.18914133 |
| 1  | 1.05445075  | -0.98825592 | 3.60785866  | 8         | 1.57025075  | 2.92744398  | -1.76704133 |
| 6  | -2.68734932 | -0.06195597 | -0.21684134 | 8         | 3.44295073  | 2.70274401  | -0.24764132 |
| 6  | -3.71524906 | 0.47494403  | 0.62185866  | 6         | 2.75785089  | 2.58334398  | -2.51904130 |
| 6  | -5.04834938 | 0.27384403  | 0.25275868  | 6         | 3.77115083  | 2.04324412  | -1.50104129 |
| 1  | -5.84524918 | 0.66924405  | 0.87385869  | 1         | 3.10675073  | 3.48874402  | -3.02304125 |
| 6  | -5.39964914 | -0.42285597 | -0.89884132 | 1         | 2.47655082  | 1.83074403  | -3.25544143 |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -4.39484930 | -0.93205601 | -1.71394134 | 1  | 3.66755080  | 0.96604401  | -1.35974133 |
| 1 | -4.68664932 | -1.46955609 | -2.61034131 | 1  | 4.79785061  | 2.31524396  | -1.74664128 |
| 6 | -3.03974915 | -0.77125597 | -1.40884137 | 8  | 1.68635082  | 4.46114397  | 0.34075868  |
| 6 | -3.38214922 | 1.26914406  | 1.89865863  | 6  | 2.35285068  | 5.56894398  | -0.29484132 |
| 6 | -1.96684933 | -1.35285592 | -2.34784126 | 1  | 3.43525076  | 5.42224407  | -0.27984133 |
| 6 | -2.57604933 | 2.53564405  | 1.54535866  | 1  | 1.99105084  | 5.68804407  | -1.31894135 |
| 1 | -1.64724922 | 2.29684401  | 1.02725863  | 1  | 2.09055066  | 6.44804430  | 0.29125869  |
| 1 | -2.32734919 | 3.09714389  | 2.45485878  | 8  | 2.08045077  | -0.42135596 | -0.50814134 |
| 1 | -3.16654921 | 3.19164395  | 0.89585871  | 15 | 2.79535079  | -1.35045600 | 0.50555867  |
| 6 | -2.59784913 | 0.39234403  | 2.89525867  | 8  | 4.18625069  | -1.65595603 | -0.44914132 |
| 1 | -1.67254925 | 0.01654403  | 2.45655870  | 8  | 2.45885086  | -2.96635604 | 0.55045867  |
| 1 | -3.19764924 | -0.47205597 | 3.20095873  | 6  | 4.00825071  | -2.83215594 | -1.20814133 |
| 1 | -2.34644914 | 0.96554404  | 3.79645872  | 6  | 3.31445074  | -3.78915596 | -0.24654132 |
| 6 | -4.64474916 | 1.74384403  | 2.64025879  | 1  | 4.98425102  | -3.20155597 | -1.53484130 |
| 1 | -5.27504921 | 0.90924400  | 2.96625876  | 1  | 3.38335085  | -2.63475609 | -2.09034133 |
| 1 | -5.25504923 | 2.41934395  | 2.03115869  | 1  | 2.69275069  | -4.53425598 | -0.74814135 |
| 1 | -4.34694910 | 2.29644394  | 3.53865862  | 1  | 4.03095055  | -4.29235601 | 0.41205868  |
| 6 | -2.57644916 | -2.05665612 | -3.57384133 | 8  | 3.68005085  | -0.71055597 | 1.71355867  |
| 1 | -3.17654920 | -1.37605596 | -4.18724155 | 6  | 5.10645056  | -0.60865599 | 1.74125862  |
| 1 | -3.20284915 | -2.90985608 | -3.29314137 | 1  | 5.57895088  | -1.59195590 | 1.69365871  |
| 1 | -1.76834917 | -2.43995595 | -4.20754147 | 1  | 5.48005056  | 0.00764403  | 0.92145866  |
| 6 | -1.12894917 | -2.41915607 | -1.61344135 | 1  | 5.34075069  | -0.13295597 | 2.69595861  |
| 1 | -0.66624916 | -2.03695607 | -0.70294130 | 1  | 0.06895077  | -3.25945592 | 3.88075876  |
| 1 | -0.33344921 | -2.80135608 | -2.26514125 | 1  | -0.79834926 | -2.39145613 | 2.60295868  |
| 1 | -1.76394916 | -3.26345611 | -1.32354128 | 1  | 0.39985076  | -3.62695599 | 2.17275858  |
| 6 | -1.07044923 | -0.22625598 | -2.90234137 | 1  | -6.44584942 | -0.56425595 | -1.15974128 |
| 1 | -1.65874910 | 0.44984403  | -3.53254128 |    |             |             |             |

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# MTS-23



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1643386.5 (Joules/Mol)      |
|                                              | 392.77879 (Kcal/Mol)        |
| Zero-point correction=                       | 0.625933 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.666641                    |
| Thermal correction to Enthalpy=              | 0.667585                    |
| Thermal correction to Gibbs Free Energy=     | 0.550969                    |
| Sum of electronic and zero-point Energies=   | -2496.472669                |
| Sum of electronic and thermal Energies=      | -2496.431961                |
| Sum of electronic and thermal Enthalpies=    | -2496.431016                |
| Sum of electronic and thermal Free Energies= | -2496.547633                |

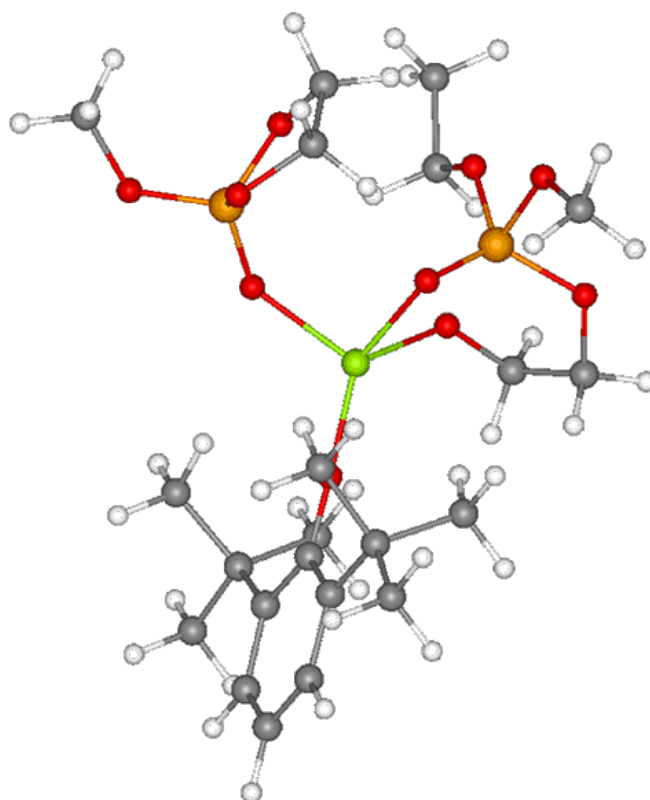
| cartesian |             |             |             |    |             |             |             |  |  |  |  |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|--|--|
| 12        | -0.46078813 | -0.07986808 | -0.08209602 | 1  | 0.91301191  | 1.99273193  | 3.36870384  |  |  |  |  |
| 8         | -2.48428822 | -1.05306804 | -1.10749602 | 1  | 0.91201186  | 1.78903198  | 1.60400391  |  |  |  |  |
| 8         | 1.38161194  | 0.08873192  | 0.01360398  | 6  | -2.78728819 | -0.75856811 | -3.46929598 |  |  |  |  |
| 6         | -2.75938821 | -1.75566804 | -2.32859612 | 8  | -1.19088817 | 1.73093200  | -0.60479605 |  |  |  |  |
| 1         | -3.72698808 | -2.26016808 | -2.22699594 | 15 | -2.36728811 | 2.54853177  | -0.20409602 |  |  |  |  |
| 1         | -1.98288810 | -2.51246810 | -2.49289608 | 8  | -2.74498820 | 2.51143193  | 1.34900391  |  |  |  |  |
| 6         | 2.69871187  | 0.22153193  | 0.09280398  | 8  | -3.79758811 | 2.13223195  | -0.79209602 |  |  |  |  |
| 6         | 3.50461197  | 0.11553192  | -1.08599603 | 6  | -3.96658802 | 1.76873195  | 1.58040392  |  |  |  |  |
| 6         | 4.89331198  | 0.21093193  | -0.95479608 | 6  | -4.52028799 | 1.35403192  | 0.19620398  |  |  |  |  |
| 1         | 5.52511168  | 0.12433192  | -1.83249605 | 1  | -4.64158821 | 2.43453193  | 2.12210393  |  |  |  |  |
| 6         | 5.50731182  | 0.41823190  | 0.27570397  | 1  | -3.71168804 | 0.89563191  | 2.18000388  |  |  |  |  |
| 6         | 4.71571207  | 0.55553192  | 1.41080391  | 1  | -4.35138798 | 0.29703194  | -0.01009602 |  |  |  |  |

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|   |            |             |             |    |             |             |             |
|---|------------|-------------|-------------|----|-------------|-------------|-------------|
| 1 | 5.21011209 | 0.73443192  | 2.35990405  | 1  | -5.57568789 | 1.60313201  | 0.07920398  |
| 6 | 3.32121181 | 0.47253191  | 1.35770392  | 8  | -2.10258818 | 4.04253197  | -0.63319600 |
| 6 | 2.87721181 | -0.08456808 | -2.47829604 | 6  | -3.06578803 | 5.07783222  | -0.35169601 |
| 6 | 2.49121189 | 0.66803193  | 2.64060402  | 1  | -4.01688814 | 4.85243225  | -0.83899605 |
| 6 | 1.93631196 | 1.09133196  | -2.81299615 | 1  | -3.19948816 | 5.18393230  | 0.72700393  |
| 1 | 1.16201186 | 1.23183191  | -2.05769610 | 1  | -2.64418817 | 5.99283218  | -0.76419604 |
| 1 | 1.45181191 | 0.93043190  | -3.78469610 | 8  | -1.93638813 | -0.66336811 | 1.22650397  |
| 1 | 2.50411177 | 2.02623200  | -2.87339616 | 15 | -2.33268809 | -1.88506806 | 0.37540397  |
| 6 | 2.11921191 | -1.42506802 | -2.54819608 | 8  | -2.15548801 | -3.28226805 | 1.26180398  |
| 1 | 1.32821190 | -1.49046803 | -1.80049610 | 8  | -0.69828808 | -2.23676825 | -0.30899602 |
| 1 | 2.80731177 | -2.26076818 | -2.37699604 | 6  | -0.80588812 | -3.57026815 | 1.60860395  |
| 1 | 1.66931200 | -1.55966806 | -3.54029608 | 6  | 0.00811189  | -3.27786803 | 0.34980398  |
| 6 | 3.93321180 | -0.12516807 | -3.59779596 | 1  | -0.75458813 | -4.61816788 | 1.90980399  |
| 1 | 4.62861204 | -0.96406811 | -3.48509598 | 1  | -0.50138813 | -2.93066812 | 2.44340396  |
| 1 | 4.51591206 | 0.80043191  | -3.65199614 | 1  | 1.02341187  | -2.94686818 | 0.57900393  |
| 1 | 3.42891192 | -0.24916808 | -4.56309605 | 1  | 0.04901189  | -4.14746809 | -0.31559601 |
| 6 | 3.36911178 | 0.95323193  | 3.87230396  | 8  | -3.96598816 | -2.11186814 | 0.33580399  |
| 1 | 3.96691179 | 1.86293197  | 3.75290394  | 6  | -4.69828796 | -2.84896827 | 1.31940401  |
| 1 | 4.04631186 | 0.12363192  | 4.10240412  | 1  | -4.53238821 | -3.92236805 | 1.20970392  |
| 1 | 2.72491193 | 1.09993196  | 4.74690390  | 1  | -4.42638826 | -2.54566813 | 2.33400393  |
| 6 | 1.68521190 | -0.60426807 | 2.96880388  | 1  | -5.75148821 | -2.62006807 | 1.13760400  |
| 1 | 0.99731183 | -0.86216807 | 2.16320395  | 1  | -3.01908803 | -1.27436805 | -4.40659618 |
| 1 | 1.09901190 | -0.46506810 | 3.88550401  | 1  | -3.54798818 | 0.00793192  | -3.29829597 |
| 1 | 2.36111188 | -1.45306802 | 3.12310386  | 1  | -1.81888807 | -0.26376808 | -3.58309603 |
| 6 | 1.55111194 | 1.88073194  | 2.48340392  | 1  | 6.59051180  | 0.48293191  | 0.34750399  |
| 1 | 2.13561177 | 2.80023193  | 2.36880398  |    |             |             |             |

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### MI-3



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1643197.0 (Joules/Mol)      |
|                                              | 392.73350 (Kcal/Mol)        |
| Zero-point correction=                       | 0.625861 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.667501                    |
| Thermal correction to Enthalpy=              | 0.668446                    |
| Thermal correction to Gibbs Free Energy=     | 0.549508                    |
| Sum of electronic and zero-point Energies=   | -2496.490683                |
| Sum of electronic and thermal Energies=      | -2496.449042                |
| Sum of electronic and thermal Enthalpies=    | -2496.448098                |
| Sum of electronic and thermal Free Energies= | -2496.567035                |

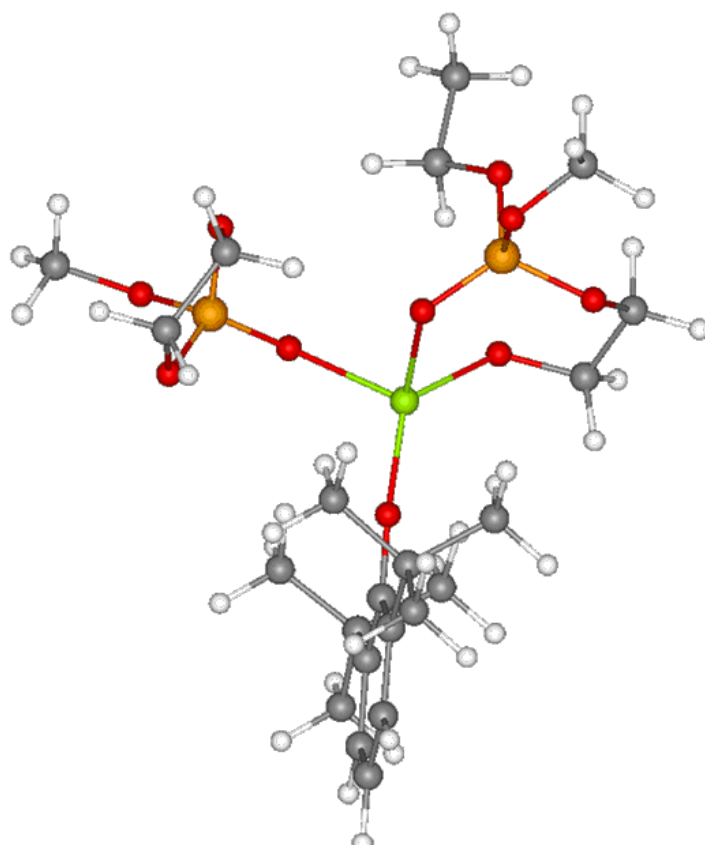
| cartesian |             |             |             |    |             |             |             |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 12        | 0.26832652  | 0.02891735  | 0.22843331  | 1  | -0.89907342 | -0.87418264 | -3.62356663 |
| 8         | 3.69682670  | -1.03028262 | 1.22113335  | 1  | -0.97147352 | 0.19851735  | -2.21186662 |
| 8         | -1.57337356 | 0.05761734  | 0.09073333  | 1  | 2.99442649  | 0.64781737  | 2.22873354  |
| 6         | 3.61282659  | -0.23198265 | 2.41413355  | 8  | 1.13502645  | 1.83421731  | -0.07396667 |
| 6         | 5.02822638  | 0.15801734  | 2.79023337  | 15 | 2.30052662  | 2.34731722  | -0.84406668 |
| 1         | 3.14902663  | -0.81368262 | 3.21433353  | 8  | 2.44092655  | 1.90691733  | -2.37596655 |
| 6         | -2.88367343 | 0.09791735  | -0.12576666 | 8  | 3.73302650  | 1.85031736  | -0.32856667 |
| 6         | -3.73677349 | 0.80691737  | 0.77853334  | 6  | 3.44752669  | 0.86461735  | -2.49686646 |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -5.11367321 | 0.80421734  | 0.53603333  | 6  | 4.44272661  | 1.09821737  | -1.34706664 |
| 1 | -5.78077364 | 1.33021736  | 1.21073329  | 1  | 3.90732670  | 0.97901738  | -3.47866654 |
| 6 | -5.67097330 | 0.14531735  | -0.55456668 | 1  | 2.94822669  | -0.09948265 | -2.40276647 |
| 6 | -4.83347321 | -0.52508265 | -1.43906665 | 1  | 4.76852655  | 0.15991735  | -0.89776665 |
| 1 | -5.28387356 | -1.02558267 | -2.28966665 | 1  | 5.30332661  | 1.69971740  | -1.65056670 |
| 6 | -3.44737339 | -0.56758261 | -1.26056671 | 8  | 2.24772644  | 3.92411733  | -0.80686671 |
| 6 | -3.17327332 | 1.57501733  | 1.98953331  | 6  | 3.25982666  | 4.72041702  | -1.45456672 |
| 6 | -2.56567335 | -1.31468260 | -2.27936649 | 1  | 4.23022652  | 4.55481720  | -0.98056668 |
| 6 | -2.22547340 | 2.69541717  | 1.51593328  | 1  | 3.30352664  | 4.48571730  | -2.52036667 |
| 1 | -1.40347338 | 2.31101727  | 0.91163331  | 1  | 2.95402670  | 5.75601721  | -1.31646669 |
| 1 | -1.80107331 | 3.22901726  | 2.37593341  | 8  | 1.72392654  | -1.00528264 | -0.66266668 |
| 1 | -2.77217340 | 3.42291737  | 0.90583330  | 15 | 2.52572656  | -1.78088260 | 0.40713331  |
| 6 | -2.43817329 | 0.61571735  | 2.94693351  | 8  | 2.02012658  | -3.21408272 | 0.99613333  |
| 1 | -1.62617350 | 0.09311734  | 2.44013333  | 8  | 1.16712654  | -1.01538265 | 1.69013333  |
| 1 | -3.12947345 | -0.13818264 | 3.34023333  | 6  | 0.81632650  | -3.30688286 | 1.76293337  |
| 1 | -2.01907349 | 1.16701734  | 3.79813337  | 6  | 0.69402653  | -2.01478267 | 2.55683351  |
| 6 | -4.27647352 | 2.25521731  | 2.81883335  | 1  | 0.90812653  | -4.19448280 | 2.39253354  |
| 1 | -4.98867321 | 1.53441739  | 3.23453355  | 1  | -0.02687347 | -3.43258286 | 1.07593334  |
| 1 | -4.83557320 | 2.99581718  | 2.23723340  | 1  | -0.34417349 | -1.82828259 | 2.84913349  |
| 1 | -3.81747341 | 2.78351736  | 3.66223335  | 1  | 1.30932653  | -2.05748272 | 3.46803355  |
| 6 | -3.38597345 | -1.94148266 | -3.42106652 | 8  | 3.68002653  | -2.48408270 | -0.53786665 |
| 1 | -3.93707323 | -1.19048262 | -3.99656653 | 6  | 3.25802660  | -3.35738277 | -1.58016670 |
| 1 | -4.09937334 | -2.68878269 | -3.05796647 | 1  | 2.80382657  | -4.26558256 | -1.17096663 |
| 1 | -2.70677352 | -2.45028281 | -4.11506701 | 1  | 2.54432654  | -2.86478281 | -2.25016665 |
| 6 | -1.81787348 | -2.47738266 | -1.59666669 | 1  | 4.15442657  | -3.62948275 | -2.14206648 |
| 1 | -1.20657349 | -2.13058281 | -0.76266670 | 1  | 5.01112652  | 0.75081736  | 3.71033335  |
| 1 | -1.16347337 | -2.99008274 | -2.31206656 | 1  | 5.64592648  | -0.72808266 | 2.95933342  |
| 1 | -2.53227329 | -3.20958281 | -1.20436668 | 1  | 5.49062681  | 0.76041734  | 2.00393343  |
| 6 | -1.57477355 | -0.33848265 | -2.94556665 | 1  | -6.74617338 | 0.15901735  | -0.71646667 |
| 1 | -2.11707330 | 0.41211733  | -3.53066659 |    |             |             |             |

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# MI-4



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1640580.5 (Joules/Mol)      |
|                                              | 392.10815 (Kcal/Mol)        |
| Zero-point correction=                       | 0.624864 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.667099                    |
| Thermal correction to Enthalpy=              | 0.668043                    |
| Thermal correction to Gibbs Free Energy=     | 0.546623                    |
| Sum of electronic and zero-point Energies=   | -2496.494176                |
| Sum of electronic and thermal Energies=      | -2496.451941                |
| Sum of electronic and thermal Enthalpies=    | -2496.450997                |
| Sum of electronic and thermal Free Energies= | -2496.572417                |

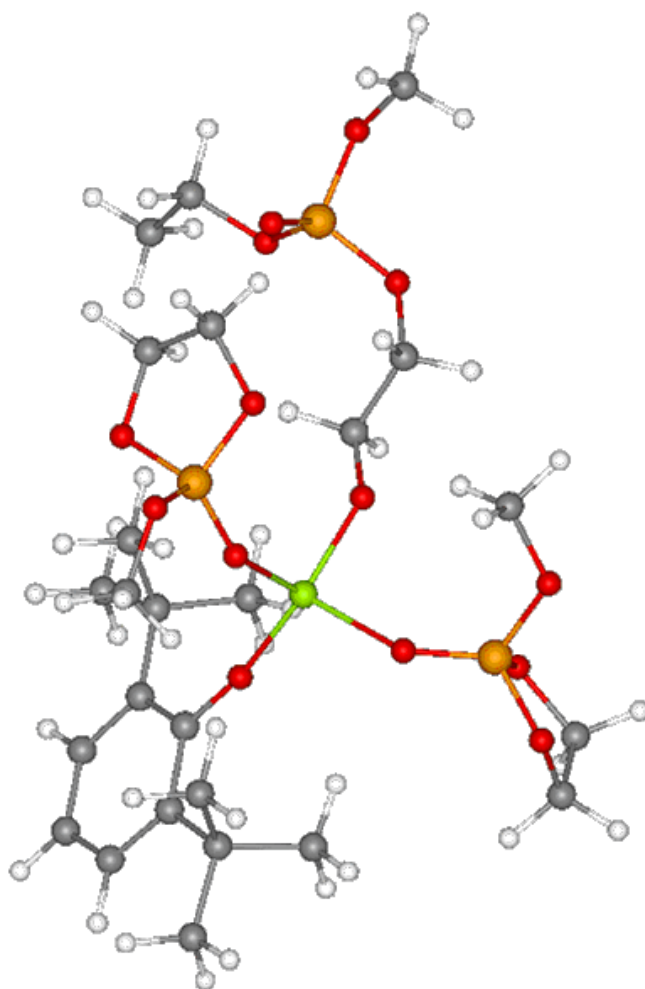
| cartesian |             |             |             |    |             |             |             |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 12        | 0.39618522  | -0.00831600 | 0.80612534  | 1  | -0.33831477 | -0.68631601 | -3.48837471 |
| 8         | 3.54258537  | -2.15861607 | -1.44747472 | 1  | -0.63811475 | 0.18698400  | -1.96587467 |
| 8         | -1.36531472 | -0.18701601 | 0.21162534  | 1  | 5.41748524  | -2.85931611 | -0.85347468 |
| 6         | 4.53808498  | -3.19411612 | -1.40997469 | 8  | 0.95178527  | 1.96198404  | 0.72722536  |
| 1         | 4.81038523  | -3.38791609 | -2.44717479 | 15 | 1.35068536  | 2.95688391  | -0.29767466 |
| 1         | 4.12698507  | -4.10021591 | -0.95947468 | 8  | 0.39468524  | 3.05168390  | -1.58157468 |
| 6         | -2.64871478 | -0.36481601 | -0.06987467 | 8  | 2.73628521  | 2.69568396  | -1.07477462 |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -3.66251469 | 0.07508401  | 0.84232533  | 6  | 1.11698532  | 2.76018405  | -2.80207467 |
| 6 | -5.00301504 | -0.12451599 | 0.49862534  | 6  | 2.43178535  | 2.10508394  | -2.36687469 |
| 1 | -5.78631496 | 0.20168400  | 1.17482531  | 1  | 1.27628517  | 3.70498395  | -3.32907486 |
| 6 | -5.38011503 | -0.73411602 | -0.69337469 | 1  | 0.49808526  | 2.09408402  | -3.40257478 |
| 6 | -4.39211512 | -1.16281605 | -1.57307470 | 1  | 2.33418536  | 1.02518404  | -2.23507476 |
| 1 | -4.70201492 | -1.64001596 | -2.49717474 | 1  | 3.26118541  | 2.33858395  | -3.03437471 |
| 6 | -3.03171468 | -0.99821603 | -1.29727471 | 8  | 1.46518517  | 4.37308407  | 0.38792533  |
| 6 | -3.30861473 | 0.75348401  | 2.17912531  | 6  | 1.75338531  | 5.55788422  | -0.38107467 |
| 6 | -1.98071480 | -1.50101602 | -2.30407476 | 1  | 2.72298527  | 5.46388435  | -0.87557465 |
| 6 | -2.52911472 | 2.05998397  | 1.92722535  | 1  | 0.95998526  | 5.73498440  | -1.11077464 |
| 1 | -1.63121486 | 1.89248395  | 1.33272529  | 1  | 1.78208518  | 6.37598419  | 0.33662534  |
| 1 | -2.23391461 | 2.52318406  | 2.87722516  | 8  | 1.87628531  | -0.57601601 | -0.52157468 |
| 1 | -3.15691471 | 2.77548409  | 1.38372529  | 15 | 2.88228536  | -1.61151600 | -0.10287467 |
| 6 | -2.49721479 | -0.20691600 | 3.07182527  | 8  | 2.38328528  | -2.94841599 | 0.58532536  |
| 1 | -1.58361483 | -0.55391598 | 2.58772516  | 8  | 1.26348519  | -0.94961596 | 2.21922517  |
| 1 | -3.09581470 | -1.09091604 | 3.31862521  | 6  | 2.24408531  | -3.11081600 | 2.02972531  |
| 1 | -2.21691465 | 0.28428400  | 4.01192522  | 6  | 1.08688521  | -2.27861595 | 2.55992532  |
| 6 | -4.55741501 | 1.14458394  | 2.99002528  | 1  | 3.18908525  | -2.80691600 | 2.48962522  |
| 1 | -5.16711473 | 0.27548400  | 3.25942516  | 1  | 2.09378529  | -4.18401575 | 2.17062521  |
| 1 | -5.19241476 | 1.86008406  | 2.45662522  | 1  | 0.14578524  | -2.70831609 | 2.17102528  |
| 1 | -4.24181509 | 1.62268400  | 3.92452526  | 1  | 1.06778526  | -2.43271589 | 3.65522528  |
| 6 | -2.61491466 | -2.13541603 | -3.55437469 | 8  | 4.10738516  | -1.08261597 | 0.76332533  |
| 1 | -3.24151468 | -1.42761600 | -4.10787487 | 6  | 4.10708523  | 0.20038401  | 1.46172535  |
| 1 | -3.22171474 | -3.01371598 | -3.31037474 | 1  | 3.97438526  | 0.98998398  | 0.71772534  |
| 1 | -1.81931472 | -2.46761608 | -4.23167467 | 1  | 3.25978541  | 0.20028400  | 2.15102530  |
| 6 | -1.10101485 | -2.58901596 | -1.65707469 | 6  | 5.43298483  | 0.32948402  | 2.17612529  |
| 1 | -0.61651474 | -2.22701597 | -0.75047469 | 1  | 5.46268511  | 1.28628397  | 2.70632529  |
| 1 | -0.32201475 | -2.92431593 | -2.35317469 | 1  | 5.56278515  | -0.47031599 | 2.91002512  |
| 1 | -1.71221471 | -3.45731592 | -1.38757467 | 1  | 6.26998520  | 0.29908401  | 1.47282529  |
| 6 | -1.11541486 | -0.32541600 | -2.80157471 | 1  | -6.43161488 | -0.87481600 | -0.93257469 |
| 1 | -1.73981476 | 0.40008399  | -3.33647490 |    |             |             |             |

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## MI-1m

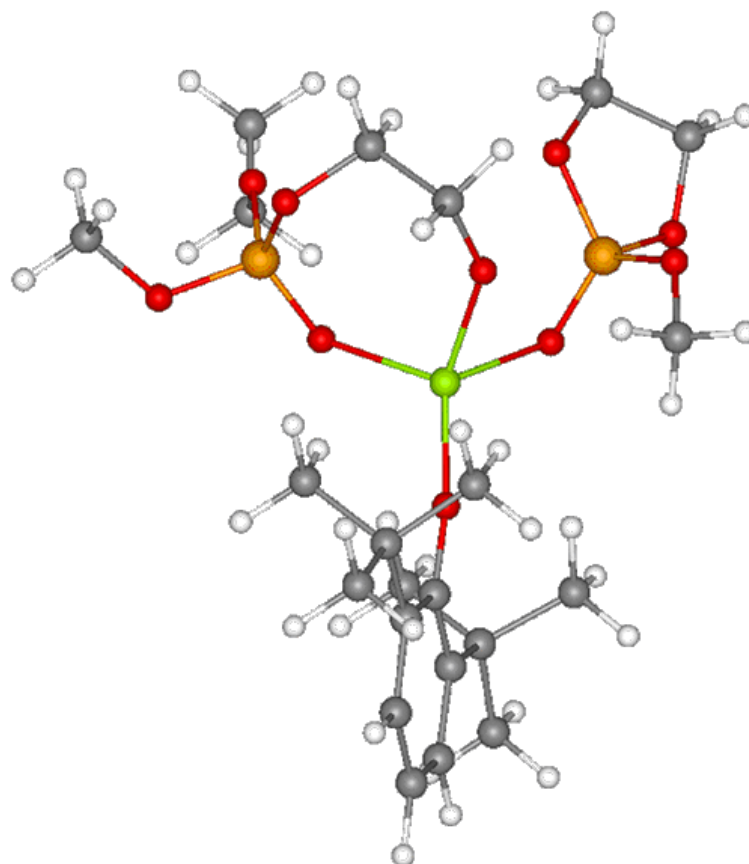


|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1944471.0 (Joules/Mol)      |
|                                              | 464.73972 (Kcal/Mol)        |
| Zero-point correction=                       | 0.740610 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.793970                    |
| Thermal correction to Enthalpy=              | 0.794915                    |
| Thermal correction to Gibbs Free Energy=     | 0.643328                    |
| Sum of electronic and zero-point Energies=   | -3257.061075                |
| Sum of electronic and thermal Energies=      | -3257.007714                |
| Sum of electronic and thermal Enthalpies=    | -3257.006770                |
| Sum of electronic and thermal Free Energies= | -3257.158357                |

| cartesian |             |             |             |   |            |             |            |
|-----------|-------------|-------------|-------------|---|------------|-------------|------------|
| 12        | -0.78191978 | 0.80300331  | 0.25762117  | 6 | 3.13168025 | 0.86020327  | 3.39682126 |
| 8         | 0.83498025  | 1.41350329  | -0.52077883 | 6 | 2.86308026 | -0.56529677 | 2.91732121 |
| 8         | -1.97581971 | -0.58359671 | -0.17047884 | 1 | 3.42058015 | 0.90120327  | 4.45042086 |
| 6         | 1.98348033  | 0.91010332  | -1.10357881 | 1 | 3.86988020 | 1.35500324  | 2.76872134 |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1  | 1.86898029  | 0.72880328  | -2.18597865 | 1  | 2.99818015  | -0.65699673 | 1.83972120  |
| 1  | 2.30588007  | -0.05429673 | -0.66697884 | 1  | 3.47338009  | -1.30459678 | 3.43492126  |
| 6  | -2.67501974 | -1.69249678 | -0.35637885 | 8  | 0.04948026  | 0.65800327  | 4.76662111  |
| 6  | -2.06531978 | -2.85199666 | -0.93887889 | 6  | -1.32901967 | 0.31890327  | 5.04992104  |
| 6  | -2.83681989 | -4.00569677 | -1.10437882 | 1  | -1.98221982 | 0.68850327  | 4.25912094  |
| 1  | -2.39181972 | -4.89329672 | -1.54187882 | 1  | -1.42581975 | -0.76419675 | 5.14692116  |
| 6  | -4.17431974 | -4.06279659 | -0.72737885 | 1  | -1.56361973 | 0.80240327  | 5.99712086  |
| 6  | -4.76741982 | -2.93019676 | -0.17997883 | 8  | -1.77261972 | 2.58810329  | 0.15462117  |
| 1  | -5.81441975 | -2.98629665 | 0.09952117  | 15 | -1.81491971 | 3.70770335  | -0.82487887 |
| 6  | -4.06011963 | -1.74009681 | 0.01262116  | 8  | -3.18701982 | 4.53910303  | -0.89547884 |
| 6  | -0.59221977 | -2.84669685 | -1.38607883 | 8  | -1.75891972 | 3.23600316  | -2.35997868 |
| 6  | -4.78031969 | -0.50989676 | 0.59402114  | 6  | -3.89301991 | 4.21950340  | -2.11417866 |
| 6  | 0.33268026  | -2.62909675 | -0.17207883 | 6  | -2.80141973 | 3.87070322  | -3.12727880 |
| 1  | 0.08858025  | -1.71499681 | 0.37112117  | 1  | -4.47271967 | 5.09790325  | -2.39887881 |
| 1  | 1.38138032  | -2.57369685 | -0.48997885 | 1  | -4.55891943 | 3.37460327  | -1.92227876 |
| 1  | 0.23568025  | -3.46039677 | 0.53512114  | 1  | -3.13741994 | 3.15920329  | -3.88177896 |
| 6  | -0.35921979 | -1.76519680 | -2.46047878 | 1  | -2.38731980 | 4.76090336  | -3.60927868 |
| 1  | -0.62621975 | -0.76899672 | -2.10657883 | 8  | -0.72921973 | 4.82210302  | -0.57177883 |
| 1  | -0.96761972 | -1.97889686 | -3.34657884 | 6  | 0.40698025  | 4.58150339  | 0.30762118  |
| 1  | 0.69298023  | -1.75059676 | -2.76957870 | 1  | 0.08268026  | 4.70280313  | 1.34242117  |
| 6  | -0.16281976 | -4.18299675 | -2.01817870 | 1  | 0.81228024  | 3.58060336  | 0.13912116  |
| 1  | -0.74441975 | -4.42299652 | -2.91477871 | 1  | 1.13378024  | 5.35040331  | 0.04802117  |
| 1  | -0.24641974 | -5.02189684 | -1.31877887 | 8  | 4.39028025  | 1.47060323  | -1.43347883 |
| 1  | 0.88838023  | -4.11509657 | -2.32167864 | 1  | 2.89718008  | 2.84540319  | -1.43727887 |
| 6  | -6.26611948 | -0.77999675 | 0.89072114  | 1  | 3.22478008  | 2.14110327  | 0.16622117  |
| 1  | -6.40481949 | -1.56969678 | 1.63712120  | 1  | -4.74891949 | -4.97559690 | -0.86547887 |
| 1  | -6.82571936 | -1.05659676 | -0.00927883 | 15 | 5.32568026  | 0.49280328  | -0.60427886 |
| 1  | -6.72401953 | 0.13130328  | 1.29262114  | 8  | 5.15968037  | -0.90089679 | -1.35967886 |
| 6  | -4.73731947 | 0.65070331  | -0.42107886 | 8  | 6.80798054  | 0.91180325  | -1.05567884 |
| 1  | -3.70921993 | 0.90680325  | -0.67797887 | 8  | 5.10408020  | 0.48060328  | 0.86602116  |
| 1  | -5.22951937 | 1.53960323  | -0.00387883 | 6  | 7.39258051  | 2.09380341  | -0.48817885 |
| 1  | -5.26451969 | 0.36560327  | -1.33907890 | 6  | 5.92628050  | -2.04749680 | -0.91587889 |
| 6  | -4.13671970 | -0.08379671 | 1.92862117  | 6  | 5.49418020  | -3.24299669 | -1.73557889 |
| 1  | -4.24311972 | -0.88479674 | 2.66942120  | 1  | 6.98948050  | -1.83019686 | -1.05937886 |
| 1  | -4.62931967 | 0.81360328  | 2.32482123  | 1  | 5.74068022  | -2.20559669 | 0.15122117  |
| 1  | -3.07411981 | 0.12820329  | 1.81142116  | 1  | 6.85728025  | 2.98380327  | -0.83137888 |
| 6  | 3.11018014  | 1.91980326  | -0.89847887 | 1  | 7.37968063  | 2.04400325  | 0.60362118  |
| 8  | -0.40501976 | 0.71120328  | 2.26802135  | 1  | 8.42168045  | 2.12820339  | -0.84587884 |
| 15 | 0.64738023  | 0.53580326  | 3.30532122  | 1  | 6.06318045  | -4.12519693 | -1.42677879 |
| 8  | 1.86738026  | 1.56330323  | 3.25702119  | 1  | 4.43068027  | -3.44959664 | -1.59247887 |
| 8  | 1.47488034  | -0.83399677 | 3.24612117  | 1  | 5.67478037  | -3.06909680 | -2.79937863 |

# MTS-45



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1639699.4 (Joules/Mol)      |
|                                              | 391.89757 (Kcal/Mol)        |
| Zero-point correction=                       | 0.624529 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.665930                    |
| Thermal correction to Enthalpy=              | 0.666874                    |
| Thermal correction to Gibbs Free Energy=     | 0.547817                    |
| Sum of electronic and zero-point Energies=   | -2496.495346                |
| Sum of electronic and thermal Energies=      | -2496.453944                |
| Sum of electronic and thermal Enthalpies=    | -2496.453000                |
| Sum of electronic and thermal Free Energies= | -2496.572057                |

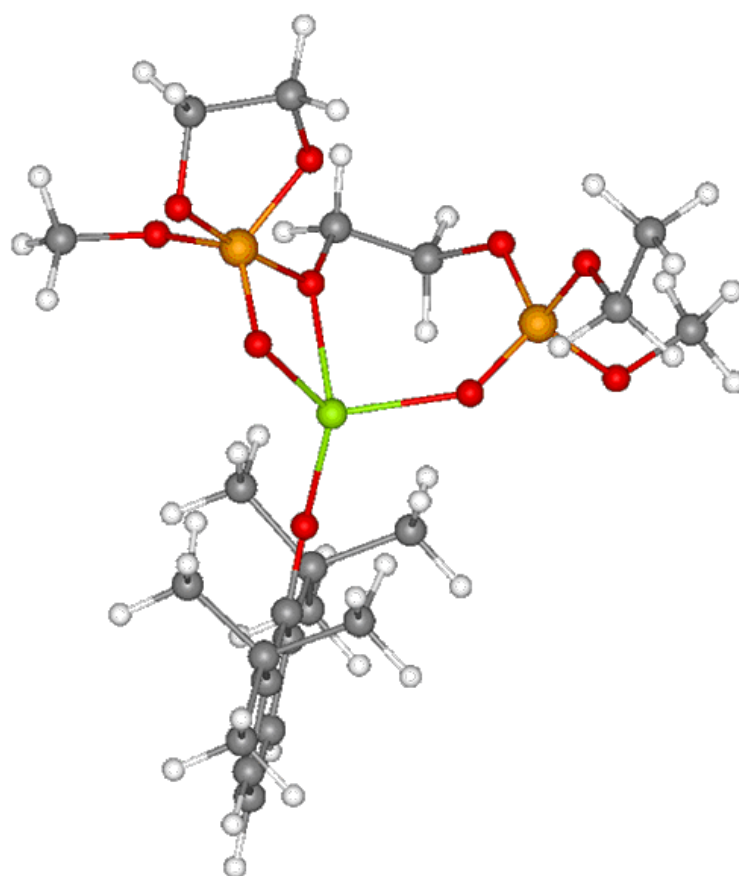
|    |             |             |             | cartesian |             |             |             |
|----|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 12 | -0.30504012 | -0.26997203 | 0.07067200  | 1         | 1.46065986  | 2.71562815  | 2.46107197  |
| 8  | -1.45064020 | 3.77982807  | -0.75682801 | 1         | 1.22625983  | 1.88042796  | 0.91127199  |
| 8  | 1.55065989  | -0.31307203 | 0.00417200  | 1         | -3.12283993 | 5.03772831  | -0.76342803 |
| 6  | -2.11214018 | 4.99322796  | -0.34952801 | 8         | -1.26494014 | -1.99667203 | -0.42202801 |
| 1  | -1.51104009 | 5.80832815  | -0.75002801 | 15        | -2.31073999 | -2.49837208 | 0.53067201  |
| 1  | -2.14654016 | 5.05272818  | 0.73977202  | 8         | -3.02424002 | -3.76087189 | -0.21942800 |
| 6  | 2.86236000  | -0.18627203 | -0.14542800 | 8         | -3.69343996 | -1.70147204 | 0.82997197  |

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|   |            |             |             |    |             |             |             |
|---|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 3.51796007 | -0.76787204 | -1.27792799 | 6  | -4.38334036 | -3.87587214 | 0.19787200  |
| 6 | 4.90455961 | -0.63027203 | -1.39012802 | 6  | -4.84944010 | -2.43257189 | 0.36997199  |
| 1 | 5.42265987 | -1.06577206 | -2.23822784 | 1  | -4.43884039 | -4.43587208 | 1.13827205  |
| 6 | 5.65915966 | 0.05292796  | -0.44212800 | 1  | -4.93624020 | -4.40857172 | -0.57722801 |
| 6 | 5.01495981 | 0.62272799  | 0.65087199  | 1  | -5.17574024 | -1.99557209 | -0.57822800 |
| 1 | 5.61765957 | 1.15542793  | 1.37917197  | 1  | -5.63394022 | -2.32067204 | 1.12027204  |
| 6 | 3.63165998 | 0.52662796  | 0.82967198  | 8  | -1.83574009 | -3.16087198 | 1.89127195  |
| 6 | 2.73176003 | -1.53137207 | -2.35952806 | 6  | -0.49244010 | -3.05767202 | 2.41087198  |
| 6 | 2.96815991 | 1.18592799  | 2.05297184  | 1  | 0.24055991  | -3.20447206 | 1.61527205  |
| 6 | 1.71425974 | -0.59507203 | -3.04272795 | 1  | -0.36124012 | -2.08047199 | 2.87237215  |
| 1 | 1.04075980 | -0.12517203 | -2.32472801 | 1  | -0.40354010 | -3.85777187 | 3.14567184  |
| 1 | 1.11075985 | -1.14837205 | -3.77322817 | 8  | -1.12524009 | 1.29762793  | -0.90402800 |
| 1 | 2.23456001 | 0.20982796  | -3.57382822 | 15 | -2.07084012 | 2.35712814  | -0.44032800 |
| 6 | 2.02376008 | -2.75717211 | -1.74742806 | 8  | -2.42584014 | 2.43552780  | 1.09037197  |
| 1 | 1.32795990 | -2.47457218 | -0.95782799 | 8  | -1.51014018 | -0.39027202 | 1.57367194  |
| 1 | 2.76225996 | -3.44467211 | -1.31962800 | 6  | -3.14213991 | 1.38792801  | 1.82967198  |
| 1 | 1.46155989 | -3.30097198 | -2.51662779 | 6  | -2.18004012 | 0.40752795  | 2.48117208  |
| 6 | 3.64195991 | -2.06947184 | -3.47822809 | 1  | -3.81724000 | 0.87202799  | 1.14447200  |
| 1 | 4.38175964 | -2.78487206 | -3.10302782 | 1  | -3.72244000 | 1.93702805  | 2.57567215  |
| 1 | 4.17275953 | -1.26927209 | -4.00522804 | 1  | -1.48234010 | 0.98022795  | 3.11587191  |
| 1 | 3.02745986 | -2.59457207 | -4.21852827 | 1  | -2.80134010 | -0.19907203 | 3.16507196  |
| 6 | 3.98715997 | 1.88272798  | 2.97267199  | 8  | -3.49544001 | 2.26282787  | -1.15632796 |
| 1 | 4.52675962 | 2.68812799  | 2.46307182  | 6  | -3.56944013 | 1.87992799  | -2.56052780 |
| 1 | 4.72235966 | 1.18202794  | 3.38287210  | 1  | -3.05944014 | 2.64302778  | -3.15642786 |
| 1 | 3.45756006 | 2.33222818  | 3.82067204  | 1  | -3.04313993 | 0.93102795  | -2.68752813 |
| 6 | 2.25345993 | 0.12822796  | 2.91747189  | 6  | -5.02914047 | 1.77182794  | -2.93752813 |
| 1 | 1.48795986 | -0.40207204 | 2.35027218  | 1  | -5.11184025 | 1.48182797  | -3.98902798 |
| 1 | 1.77825987 | 0.60032797  | 3.78697205  | 1  | -5.53374004 | 1.01552796  | -2.33092785 |
| 1 | 2.97375989 | -0.61057204 | 3.28637218  | 1  | -5.54364014 | 2.72672796  | -2.80222797 |
| 6 | 1.97605979 | 2.27542782  | 1.59797204  | 1  | 6.73715973  | 0.14172797  | -0.55492800 |
| 1 | 2.50616002 | 3.07862806  | 1.07447195  |    |             |             |             |

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## MI-5



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1642692.3 (Joules/Mol)      |
|                                              | 392.61288 (Kcal/Mol)        |
| Zero-point correction=                       | 0.625668 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.667186                    |
| Thermal correction to Enthalpy=              | 0.668130                    |
| Thermal correction to Gibbs Free Energy=     | 0.547247                    |
| Sum of electronic and zero-point Energies=   | -2496.494973                |
| Sum of electronic and thermal Energies=      | -2496.453455                |
| Sum of electronic and thermal Enthalpies=    | -2496.452511                |
| Sum of electronic and thermal Free Energies= | -2496.573394                |

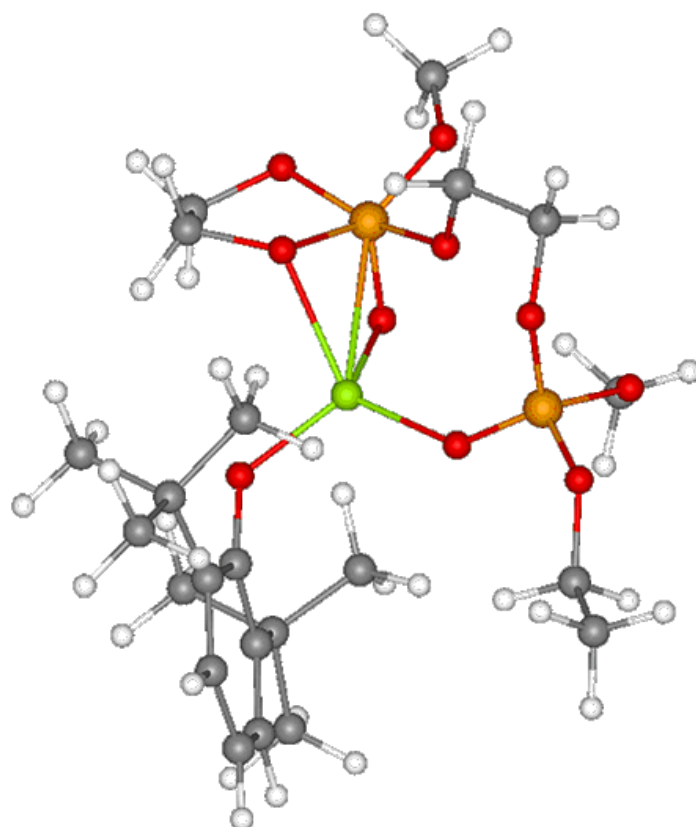
| cartesian |             |             |             |    |             |                         |
|-----------|-------------|-------------|-------------|----|-------------|-------------------------|
| 12        | -0.28790274 | -0.37243477 | -0.22901058 | 1  | 1.43029714  | -3.02943468 -2.74811053 |
| 8         | -1.45250273 | 3.79756522  | -0.24011061 | 1  | 1.34929729  | -2.36803460 -1.11051059 |
| 8         | 1.54509735  | -0.21953475 | -0.03601059 | 1  | -3.07170272 | 5.11586523 -0.36891058  |
| 6         | -2.18480277 | 4.93866539  | 0.24478941  | 8  | -1.33290267 | -1.98763478 -0.65801060 |
| 1         | -1.50480270 | 5.78576517  | 0.16848941  | 15 | -2.35600281 | -2.20033479 0.46668941  |
| 1         | -2.47880268 | 4.79086542  | 1.28658938  | 8  | -3.06700277 | -3.58933473 -0.20071059 |
| 6         | 2.86729741  | -0.15133476 | -0.13311060 | 8  | -3.82730269 | -1.45853484 0.56378943  |

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|   |            |             |             |    |             |             |             |
|---|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 3.62339735 | 0.44676524  | 0.92398942  | 6  | -4.43580294 | -3.68043470 | 0.12608941  |
| 6 | 5.01479721 | 0.50106525  | 0.80438942  | 6  | -4.92530298 | -2.23953462 | 0.08568941  |
| 1 | 5.60829687 | 0.94816524  | 1.59528935  | 1  | -4.58210278 | -4.11583471 | 1.12668943  |
| 6 | 5.67799711 | -0.00373476 | -0.30931059 | 1  | -4.93630314 | -4.31463480 | -0.61011058 |
| 6 | 4.93589687 | -0.57903475 | -1.33551061 | 1  | -5.15870285 | -1.92293477 | -0.93611062 |
| 1 | 5.46929693 | -0.96713477 | -2.19701052 | 1  | -5.78340292 | -2.05023479 | 0.73498940  |
| 6 | 3.54169726 | -0.67033476 | -1.28341055 | 8  | -1.88990283 | -2.89903474 | 1.86588943  |
| 6 | 2.93039727 | 1.03426516  | 2.16678929  | 6  | -1.58460283 | -4.29873466 | 1.94058943  |
| 6 | 2.76869726 | -1.32763481 | -2.44131064 | 1  | -2.49060273 | -4.90893459 | 1.91238940  |
| 6 | 2.13569736 | -0.05753476 | 2.91218948  | 1  | -0.92020273 | -4.60213470 | 1.12878942  |
| 1 | 1.39639735 | -0.53333479 | 2.26698947  | 1  | -1.07890272 | -4.43583488 | 2.89808941  |
| 1 | 1.62259722 | 0.36896524  | 3.78448939  | 8  | -1.09710276 | 1.39586520  | -0.78481060 |
| 1 | 2.81239724 | -0.83933473 | 3.27438951  | 15 | -2.12250280 | 2.35206532  | -0.27191058 |
| 6 | 2.00499725 | 2.19436526  | 1.74638939  | 8  | -2.74890280 | 2.07666540  | 1.15368938  |
| 1 | 1.28029728 | 1.87746513  | 0.99408942  | 8  | -1.71660280 | -0.62393475 | 1.20108938  |
| 1 | 2.59149742 | 3.01076531  | 1.31078947  | 6  | -1.97850275 | 1.50306523  | 2.25068951  |
| 1 | 1.47089720 | 2.59706521  | 2.61818933  | 6  | -2.22050285 | 0.01266524  | 2.35198951  |
| 6 | 3.93089747 | 1.61696517  | 3.18008947  | 1  | -2.33490276 | 2.01166534  | 3.14938951  |
| 1 | 4.51879692 | 2.43836522  | 2.75708938  | 1  | -0.91640276 | 1.72886515  | 2.11988950  |
| 1 | 4.62249708 | 0.85846525  | 3.56168938  | 1  | -1.71500278 | -0.35783476 | 3.25448942  |
| 1 | 3.38089728 | 2.01856542  | 4.03918934  | 1  | -3.29350281 | -0.17713475 | 2.44668937  |
| 6 | 3.69649720 | -1.80253482 | -3.57441068 | 8  | -3.44720268 | 2.45426536  | -1.13561058 |
| 1 | 4.40549707 | -2.56553459 | -3.23641062 | 6  | -3.35400271 | 2.47386527  | -2.59141064 |
| 1 | 4.26319695 | -0.97873473 | -4.02141047 | 1  | -2.75050259 | 1.62066519  | -2.91031051 |
| 1 | 3.09049726 | -2.25173473 | -4.36951065 | 6  | -4.75870275 | 2.40266538  | -3.14331055 |
| 6 | 1.79649734 | -0.31713477 | -3.08571053 | 1  | -2.84830260 | 3.39576530  | -2.89521050 |
| 1 | 1.13959718 | 0.15796524  | -2.35421062 | 1  | -4.71870279 | 2.41456532  | -4.23641062 |
| 1 | 1.17689729 | -0.80783474 | -3.84631062 | 1  | -5.25290298 | 1.48196518  | -2.82491064 |
| 1 | 2.35529733 | 0.48956525  | -3.57271051 | 1  | -5.35680294 | 3.25466537  | -2.81021070 |
| 6 | 2.02229738 | -2.58143473 | -1.94101059 | 1  | 6.76189709  | 0.05066524  | -0.37701058 |
| 1 | 2.74209738 | -3.33063459 | -1.59341061 |    |             |             |             |

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# MTS-56



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1644056.5 (Joules/Mol)      |
|                                              | 392.93894 (Kcal/Mol)        |
| Zero-point correction=                       | 0.626188 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.666465                    |
| Thermal correction to Enthalpy=              | 0.667409                    |
| Thermal correction to Gibbs Free Energy=     | 0.551891                    |
| Sum of electronic and zero-point Energies=   | -2496.482601                |
| Sum of electronic and thermal Energies=      | -2496.442324                |
| Sum of electronic and thermal Enthalpies=    | -2496.441380                |
| Sum of electronic and thermal Free Energies= | -2496.556898                |

cartesian

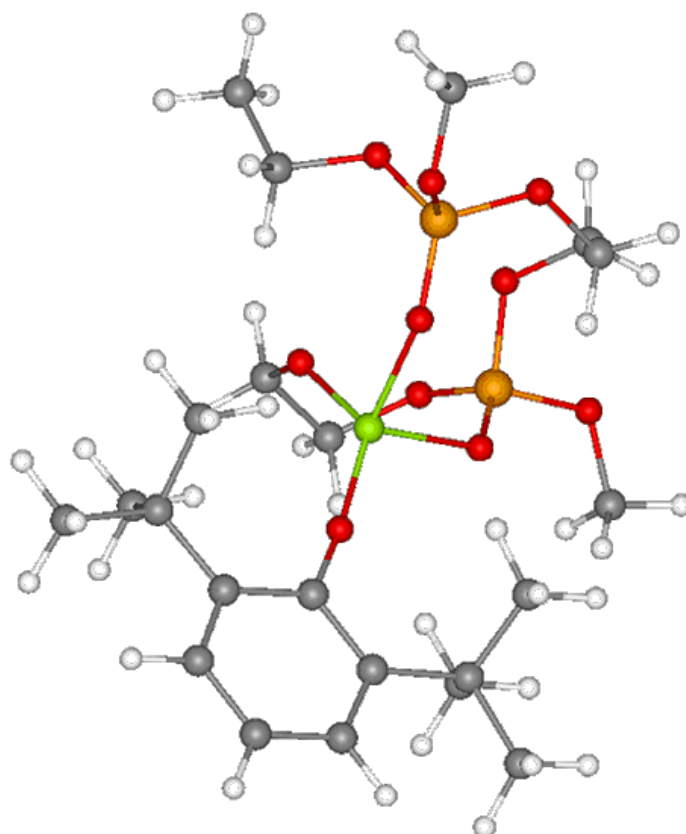
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 12 | -0.81081843 | -0.35784656 | 0.18830393  | 1  | 1.19228148  | -2.46884656 | -2.18579602 |
| 8  | -2.04101849 | 3.30685353  | 1.43130386  | 1  | -2.79001832 | 1.47135341  | 2.12430406  |
| 8  | 0.77068156  | -1.33184659 | -0.16919607 | 8  | -2.40371847 | -1.02724659 | 1.25570393  |
| 6  | -2.34831834 | 2.38915348  | 2.51310396  | 15 | -3.39051843 | -0.99164653 | 0.07590393  |
| 1  | -1.44191837 | 2.16395354  | 3.07770395  | 8  | -3.89701843 | -2.56954646 | -0.16579607 |
| 6  | 2.04558158  | -0.94294655 | -0.05739607 | 8  | -2.26351833 | -1.22924650 | -1.28219604 |
| 6  | 2.71358156  | -1.02894652 | 1.20380390  | 6  | -2.86111832 | -3.40614653 | -0.65509611 |
| 6  | 4.00568151  | -0.50324655 | 1.30930388  | 6  | -2.17911839 | -2.57984662 | -1.74009609 |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1 | 4.52618122  | -0.52874655 | 2.26100397  | 1  | -3.31501842 | -4.31924677 | -1.04529607 |
| 6 | 4.66518164  | 0.05475347  | 0.21870393  | 1  | -2.16861844 | -3.65654659 | 0.15630393  |
| 6 | 4.04468155  | 0.04155347  | -1.02639604 | 1  | -1.12901843 | -2.84494662 | -1.87389612 |
| 1 | 4.59418154  | 0.43445349  | -1.87529612 | 1  | -2.70621824 | -2.65474653 | -2.69719601 |
| 6 | 2.75368166  | -0.46594656 | -1.20519614 | 8  | -4.92571878 | -0.53104657 | 0.38970396  |
| 6 | 2.06138158  | -1.72384655 | 2.41530395  | 6  | -5.96411848 | -1.41514659 | 0.83400393  |
| 6 | 2.14988160  | -0.55504656 | -2.62059593 | 1  | -6.29831839 | -2.06514645 | 0.02370393  |
| 6 | 1.74978161  | -3.19254661 | 2.06020403  | 1  | -5.63061857 | -2.02544665 | 1.67570388  |
| 1 | 1.09988165  | -3.25284648 | 1.18500388  | 1  | -6.78131866 | -0.76384652 | 1.15140390  |
| 1 | 1.25238156  | -3.69304657 | 2.90070415  | 8  | -0.41801843 | 1.57695341  | 0.43240395  |
| 1 | 2.67378163  | -3.73834658 | 1.84060395  | 15 | -1.09041834 | 2.90265346  | 0.22310393  |
| 6 | 0.76238161  | -1.01884651 | 2.86680412  | 8  | -1.92911839 | 3.10295343  | -1.10299611 |
| 1 | -0.10141841 | -1.33354652 | 2.27720404  | 8  | -3.07651830 | 0.67585343  | -0.28739604 |
| 1 | 0.86258155  | 0.07155347  | 2.82410407  | 6  | -3.34411836 | 2.81765342  | -1.22129607 |
| 1 | 0.52008158  | -1.28704655 | 3.90220404  | 6  | -3.59871840 | 1.34085345  | -1.42129612 |
| 6 | 2.99708176  | -1.74254656 | 3.63770413  | 1  | -3.67531824 | 3.39185357  | -2.08859587 |
| 1 | 3.21428156  | -0.73524654 | 4.01120377  | 1  | -3.85481834 | 3.18225336  | -0.32659605 |
| 1 | 3.94678187  | -2.24324656 | 3.42460394  | 1  | -4.68321848 | 1.18885350  | -1.50079608 |
| 1 | 2.51448154  | -2.29504657 | 4.45140409  | 1  | -3.11491847 | 0.97915345  | -2.33679605 |
| 6 | 3.12488174  | -0.04914653 | -3.69889593 | 8  | -0.04621843 | 4.07295370  | 0.03910393  |
| 1 | 4.06858158  | -0.60394657 | -3.69659591 | 6  | 1.19918156  | 4.07435369  | 0.79870391  |
| 1 | 3.35118175  | 1.01725352  | -3.58759594 | 1  | 1.64618158  | 3.07935357  | 0.73940390  |
| 1 | 2.67108154  | -0.18414654 | -4.68709612 | 6  | 2.09948158  | 5.13085365  | 0.20170394  |
| 6 | 0.86658162  | 0.28805345  | -2.76269603 | 1  | 0.95838159  | 4.30015326  | 1.84230387  |
| 1 | 0.02728158  | -0.16314654 | -2.23109603 | 1  | 5.66698122  | 0.46305346  | 0.33080393  |
| 1 | 0.57228160  | 0.35775346  | -3.81739593 | 1  | -3.05891848 | 2.91995335  | 3.14570403  |
| 1 | 1.01608157  | 1.30575347  | -2.38819599 | 1  | 3.03958154  | 5.16065359  | 0.76030391  |
| 6 | 1.84078169  | -2.03084660 | -2.94699597 | 1  | 2.32648158  | 4.90095329  | -0.84199607 |
| 1 | 2.76518154  | -2.61724663 | -2.98449588 | 1  | 1.63358164  | 6.11825323  | 0.25180393  |
| 1 | 1.34758162  | -2.11414647 | -3.92409587 |    |             |             |             |

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## MI-6



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1640789.1 (Joules/Mol)      |
|                                              | 392.15801 (Kcal/Mol)        |
| Zero-point correction=                       | 0.624944 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.666902                    |
| Thermal correction to Enthalpy=              | 0.667846                    |
| Thermal correction to Gibbs Free Energy=     | 0.547219                    |
| Sum of electronic and zero-point Energies=   | -2496.501729                |
| Sum of electronic and thermal Energies=      | -2496.459770                |
| Sum of electronic and thermal Enthalpies=    | -2496.458826                |
| Sum of electronic and thermal Free Energies= | -2496.579453                |

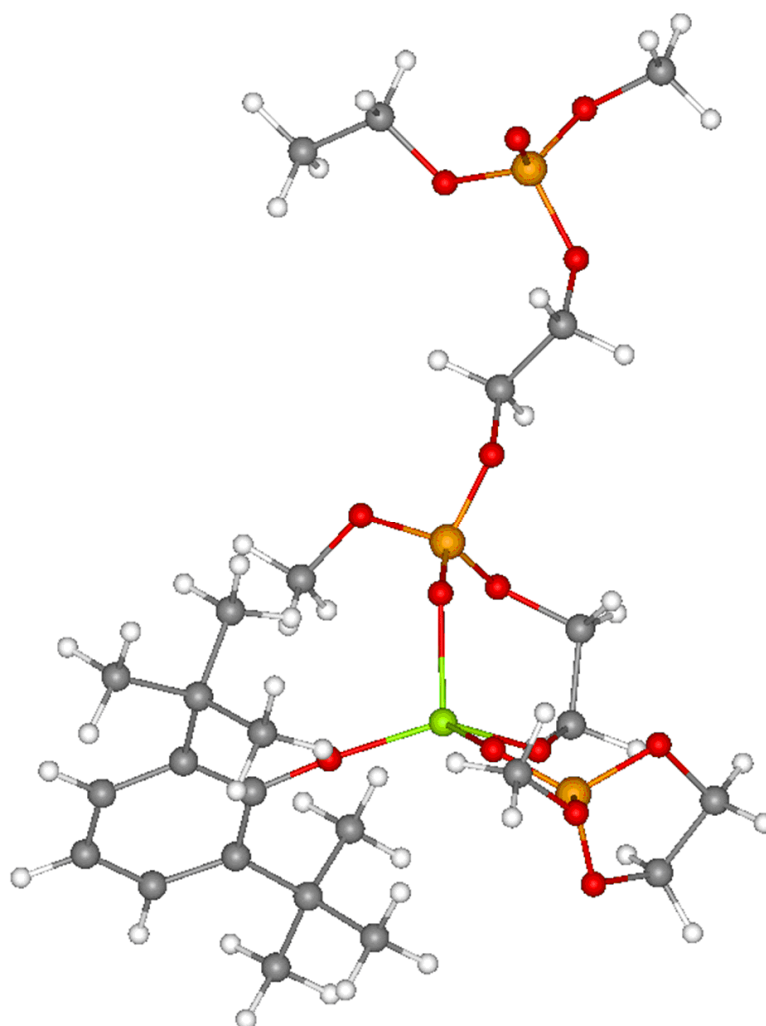
| cartesian |             |             |             |    |             |             |             |  |  |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|
| 12        | 0.32792419  | 0.15321603  | -0.32939997 | 1  | -1.56357586 | -2.55158401 | -2.89409995 |  |  |
| 8         | 2.39532423  | -2.65828395 | 2.48600006  | 1  | -1.39867580 | -0.94308400 | -2.17269993 |  |  |
| 8         | -1.50977576 | 0.15041603  | -0.04820000 | 1  | 4.07962418  | -3.88158393 | 2.27340007  |  |  |
| 6         | 3.47182417  | -3.42458391 | 3.05820012  | 8  | 1.21752417  | 2.00781608  | -0.10550000 |  |  |
| 1         | 3.00002432  | -4.19928408 | 3.66090012  | 15 | 2.55792427  | 2.29231596  | -0.71880001 |  |  |
| 1         | 4.09292412  | -2.78638411 | 3.69070005  | 8  | 2.63482428  | 2.27521610  | -2.28889990 |  |  |
| 6         | -2.80837584 | -0.01448397 | 0.15940000  | 8  | 1.37912416  | -0.30178395 | -1.85080004 |  |  |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -3.55267572 | 0.99111599  | 0.85659999  | 6  | 1.60152423  | 1.70561600  | -3.15910006 |
| 6 | -4.92207575 | 0.79411602  | 1.05550003  | 6  | 1.60942423  | 0.18651603  | -3.11529994 |
| 1 | -5.50477600 | 1.54371595  | 1.58089995  | 1  | 1.84832418  | 2.09611607  | -4.14919996 |
| 6 | -5.57787609 | -0.34428397 | 0.59869999  | 1  | 0.63342416  | 2.10621595  | -2.84189987 |
| 6 | -4.84917593 | -1.31838393 | -0.07550000 | 1  | 0.84822416  | -0.13398397 | -3.85389996 |
| 1 | -5.37657595 | -2.19988394 | -0.42499998 | 1  | 2.58452415  | -0.15688396 | -3.50749993 |
| 6 | -3.47687578 | -1.19078398 | -0.31039998 | 8  | 1.38902426  | -0.83308399 | 1.09669995  |
| 6 | -2.87497568 | 2.27051592  | 1.38090003  | 15 | 2.67802429  | -1.48658395 | 1.45280004  |
| 6 | -2.72037601 | -2.30428410 | -1.05859995 | 8  | 3.72052431  | -0.53638399 | 2.19610000  |
| 6 | -2.27767563 | 3.07681608  | 0.20999999  | 8  | 3.76062441  | 1.36761606  | -0.23480000 |
| 1 | -1.54617584 | 2.49161601  | -0.34759998 | 6  | 3.61462402  | 0.90161604  | 2.19140005  |
| 1 | -1.78447592 | 3.98381591  | 0.58350003  | 6  | 4.38662434  | 1.53541601  | 1.05349994  |
| 1 | -3.06927586 | 3.38371611  | -0.48280001 | 1  | 4.06392431  | 1.22141600  | 3.13490009  |
| 6 | -1.78247583 | 1.91681600  | 2.41059995  | 1  | 2.56322432  | 1.19961596  | 2.18420005  |
| 1 | -1.03277576 | 1.24631596  | 1.98940003  | 1  | 4.52302408  | 2.60061598  | 1.26110005  |
| 1 | -2.22597599 | 1.41851604  | 3.27979994  | 1  | 5.36592388  | 1.06441605  | 0.95530003  |
| 1 | -1.27767575 | 2.82611609  | 2.76239991  | 8  | 3.55542421  | -2.08388400 | 0.28460002  |
| 6 | -3.86347580 | 3.20691609  | 2.09829998  | 6  | 2.94192410  | -2.86038399 | -0.80320001 |
| 1 | -4.32147598 | 2.73521590  | 2.97429991  | 1  | 2.27312422  | -2.18258405 | -1.34309995 |
| 1 | -4.66397572 | 3.55251598  | 1.43519998  | 6  | 4.06262398  | -3.37028408 | -1.67799997 |
| 1 | -3.32647562 | 4.09531593  | 2.45050001  | 1  | 2.37352419  | -3.68408394 | -0.35889998 |
| 6 | -3.64277601 | -3.46428394 | -1.47659993 | 1  | -6.64487600 | -0.47118399 | 0.76660001  |
| 1 | -4.43017578 | -3.14008403 | -2.16549993 | 8  | 3.09002399  | 3.73811603  | -0.29439998 |
| 1 | -4.11527586 | -3.95138407 | -0.61680001 | 6  | 2.21732426  | 4.87691593  | -0.44679999 |
| 1 | -3.04867601 | -4.22528410 | -1.99559999 | 1  | 2.71562433  | 5.70821619  | 0.05060000  |
| 6 | -1.63917577 | -2.91938400 | -0.14690000 | 1  | 2.08842421  | 5.10631609  | -1.50740004 |
| 1 | -0.95567584 | -2.16768408 | 0.25020000  | 1  | 1.25082421  | 4.68161583  | 0.02230000  |
| 1 | -1.05347586 | -3.66908407 | -0.69449997 | 1  | 3.63502407  | -3.94048405 | -2.50810003 |
| 1 | -2.10547590 | -3.41658401 | 0.71090001  | 1  | 4.63502407  | -2.53758407 | -2.09389997 |
| 6 | -2.09967566 | -1.75688398 | -2.36019993 | 1  | 4.74272394  | -4.02448416 | -1.12500000 |
| 1 | -2.88667583 | -1.37728393 | -3.02149987 |    |             |             |             |

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## MI-4m



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 1946318.9 (Joules/Mol)      |
|                                              | 465.18137 (Kcal/Mol)        |
| Zero-point correction=                       | 0.741314 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.794161                    |
| Thermal correction to Enthalpy=              | 0.795105                    |
| Thermal correction to Gibbs Free Energy=     | 0.644976                    |
| Sum of electronic and zero-point Energies=   | -3257.067540                |
| Sum of electronic and thermal Energies=      | -3257.014693                |
| Sum of electronic and thermal Enthalpies=    | -3257.013749                |
| Sum of electronic and thermal Free Energies= | -3257.163878                |

| cartesian |             |             |             |   |             |             |             |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 12        | -1.61996853 | 0.97902334  | -0.00587332 | 1 | -0.77956855 | 1.40142334  | -3.37387323 |
| 8         | -2.48966837 | -0.67927670 | 0.14692667  | 1 | -0.67526853 | 3.14852333  | -3.15357327 |
| 6         | -3.17336845 | -1.81527662 | 0.15302669  | 8 | 1.79513144  | -1.26977670 | -0.54267329 |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | -3.89266825 | -2.23897672 | -1.01307321 | 6  | 0.80103147  | -2.18807673 | -1.07017326 |
| 6  | -4.53546858 | -3.48057675 | -0.98907334 | 1  | 0.68843150  | -2.02297664 | -2.14287329 |
| 1  | -5.07386827 | -3.82587647 | -1.86537337 | 1  | -0.15296853 | -2.05807662 | -0.55667329 |
| 6  | -4.51686859 | -4.30187702 | 0.13272668  | 1  | 1.19373155  | -3.18537664 | -0.87987334 |
| 6  | -3.86316824 | -3.86187673 | 1.27862668  | 8  | -2.39636850 | 2.32942319  | 1.29742670  |
| 1  | -3.88256836 | -4.50277710 | 2.15392685  | 15 | -2.90546846 | 3.71762323  | 1.08962679  |
| 6  | -3.19756842 | -2.63317657 | 1.33102679  | 8  | -1.78506863 | 4.77142286  | 0.63772666  |
| 6  | -3.99586821 | -1.35367668 | -2.26977324 | 8  | -3.95876837 | 3.96832323  | -0.08177331 |
| 6  | -2.53566837 | -2.18087673 | 2.64692664  | 6  | -2.19856834 | 5.47262287  | -0.55767334 |
| 6  | -4.66296864 | -0.00927672 | -1.91527343 | 6  | -3.28306866 | 4.60332298  | -1.20027328 |
| 1  | -4.13076830 | 0.51502329  | -1.12137341 | 1  | -2.57086849 | 6.45662308  | -0.25927332 |
| 1  | -4.69886827 | 0.64712328  | -2.79337335 | 1  | -1.32286859 | 5.57932329  | -1.19747329 |
| 1  | -5.69006824 | -0.17667672 | -1.57287335 | 1  | -2.85096836 | 3.81212330  | -1.81797338 |
| 6  | -2.60746861 | -1.12457669 | -2.89817333 | 1  | -4.03076839 | 5.18632317  | -1.73807335 |
| 1  | -1.92646849 | -0.62827671 | -2.20647335 | 8  | -3.63046837 | 4.26522303  | 2.38112664  |
| 1  | -2.16206837 | -2.08177662 | -3.19387317 | 6  | -3.51136875 | 3.61352324  | 3.66882682  |
| 1  | -2.69096851 | -0.49927673 | -3.79567337 | 1  | -2.64116859 | 4.01382303  | 4.19222689  |
| 6  | -4.86566830 | -1.99087667 | -3.36877322 | 1  | -3.41866875 | 2.53462338  | 3.54582667  |
| 1  | -4.44876862 | -2.93487668 | -3.73607326 | 1  | -4.42286825 | 3.86002326  | 4.21122694  |
| 1  | -5.89106846 | -2.17527676 | -3.03127337 | 8  | 2.81313133  | 0.87982333  | 0.18682668  |
| 1  | -4.92176819 | -1.30627668 | -4.22287321 | 6  | 4.10053158  | 0.58402330  | -0.39677331 |
| 6  | -2.74146843 | -3.19597673 | 3.78552675  | 1  | 4.06323147  | 0.70482326  | -1.48307323 |
| 1  | -3.80056858 | -3.36237669 | 4.00902653  | 1  | 4.37693167  | -0.44527671 | -0.15857331 |
| 1  | -2.27896833 | -4.16467714 | 3.56672668  | 6  | 5.07613182  | 1.57432330  | 0.21762668  |
| 1  | -2.27156830 | -2.81157660 | 4.69802666  | 8  | 6.37403154  | 1.36782336  | -0.36387330 |
| 6  | -1.01286852 | -2.02027678 | 2.47562671  | 1  | 4.78293180  | 2.59782338  | -0.02557332 |
| 1  | -0.76436853 | -1.26817667 | 1.72762680  | 1  | 5.11423159  | 1.46782327  | 1.30482674  |
| 1  | -0.55006856 | -1.71907663 | 3.42402673  | 15 | 7.49903154  | 0.55652332  | 0.44972667  |
| 1  | -0.56156856 | -2.97267675 | 2.17342663  | 8  | 7.27573156  | -0.93537664 | -0.07367332 |
| 6  | -3.16266870 | -0.85417664 | 3.12322664  | 8  | 8.83723068  | 0.98142326  | -0.31437331 |
| 1  | -4.22796822 | -0.99337673 | 3.33982682  | 8  | 7.48813152  | 0.75702327  | 1.91402674  |
| 1  | -2.67176867 | -0.51057673 | 4.04312658  | 6  | 9.48563099  | 2.21282315  | 0.05522668  |
| 1  | -3.07186842 | -0.07227671 | 2.36842680  | 6  | 8.03053093  | -2.01497674 | 0.53992665  |
| 1  | -5.02186823 | -5.26487684 | 0.12062668  | 6  | 7.49363136  | -3.32297659 | 0.00372668  |
| 8  | 0.33113146  | 0.64302325  | 0.47262669  | 1  | 9.08643150  | -1.88367677 | 0.28352669  |
| 15 | 1.47423148  | 0.27292329  | -0.41167331 | 1  | 7.91893148  | -1.94737673 | 1.62572670  |
| 8  | 1.32503152  | 0.73702329  | -1.92107344 | 1  | 8.90573120  | 3.06572342  | -0.30737332 |
| 8  | -1.39746857 | 2.11202335  | -1.52627325 | 1  | 9.60713100  | 2.27252316  | 1.13902664  |
| 6  | 0.91953146  | 2.09802318  | -2.29047322 | 1  | 10.46063137 | 2.19932318  | -0.43127334 |
| 6  | -0.56626856 | 2.18062329  | -2.61827326 | 1  | 8.05293179  | -4.15487671 | 0.44222668  |
| 1  | 1.17083144  | 2.78422332  | -1.47537327 | 1  | 6.43813181  | -3.44547677 | 0.26032668  |

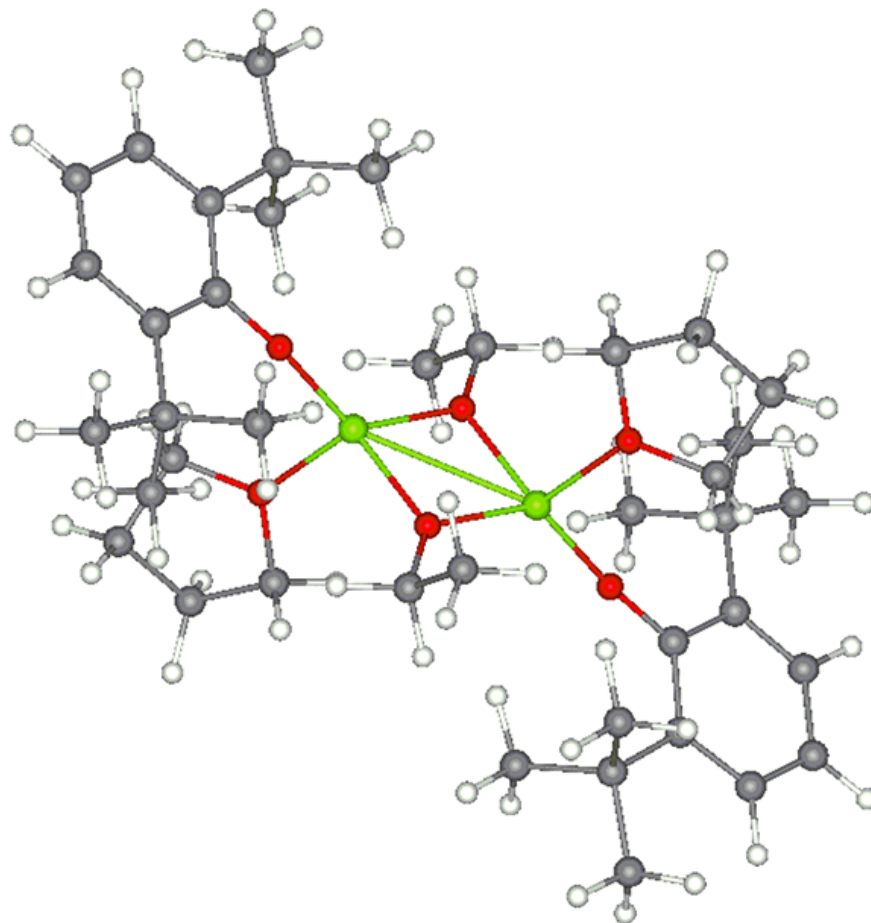
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|   |            |            |             |   |            |             |             |
|---|------------|------------|-------------|---|------------|-------------|-------------|
| 1 | 1.53243148 | 2.33222318 | -3.16547322 | 1 | 7.59763145 | -3.37157679 | -1.08317327 |
|---|------------|------------|-------------|---|------------|-------------|-------------|

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### S1.3. Molecular structures, energies and cartesian coordinates for binuclear mechanism

DI-1\_\_THF



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2688289.1 (Joules/Mol)      |
|                                              | 642.51652 (Kcal/Mol)        |
| Zero-point correction=                       | 1.023915 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.082452                    |
| Thermal correction to Enthalpy=              | 1.083396                    |
| Thermal correction to Gibbs Free Energy=     | 0.927286                    |
| Sum of electronic and zero-point Energies=   | -2415.288266                |
| Sum of electronic and thermal Energies=      | -2415.229729                |
| Sum of electronic and thermal Enthalpies=    | -2415.228785                |
| Sum of electronic and thermal Free Energies= | -2415.384895                |

| cartesian |             |             |            |                                       |
|-----------|-------------|-------------|------------|---------------------------------------|
| 12        | -1.42806900 | -0.14603621 | 0.36572510 | 6 0.01873104 -2.29913616 -2.76147485  |
| 8         | 0.03603104  | 1.16836381  | 0.59032512 | 1 -1.03836906 -2.92593622 -1.00187492 |

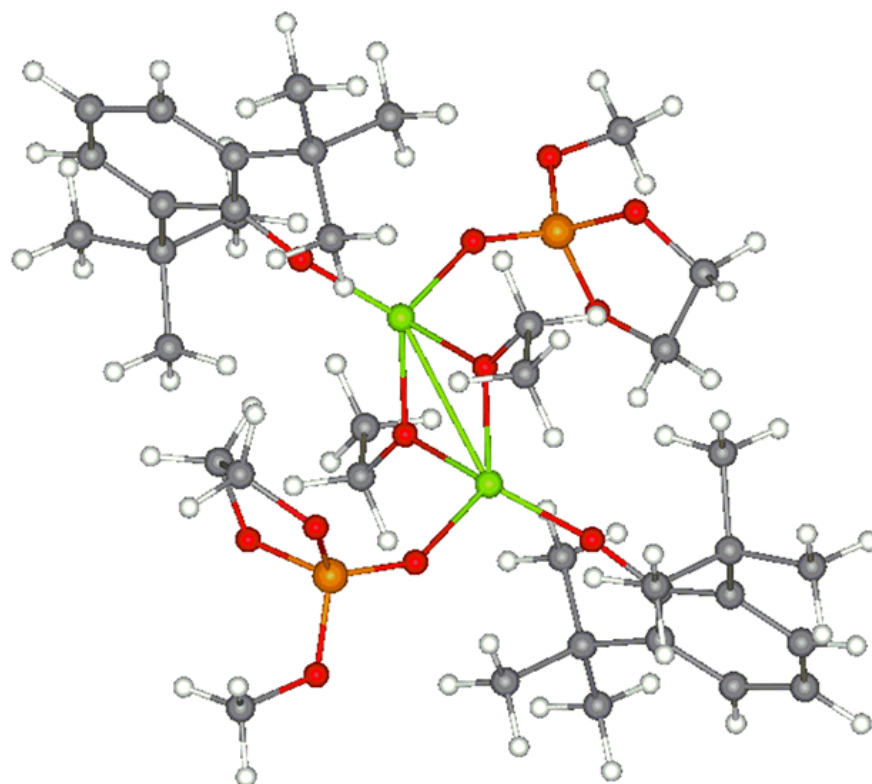
|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 8 | -3.21136904 | 0.09606380  | -0.16957490 | 6 | 2.83813095  | 1.05076373  | -3.05007505 |
| 8 | -1.64806902 | -1.07903624 | 2.21852493  | 1 | 2.81733108  | 0.13526379  | -3.65197492 |
| 6 | 0.09403104  | 2.42176366  | 1.24842501  | 1 | 3.70273089  | 1.02526379  | -2.38627505 |
| 1 | -0.71176893 | 3.06946373  | 0.87622511  | 6 | 2.72543097  | 2.29326367  | -3.91567492 |
| 6 | -0.01756896 | 2.29806376  | 2.76202512  | 1 | 3.07663107  | 3.17196369  | -3.36607504 |
| 6 | -2.84016895 | -1.05043626 | 3.04942513  | 1 | 3.30763102  | 2.20726371  | -4.83637476 |
| 1 | -2.81956911 | -0.13443621 | 3.65062499  | 6 | 1.21633101  | 2.37116385  | -4.16427469 |
| 1 | -3.70416903 | -1.02513623 | 2.38472509  | 1 | 0.92603105  | 1.68256378  | -4.96387482 |
| 6 | -2.72876906 | -2.29223633 | 3.91602492  | 1 | 0.87563103  | 3.37176371  | -4.43997478 |
| 1 | -3.07986903 | -3.17123628 | 3.36682510  | 6 | 0.62823105  | 1.92046380  | -2.82997489 |
| 1 | -3.31156898 | -2.20523620 | 4.83622551  | 1 | 0.44233105  | 2.75726366  | -2.15177488 |
| 6 | -1.21976900 | -2.37063622 | 4.16582537  | 1 | -0.28656894 | 1.33286381  | -2.93047500 |
| 1 | -0.92976892 | -1.68133628 | 4.96482515  | 6 | 4.52913094  | -0.22573622 | 0.30762509  |
| 1 | -0.87986892 | -3.37123632 | 4.44282532  | 6 | 5.16613102  | -1.48223627 | 0.04282509  |
| 6 | -0.63066894 | -1.92163622 | 2.83152509  | 6 | 6.55943108  | -1.56073630 | 0.12762509  |
| 1 | -0.44546893 | -2.75933623 | 2.15402508  | 1 | 7.06013107  | -2.49953628 | -0.08257490 |
| 1 | 0.28483105  | -1.33503628 | 2.93182492  | 6 | 7.34183121  | -0.46713620 | 0.47882509  |
| 6 | -4.52836895 | 0.22586378  | -0.30797490 | 6 | 6.71563101  | 0.73316383  | 0.79302508  |
| 6 | -5.16536903 | 1.48226380  | -0.04277491 | 1 | 7.33803082  | 1.56776381  | 1.09682500  |
| 6 | -6.55866909 | 1.56076372  | -0.12707491 | 6 | 5.32673120  | 0.88646382  | 0.73642510  |
| 1 | -7.05936909 | 2.49946380  | 0.08352509  | 6 | 4.35913086  | -2.74263620 | -0.31887490 |
| 6 | -7.34106922 | 0.46726379  | -0.47837490 | 6 | 4.69633102  | 2.22036386  | 1.18002498  |
| 6 | -6.71486902 | -0.73293620 | -0.79307491 | 6 | 3.65083098  | -2.55313635 | -1.67267501 |
| 1 | -7.33736897 | -1.56743622 | -1.09697497 | 1 | 2.97033095  | -1.70043623 | -1.65077496 |
| 6 | -5.32606888 | -0.88613617 | -0.73687488 | 1 | 3.07313108  | -3.44563627 | -1.94167495 |
| 6 | -4.35816908 | 2.74266386  | 0.31902510  | 1 | 4.38493109  | -2.37393618 | -2.46607494 |
| 6 | -4.69566917 | -2.21993613 | -1.18107498 | 6 | 3.33933091  | -3.06213617 | 0.79282510  |
| 6 | -3.64966893 | 2.55296373  | 1.67262506  | 1 | 2.65143108  | -2.23233628 | 0.96262509  |
| 1 | -2.96896911 | 1.70046377  | 1.65052509  | 1 | 3.85933089  | -3.26423621 | 1.73572505  |
| 1 | -3.07216907 | 3.44566369  | 1.94172502  | 1 | 2.75583100  | -3.95453620 | 0.53342509  |
| 1 | -4.38356924 | 2.37356377  | 2.46612501  | 6 | 5.24633121  | -3.99233627 | -0.46427491 |
| 6 | -3.33856893 | 3.06236386  | -0.79277492 | 1 | 5.79263115  | -4.21993637 | 0.45702508  |
| 1 | -2.65076900 | 2.23256373  | -0.96267492 | 1 | 5.97073078  | -3.90023613 | -1.28047502 |
| 1 | -3.85876894 | 3.26446366  | -1.73557496 | 1 | 4.61333084  | -4.85793638 | -0.69047493 |
| 1 | -2.75516891 | 3.95476365  | -0.53337491 | 6 | 5.74393082  | 3.23266387  | 1.67802501  |
| 6 | -5.24546909 | 3.99236369  | 0.46472511  | 1 | 6.45173120  | 3.52166367  | 0.89372510  |
| 1 | -5.79196882 | 4.21996355  | -0.45647490 | 1 | 6.31223106  | 2.85216379  | 2.53272510  |
| 1 | -5.96966887 | 3.90016365  | 1.28102505  | 1 | 5.23353100  | 4.14506388  | 2.00682497  |
| 1 | -4.61246920 | 4.85786390  | 0.69072509  | 6 | 3.73423100  | 1.96776378  | 2.35662508  |
| 6 | -5.74326897 | -3.23193622 | -1.67947495 | 1 | 2.95903111  | 1.24866378  | 2.08852506  |
| 1 | -6.45106888 | -3.52133632 | -0.89537489 | 1 | 3.25413108  | 2.90276384  | 2.67112494  |

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|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1  | -6.31166887 | -2.85093617 | -2.53397489 | 1 | 4.28363085  | 1.56646371  | 3.21532512  |
| 1  | -5.23296881 | -4.14423609 | -2.00897503 | 6 | 3.95703101  | 2.90366387  | 0.01412509  |
| 6  | -3.73346901 | -1.96693623 | -2.35757494 | 1 | 4.65263081  | 3.11866379  | -0.80527490 |
| 1  | -2.95826912 | -1.24803627 | -2.08917499 | 1 | 3.51943088  | 3.85596371  | 0.33962509  |
| 1  | -3.25346899 | -2.90183616 | -2.67227507 | 1 | 3.15553093  | 2.27706385  | -0.37907490 |
| 1  | -4.28286886 | -1.56523621 | -3.21617508 | 1 | 1.03943098  | 2.92456365  | 1.00232506  |
| 6  | -3.95646906 | -2.90373635 | -0.01547491 | 1 | 0.71283108  | -3.07023621 | -0.87547493 |
| 1  | -4.65216923 | -3.11903620 | 0.80392510  | 1 | 8.42443180  | -0.55493617 | 0.52772510  |
| 1  | -3.51896906 | -3.85593629 | -0.34127492 | 1 | -8.42366886 | 0.55506384  | -0.52697492 |
| 1  | -3.15486908 | -2.27743626 | 0.37802508  | 1 | 0.03763104  | 3.28666377  | 3.23242497  |
| 12 | 1.42843103  | 0.14496379  | -0.36527491 | 1 | 0.79423106  | 1.68526375  | 3.16422510  |
| 8  | -0.03576896 | -1.16943622 | -0.58967489 | 1 | -0.97036892 | 1.84336376  | 3.05122495  |
| 8  | 3.21223092  | -0.09583620 | 0.16882509  | 1 | -0.03606896 | -3.28773618 | -3.23187494 |
| 8  | 1.64693105  | 1.07846379  | -2.21807504 | 1 | 0.97143108  | -1.84403622 | -3.05037498 |
| 6  | -0.09316895 | -2.42283630 | -1.24787498 | 1 | -0.79316896 | -1.68663621 | -3.16377497 |

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# DI-1\_\_MeOEP



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2675081.6 (Joules/Mol)      |
|                                              | 639.35986 (Kcal/Mol)        |
| Zero-point correction=                       | 1.018885 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.084481                    |
| Thermal correction to Enthalpy=              | 1.085425                    |
| Thermal correction to Gibbs Free Energy=     | 0.914368                    |
| Sum of electronic and zero-point Energies=   | -3471.863116                |
| Sum of electronic and thermal Energies=      | -3471.797521                |
| Sum of electronic and thermal Enthalpies=    | -3471.796576                |
| Sum of electronic and thermal Free Energies= | -3471.967633                |

| cartesian |             |             |            |   |             |             |             |
|-----------|-------------|-------------|------------|---|-------------|-------------|-------------|
| 12        | 1.30913222  | -0.71193415 | 0.02037165 | 6 | -3.40286779 | -1.04893410 | -2.76862836 |
| 8         | -0.01356778 | -0.04133416 | 1.33867168 | 1 | -2.67326784 | -1.01683414 | -1.95792830 |
| 8         | 3.15723205  | -0.28443417 | 0.00057165 | 1 | -3.93536782 | -2.00713420 | -2.72382832 |
| 6         | 0.00703222  | -0.18383417 | 2.74797153 | 1 | -2.86396790 | -1.01273417 | -3.72282839 |
| 6         | -0.25436780 | 1.13066590  | 3.46767163 | 6 | -5.34846783 | -0.02543417 | -3.88172841 |
| 1         | 0.98243219  | -0.57623416 | 3.06357145 | 1 | -5.86476803 | -0.99103415 | -3.91022849 |
| 6         | 4.48353195  | -0.16973417 | 0.05407165 | 1 | -6.10126781 | 0.76886582  | -3.91462851 |
| 6         | 5.15363216  | 0.02506583  | 1.30797172 | 1 | -4.75396776 | 0.05166584  | -4.79932833 |

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|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 6.53503227  | 0.24236584  | 1.30877173  | 6  | -5.69296789 | 0.59256583  | 3.63967156  |
| 1  | 7.05123234  | 0.40716583  | 2.24817157  | 1  | -6.45906782 | 1.35856581  | 3.47997165  |
| 6  | 7.28723192  | 0.24826583  | 0.14047165  | 1  | -6.19336796 | -0.37173417 | 3.77937150  |
| 6  | 6.64733219  | -0.00853417 | -1.06562829 | 1  | -5.18456793 | 0.83336586  | 4.58027172  |
| 1  | 7.24953222  | -0.03903417 | -1.96722829 | 6  | -3.62816787 | -0.52353418 | 2.89657164  |
| 6  | 5.26963234  | -0.23393416 | -1.14522827 | 1  | -2.84006786 | -0.61933416 | 2.14977145  |
| 6  | 4.40493202  | -0.02913417 | 2.65157151  | 1  | -3.16486788 | -0.28733417 | 3.86207151  |
| 6  | 4.64633226  | -0.58283418 | -2.50762844 | 1  | -4.12396765 | -1.49663413 | 2.99437165  |
| 6  | 3.74173212  | -1.41073418 | 2.81947160  | 6  | -4.00776768 | 1.95346582  | 2.46017146  |
| 1  | 3.06213212  | -1.64463413 | 1.99867165  | 1  | -4.77016783 | 2.71296573  | 2.25497150  |
| 1  | 3.18223214  | -1.46113420 | 3.76187158  | 1  | -3.54336786 | 2.19726586  | 3.42347169  |
| 1  | 4.50573206  | -2.19553423 | 2.84147167  | 1  | -3.25156784 | 2.03586578  | 1.67807174  |
| 6  | 3.36593223  | 1.10276580  | 2.73927164  | 1  | -0.73936778 | -0.92753416 | 3.05957150  |
| 1  | 2.61733222  | 1.03336585  | 1.94967175  | 1  | 0.73003221  | 0.91096586  | -3.00442839 |
| 1  | 3.86223221  | 2.07666588  | 2.65467167  | 1  | -8.37666798 | -0.35033417 | -0.19942835 |
| 1  | 2.84853220  | 1.07836580  | 3.70567155  | 1  | 8.35953236  | 0.42566583  | 0.17257164  |
| 6  | 5.34033203  | 0.14926584  | 3.86147165  | 8  | -1.05396771 | 2.72506595  | 0.02147165  |
| 1  | 5.83383226  | 1.12716579  | 3.86707163  | 15 | -0.06146779 | 3.81826591  | -0.11572835 |
| 1  | 6.11133194  | -0.62673414 | 3.91017151  | 8  | 0.55123222  | 3.99366593  | -1.59012830 |
| 1  | 4.75013208  | 0.07946583  | 4.78227186  | 8  | 1.31963229  | 3.69346595  | 0.68807161  |
| 6  | 5.68353224  | -0.64013416 | -3.64372849 | 6  | 1.99873221  | 3.93266582  | -1.57062829 |
| 1  | 6.45333195  | -1.39863420 | -3.46762848 | 6  | 2.38493204  | 3.31316590  | -0.22282836 |
| 1  | 6.17963219  | 0.32306585  | -3.80502844 | 1  | 2.37843204  | 4.95176554  | -1.68392825 |
| 1  | 5.17553234  | -0.90433419 | -4.57832813 | 1  | 2.31843209  | 3.32106590  | -2.41332841 |
| 6  | 3.61733222  | 0.48626584  | -2.91662836 | 1  | 2.45043206  | 2.22346592  | -0.26042834 |
| 1  | 2.83643222  | 0.59006584  | -2.16262841 | 1  | 3.31423211  | 3.71686578  | 0.17667164  |
| 1  | 3.14723206  | 0.23256584  | -3.87452841 | 8  | -0.74676782 | 5.16576576  | 0.34077165  |
| 1  | 4.11703205  | 1.45586586  | -3.03512836 | 8  | 1.05843222  | -2.73043418 | 0.11127165  |
| 6  | 4.00153208  | -1.98103416 | -2.43532848 | 15 | 0.09373222  | -3.83783412 | 0.31507167  |
| 1  | 4.76523209  | -2.73483419 | -2.21502852 | 8  | -0.74266779 | -4.25463438 | -0.99172837 |
| 1  | 3.53693223  | -2.24513412 | -3.39312840 | 8  | -1.14436769 | -3.58913422 | 1.30367172  |
| 1  | 3.24643207  | -2.04523420 | -1.65052831 | 6  | -2.16866779 | -4.21113443 | -0.73752838 |
| 12 | -1.31636775 | 0.70706582  | 0.05097165  | 6  | -2.34806776 | -3.36133409 | 0.52327162  |
| 8  | 0.00533222  | 0.03196584  | -1.27792835 | 1  | -2.51766777 | -5.23823452 | -0.59942836 |
| 8  | -3.16586781 | 0.29086584  | -0.01622835 | 1  | -2.64946795 | -3.76743412 | -1.60802829 |
| 6  | -0.01846778 | 0.17076585  | -2.68612838 | 1  | -2.43466783 | -2.29503417 | 0.30247167  |
| 6  | 0.24133222  | -1.14353418 | -3.40672851 | 1  | -3.19526792 | -3.67723417 | 1.13047171  |
| 1  | -0.99156779 | 0.56746584  | -3.00202847 | 8  | 0.88283223  | -5.09203434 | 0.86087161  |
| 6  | -4.49326801 | 0.19376583  | -0.06672835 | 6  | 0.21763222  | -6.34773445 | 1.09967172  |
| 6  | -5.16646767 | 0.03756583  | -1.32452834 | 6  | -0.03906778 | 6.42006540  | 0.29867166  |
| 6  | -6.55066776 | -0.16163416 | -1.33212829 | 1  | 0.84633219  | 6.37866545  | 0.93707162  |

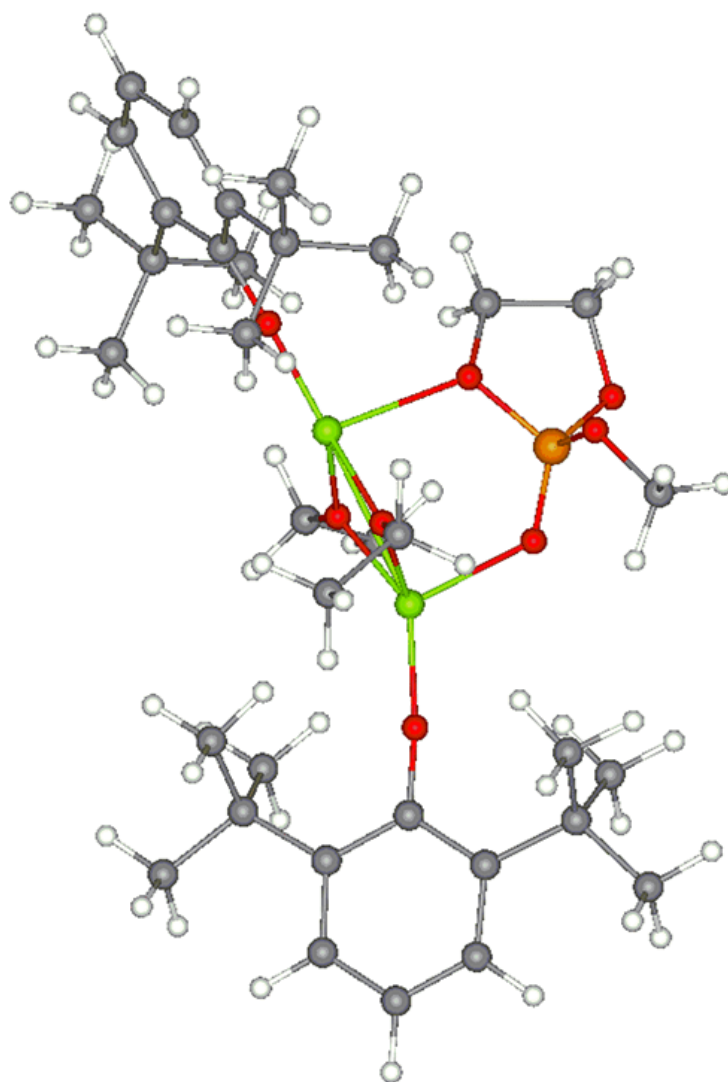
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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | -7.06866789 | -0.29603416 | -2.27532840 | 1 | 0.23433222  | 6.66556549  | -0.73042840 |
| 6 | -7.30216789 | -0.18743417 | -0.16392836 | 1 | -0.59516782 | -6.21803427 | 1.81797171  |
| 6 | -6.65846777 | 0.03116583  | 1.04787171  | 1 | -0.15646778 | -6.75983429 | 0.15947165  |
| 1 | -7.26036787 | 0.04576584  | 1.94997168  | 1 | -0.73506778 | 7.16516542  | 0.68017161  |
| 6 | -5.27836800 | 0.23886584  | 1.13417172  | 1 | 0.97523218  | -7.00993443 | 1.51527166  |
| 6 | -4.41426802 | 0.10686583  | -2.66502833 | 1 | -0.22116777 | 0.98806584  | 4.55457163  |
| 6 | -4.65376806 | 0.55456585  | 2.50417161  | 1 | 0.49613219  | 1.87826586  | 3.19547153  |
| 6 | -3.71716785 | 1.47476590  | -2.80382848 | 1 | -1.24066770 | 1.52806580  | 3.21197152  |
| 1 | -3.03536797 | 1.67536581  | -1.97642827 | 1 | 0.21223222  | -0.99973416 | -4.49342823 |
| 1 | -3.15406775 | 1.53096581  | -3.74382854 | 1 | 1.22393227  | -1.54663420 | -3.14692855 |
| 1 | -4.46346807 | 2.27656579  | -2.81272840 | 1 | -0.51176780 | -1.89043415 | -3.13972855 |

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# DI-1i



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2364823.6 (Joules/Mol)      |
|                                              | 565.20640 (Kcal/Mol)        |
| Zero-point correction=                       | 0.900714 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.957068                    |
| Thermal correction to Enthalpy=              | 0.958012                    |
| Thermal correction to Gibbs Free Energy=     | 0.805897                    |
| Sum of electronic and zero-point Energies=   | -2711.281411                |
| Sum of electronic and thermal Energies=      | -2711.225057                |
| Sum of electronic and thermal Enthalpies=    | -2711.224113                |
| Sum of electronic and thermal Free Energies= | -2711.376228                |

| cartesian |             |             |             |   |            |             |             |
|-----------|-------------|-------------|-------------|---|------------|-------------|-------------|
| 12        | -1.53715086 | -0.19066104 | 0.44635624  | 6 | 5.12244892 | -0.28676105 | -1.44454384 |
| 8         | -0.17965086 | -0.73596108 | -0.91764373 | 6 | 4.52864885 | 2.30383897  | 1.41315627  |

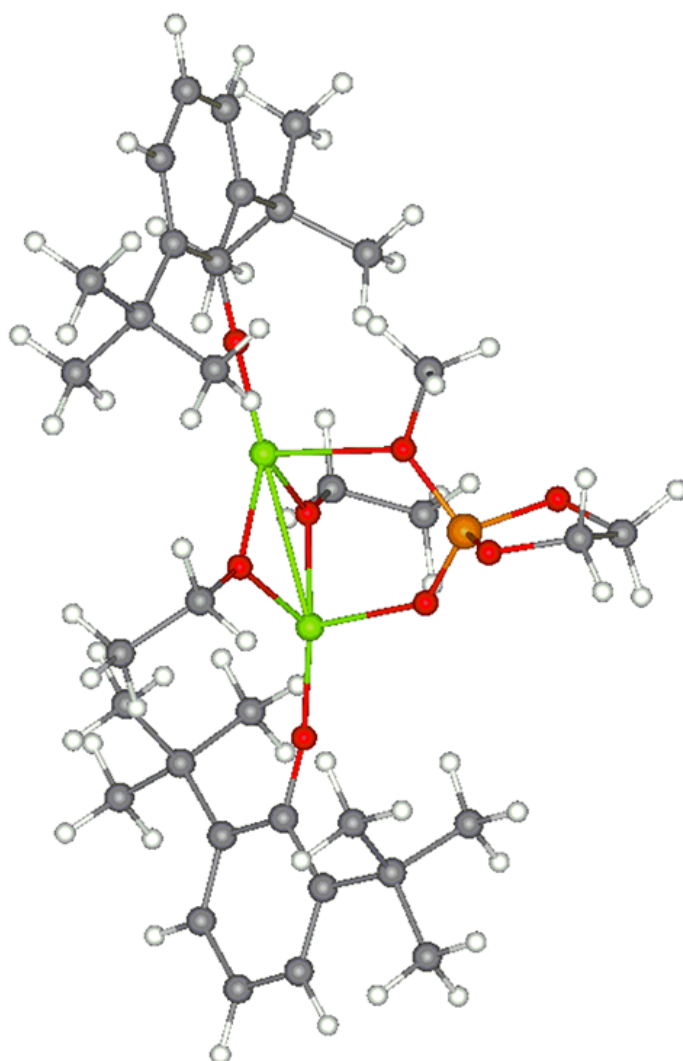
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 8  | -3.31445074 | 0.27383897  | 0.19815625  | 6  | 4.36644888  | -1.27856112 | -2.34914374 |
| 6  | -0.35385084 | -1.41176105 | -2.15344381 | 6  | 3.41214919  | 3.16133904  | 0.78435624  |
| 1  | -1.09515083 | -2.21546102 | -2.03004384 | 1  | 2.65494919  | 2.54983902  | 0.29105625  |
| 1  | 0.58754909  | -1.89786112 | -2.44104385 | 1  | 2.91724920  | 3.77403903  | 1.54755616  |
| 6  | -4.52105093 | 0.66743898  | -0.20584375 | 1  | 3.83174920  | 3.83653927  | 0.03125625  |
| 6  | -5.57645082 | -0.29016104 | -0.33964375 | 6  | 3.97184920  | 1.42313898  | 2.54805613  |
| 6  | -6.82755089 | 0.14883897  | -0.78334373 | 1  | 3.23244929  | 0.71573901  | 2.16875625  |
| 1  | -7.64025116 | -0.56056106 | -0.89674371 | 1  | 4.78014898  | 0.85033894  | 3.01715612  |
| 6  | -7.07565117 | 1.48133898  | -1.09064364 | 1  | 3.50144935  | 2.03923893  | 3.32415628  |
| 6  | -6.05185080 | 2.40933895  | -0.94064373 | 6  | 5.51264906  | 3.28713894  | 2.07165623  |
| 1  | -6.26545095 | 3.44653916  | -1.17494369 | 1  | 6.32874918  | 2.77493906  | 2.59225631  |
| 6  | -4.77585077 | 2.04543900  | -0.49944377 | 1  | 5.94854879  | 3.98363924  | 1.34815621  |
| 6  | -5.36645079 | -1.77966106 | -0.01074374 | 1  | 4.97704887  | 3.88613892  | 2.81665611  |
| 6  | -3.69885087 | 3.13143897  | -0.31864375 | 6  | 5.28444910  | -1.94336104 | -3.39094377 |
| 6  | -4.94545078 | -1.95436108 | 1.46215630  | 1  | 5.74324894  | -1.21376109 | -4.06584358 |
| 1  | -4.03635120 | -1.40006101 | 1.69405627  | 1  | 6.08204889  | -2.53276086 | -2.92654371 |
| 1  | -4.77195120 | -3.01426101 | 1.68875623  | 1  | 4.69204903  | -2.62826085 | -4.00814390 |
| 1  | -5.73875093 | -1.59566104 | 2.12695622  | 6  | 3.75484920  | -2.42566085 | -1.52154374 |
| 6  | -4.31245089 | -2.38796091 | -0.95614380 | 1  | 3.05824924  | -2.06076097 | -0.76604372 |
| 1  | -3.34965086 | -1.88276112 | -0.86094373 | 1  | 3.21744919  | -3.12696099 | -2.17194390 |
| 1  | -4.63375092 | -2.29776096 | -1.99944377 | 1  | 4.54464912  | -2.98556089 | -1.00744367 |
| 1  | -4.17565107 | -3.45546103 | -0.73814374 | 6  | 3.27674913  | -0.53326106 | -3.14514375 |
| 6  | -6.64785099 | -2.61146092 | -0.20064375 | 1  | 3.73084927  | 0.22183895  | -3.79524374 |
| 1  | -7.00515079 | -2.59866095 | -1.23584366 | 1  | 2.71364927  | -1.22906113 | -3.77864385 |
| 1  | -7.46115112 | -2.27136087 | 0.44865626  | 1  | 2.57264924  | -0.01586103 | -2.49064374 |
| 1  | -6.44105101 | -3.65616107 | 0.05925625  | 6  | -0.81225085 | -0.47856104 | -3.26314378 |
| 6  | -4.21645117 | 4.53983927  | -0.66474372 | 1  | -0.40685084 | 2.63773894  | 2.00075626  |
| 1  | -5.05685091 | 4.84073925  | -0.03064375 | 1  | 8.28434944  | 0.96573889  | -1.06494379 |
| 1  | -4.52645111 | 4.62363911  | -1.71184373 | 1  | -8.05775070 | 1.79433894  | -1.43654370 |
| 1  | -3.41195083 | 5.26663923  | -0.50514376 | 8  | -1.25385094 | -1.99466109 | 1.50055623  |
| 6  | -2.49695086 | 2.87773895  | -1.24914384 | 15 | 0.01494915  | -2.76476097 | 1.51195621  |
| 1  | -2.04225087 | 1.90003884  | -1.08334374 | 8  | 0.37964916  | -3.36796093 | 2.95295620  |
| 1  | -1.72415090 | 3.64173913  | -1.09974384 | 8  | 1.40494907  | -1.96146107 | 1.26355624  |
| 1  | -2.81105065 | 2.91653895  | -2.29784369 | 6  | 1.81864917  | -3.41746092 | 3.08755612  |
| 6  | -3.25315070 | 3.18333912  | 1.15545630  | 6  | 2.32724929  | -2.16396093 | 2.37945628  |
| 1  | -4.09885120 | 3.45003915  | 1.79855633  | 1  | 2.19124913  | -4.33436108 | 2.62245607  |
| 1  | -2.47075081 | 3.93933916  | 1.29595613  | 1  | 2.04864931  | -3.41826105 | 4.15235615  |
| 1  | -2.87325072 | 2.21873903  | 1.49435616  | 1  | 2.27114916  | -1.28076112 | 3.01685619  |
| 12 | 1.34864914  | 0.00073896  | 0.04135625  | 1  | 3.32634926  | -2.26916099 | 1.95945621  |
| 8  | 0.01224915  | 0.76453900  | 1.24505615  | 8  | 0.10874915  | -3.92876101 | 0.44905624  |
| 8  | 3.16774917  | 0.25973895  | -0.16424376 | 6  | -1.05735087 | -4.71406078 | 0.09075625  |

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 0.05474915  | 1.69343889  | 2.31655622  | 1 | -1.27355087 | -5.42966080 | 0.88685626  |
| 6 | -0.65445089 | 1.17413890  | 3.55945611  | 1 | -1.91375089 | -4.06316090 | -0.08424374 |
| 1 | 1.09864914  | 1.92273891  | 2.56345630  | 1 | -0.78675079 | -5.23886108 | -0.82344377 |
| 6 | 4.46224880  | 0.46213898  | -0.41944373 | 1 | -0.93795085 | -1.03156102 | -4.20094395 |
| 6 | 5.19844913  | 1.42733896  | 0.33815625  | 1 | -1.77015090 | -0.01446104 | -3.01054382 |
| 6 | 6.56464911  | 1.57773888  | 0.08155625  | 1 | -0.07885085 | 0.31603897  | -3.43234372 |
| 1 | 7.14334917  | 2.29913902  | 0.64785624  | 1 | -0.60375082 | 1.91363895  | 4.36635637  |
| 6 | 7.22024918  | 0.82963896  | -0.88874376 | 1 | -1.71325088 | 0.97433889  | 3.36125612  |
| 6 | 6.49204922  | -0.08326104 | -1.64204383 | 1 | -0.19765085 | 0.24553895  | 3.91815615  |
| 1 | 7.01514912  | -0.64526105 | -2.40784383 |   |             |             |             |

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# DI-1ic



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2366047.4 (Joules/Mol)      |
|                                              | 565.49889 (Kcal/Mol)        |
| Zero-point correction=                       | 0.901180 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.957280                    |
| Thermal correction to Enthalpy=              | 0.958224                    |
| Thermal correction to Gibbs Free Energy=     | 0.807264                    |
| Sum of electronic and zero-point Energies=   | -2711.280121                |
| Sum of electronic and thermal Energies=      | -2711.224021                |
| Sum of electronic and thermal Enthalpies=    | -2711.223077                |
| Sum of electronic and thermal Free Energies= | -2711.374037                |

| cartesian |            |             |             |   |             |             |             |  |
|-----------|------------|-------------|-------------|---|-------------|-------------|-------------|--|
| 12        | 1.52467597 | 0.06705249  | 0.21460950  | 6 | -5.11182404 | -0.38324749 | -1.56039047 |  |
| 8         | 0.17317595 | 0.01075250  | -1.24539042 | 6 | -4.61352396 | -1.34754753 | 2.18950939  |  |
| 8         | 3.34497595 | -0.27924752 | 0.20350951  | 6 | -4.30862427 | -0.12024750 | -2.84899068 |  |

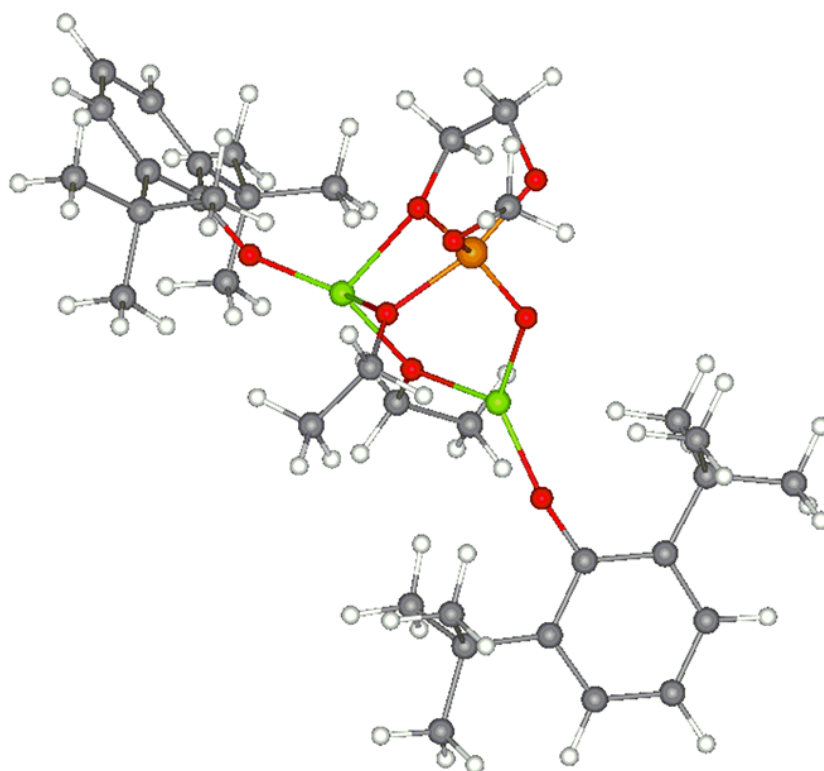
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 0.33267596  | 0.30885249  | -2.62329054 | 6  | -3.70272422 | -2.57654738 | 1.99640954  |
| 1  | 0.87357593  | 1.26075244  | -2.73409057 | 1  | -2.91302419 | -2.39134741 | 1.26590955  |
| 1  | -0.65252405 | 0.45345247  | -3.08449054 | 1  | -3.23452425 | -2.86284733 | 2.94590950  |
| 6  | 4.59787607  | -0.61624748 | -0.09199050 | 1  | -4.28762436 | -3.43104744 | 1.64010954  |
| 6  | 5.53377581  | 0.38925248  | -0.49429053 | 6  | -3.82002425 | -0.17344750 | 2.79490948  |
| 6  | 6.83617592  | -0.00214751 | -0.81969053 | 1  | -3.00032425 | 0.14375249  | 2.14830947  |
| 1  | 7.56147575  | 0.74115252  | -1.13349044 | 1  | -4.47652435 | 0.68885249  | 2.95910954  |
| 6  | 7.24637604  | -1.32894754 | -0.75409049 | 1  | -3.39312410 | -0.45714748 | 3.76440954  |
| 6  | 6.33897591  | -2.29634738 | -0.33739051 | 6  | -5.66132402 | -1.74434757 | 3.24560952  |
| 1  | 6.67997599  | -3.32444739 | -0.27849051 | 1  | -6.33592415 | -0.91804749 | 3.49470949  |
| 6  | 5.02067566  | -1.98044765 | 0.00490950  | 1  | -6.26612425 | -2.59974742 | 2.92830944  |
| 6  | 5.14297581  | 1.87765241  | -0.56529051 | 1  | -5.14892435 | -2.03424740 | 4.16970968  |
| 6  | 4.07157564  | -3.09154749 | 0.49240950  | 6  | -5.21332407 | 0.01195249  | -4.08779049 |
| 6  | 4.67717600  | 2.37255263  | 0.81910950  | 1  | -5.80782413 | -0.89044744 | -4.26329041 |
| 1  | 3.83407593  | 1.79235244  | 1.19370949  | 1  | -5.89482403 | 0.86665249  | -4.01969051 |
| 1  | 4.37787580  | 3.42765260  | 0.76690948  | 1  | -4.58782434 | 0.16625249  | -4.97399044 |
| 1  | 5.49467564  | 2.29025269  | 1.54400957  | 6  | -3.52422404 | 1.20175242  | -2.74579048 |
| 6  | 4.04457569  | 2.09685254  | -1.62449050 | 1  | -2.79482412 | 1.17825246  | -1.93449044 |
| 1  | 3.15737581  | 1.49685240  | -1.41969049 | 1  | -2.98552418 | 1.40635240  | -3.67889047 |
| 1  | 4.41157579  | 1.81775248  | -2.61809063 | 1  | -4.20862436 | 2.03835249  | -2.56399059 |
| 1  | 3.74297595  | 3.15125251  | -1.65769041 | 6  | -3.35692406 | -1.30004752 | -3.13149047 |
| 6  | 6.32347584  | 2.77585268  | -0.97629052 | 1  | -3.92992425 | -2.21874738 | -3.29549050 |
| 1  | 6.70217609  | 2.53525257  | -1.97539055 | 1  | -2.76242423 | -1.10914755 | -4.03279018 |
| 1  | 7.15627575  | 2.71345258  | -0.26789051 | 1  | -2.67342424 | -1.48454750 | -2.30099058 |
| 1  | 5.99097586  | 3.82025266  | -0.99779052 | 6  | 1.08127594  | -0.78944749 | -3.36279058 |
| 6  | 4.75987577  | -4.46694756 | 0.55940950  | 1  | 0.57927591  | -2.18714738 | 2.58670950  |
| 1  | 5.61097574  | -4.47184753 | 1.24840951  | 1  | -8.36662388 | -0.72994751 | -0.56499052 |
| 1  | 5.10797596  | -4.80604744 | -0.42199051 | 1  | 8.26487541  | -1.60464752 | -1.01649046 |
| 1  | 4.04167604  | -5.21054745 | 0.92340946  | 8  | 1.09737599  | 2.05625248  | 0.70340949  |
| 6  | 2.87877584  | -3.25544739 | -0.46979052 | 15 | -0.10492406 | 2.90775251  | 0.81180948  |
| 1  | 2.31277585  | -2.33054733 | -0.58859050 | 8  | -0.12342405 | 4.18545246  | -0.15859050 |
| 1  | 2.19177580  | -4.02944756 | -0.10609050 | 8  | -0.33032405 | 3.68285251  | 2.20020938  |
| 1  | 3.22717595  | -3.55404735 | -1.46439040 | 6  | -0.26242405 | 5.41575241  | 0.58820951  |
| 6  | 3.58357596  | -2.77824736 | 1.92070961  | 6  | 0.07187594  | 5.06345272  | 2.04200959  |
| 1  | 4.43057585  | -2.75594735 | 2.61520934  | 1  | -1.29042399 | 5.76835251  | 0.47380948  |
| 1  | 2.88437581  | -3.54984736 | 2.26650953  | 1  | 0.42847595  | 6.14405251  | 0.16290951  |
| 1  | 3.08847594  | -1.80784750 | 1.97240961  | 1  | 1.14157593  | 5.14135265  | 2.25170946  |
| 12 | -1.31592405 | -0.28834748 | -0.03959050 | 1  | -0.49222404 | 5.65485239  | 2.76250935  |
| 8  | 0.03207594  | -0.66944748 | 1.30520952  | 8  | -1.43102407 | 2.05145240  | 0.55740947  |
| 8  | -3.14812422 | -0.48784751 | -0.19089049 | 6  | -2.74202418 | 2.70165253  | 0.59600949  |
| 6  | 0.02657594  | -1.23834753 | 2.60370946  | 1  | -2.89852405 | 3.13125253  | 1.58600950  |

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 0.63997591  | -0.31294751 | 3.64520955  | 1 | -2.78802419 | 3.45945263  | -0.18739049 |
| 1 | -1.00352407 | -1.47874761 | 2.89550948  | 1 | -3.46252418 | 1.91085243  | 0.40060949  |
| 6 | -4.47272396 | -0.60904747 | -0.30029050 | 1 | 1.18637598  | -0.53414750 | -4.42349052 |
| 6 | -5.25702429 | -0.95814747 | 0.84420949  | 1 | 2.08387589  | -0.93034750 | -2.94789052 |
| 6 | -6.64932394 | -0.98304754 | 0.71230948  | 1 | 0.54397595  | -1.74004757 | -3.28959060 |
| 1 | -7.26832390 | -1.22934759 | 1.56790960  | 1 | 0.63597590  | -0.79174751 | 4.63090944  |
| 6 | -7.28192425 | -0.70744747 | -0.49409050 | 1 | 1.67967594  | -0.07164751 | 3.39840937  |
| 6 | -6.50842428 | -0.42984748 | -1.61489046 | 1 | 0.07877594  | 0.62425250  | 3.71930933  |
| 1 | -7.01802397 | -0.24984752 | -2.55499053 |   |             |             |             |

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## DTS-12i



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2366483.8 (Joules/Mol)      |
|                                              | 565.60320 (Kcal/Mol)        |
| Zero-point correction=                       | 0.901346 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.956081                    |
| Thermal correction to Enthalpy=              | 0.957025                    |
| Thermal correction to Gibbs Free Energy=     | 0.811222                    |
| Sum of electronic and zero-point Energies=   | -2711.264133                |
| Sum of electronic and thermal Energies=      | -2711.209397                |
| Sum of electronic and thermal Enthalpies=    | -2711.208453                |
| Sum of electronic and thermal Free Energies= | -2711.354256                |

| cartesian |             |             |             |   |             |             |             |  |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|--|
| 12        | 1.75231040  | 0.47863626  | 0.28072289  | 6 | -5.41218948 | -0.29436374 | -0.87317711 |  |
| 8         | -0.57038957 | 1.40593624  | -1.21627712 | 6 | -4.15588951 | -1.87606382 | 2.46162271  |  |
| 8         | 3.46151042  | -0.04436372 | -0.14227712 | 6 | -4.91578913 | 0.10103627  | -2.27727723 |  |
| 6         | -0.04518957 | 1.38343620  | -2.55817723 | 6 | -3.42378950 | -3.08866382 | 1.85122287  |  |
| 1         | 0.99171042  | 1.73903620  | -2.54127717 | 1 | -2.84558964 | -2.81056380 | 0.96902287  |  |
| 1         | -0.62808961 | 2.07803631  | -3.16717720 | 1 | -2.75088954 | -3.54506373 | 2.58832288  |  |
| 6         | 4.72651052  | -0.46066374 | -0.05547711 | 1 | -4.14968920 | -3.85016394 | 1.54692292  |  |
| 6         | 5.62621069  | 0.14513627  | 0.87572289  | 6 | -3.15218949 | -0.86546373 | 3.04952288  |  |
| 6         | 6.92291069  | -0.37016374 | 0.97422290  | 1 | -2.48698950 | -0.45606375 | 2.28612280  |  |

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|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1  | 7.62271070  | 0.06103627  | 1.68192291  | 1  | -3.68078971 | -0.02736373 | 3.51682281  |
| 6  | 7.35921049  | -1.42626369 | 0.18282288  | 1  | -2.52708960 | -1.33976376 | 3.81572270  |
| 6  | 6.49321079  | -1.96936369 | -0.75977713 | 6  | -4.96518946 | -2.41196370 | 3.65692282  |
| 1  | 6.86071062  | -2.77316380 | -1.38847709 | 1  | -5.48438931 | -1.61706376 | 4.20302296  |
| 6  | 5.18301058  | -1.50696373 | -0.91497707 | 1  | -5.70418930 | -3.15886378 | 3.35012269  |
| 6  | 5.21791077  | 1.35833621  | 1.73412287  | 1  | -4.28428936 | -2.89986372 | 4.36352301  |
| 6  | 4.28351068  | -2.10226369 | -2.01497722 | 6  | -6.07358932 | 0.39373627  | -3.24937725 |
| 6  | 4.10191059  | 0.98553628  | 2.72952271  | 1  | -6.74448919 | -0.46416372 | -3.36037731 |
| 1  | 4.44841051  | 0.21903628  | 3.43062282  | 1  | -6.66908932 | 1.26113629  | -2.94537711 |
| 1  | 3.21881032  | 0.57313627  | 2.23392272  | 1  | -5.66168928 | 0.61753625  | -4.23987722 |
| 1  | 3.78341031  | 1.86123621  | 3.30672288  | 6  | -4.07048941 | 1.38693631  | -2.21547723 |
| 6  | 4.78131056  | 2.52853632  | 0.82822287  | 1  | -3.19548965 | 1.28353631  | -1.57307708 |
| 1  | 3.96961045  | 2.25513625  | 0.15402290  | 1  | -3.71838951 | 1.66793621  | -3.21587729 |
| 1  | 5.62491083  | 2.85953617  | 0.21292290  | 1  | -4.66648912 | 2.21863627  | -1.82407713 |
| 1  | 4.44871044  | 3.38003635  | 1.43352294  | 6  | -4.11318922 | -1.05816376 | -2.90277719 |
| 6  | 6.38191080  | 1.88863623  | 2.59192276  | 1  | -4.75848913 | -1.93136382 | -3.04727721 |
| 1  | 7.23161077  | 2.20563626  | 1.97902286  | 1  | -3.72278953 | -0.76656371 | -3.88597727 |
| 1  | 6.73691082  | 1.15113628  | 3.31952286  | 1  | -3.28138971 | -1.36786377 | -2.26827717 |
| 1  | 6.04261065  | 2.76453614  | 3.15622282  | 6  | -0.12528957 | -0.02526373 | -3.11237717 |
| 6  | 5.01021051  | -3.17306376 | -2.84807730 | 1  | 0.44531044  | -2.68976378 | 0.51752287  |
| 1  | 5.31401062  | -4.03476381 | -2.24417710 | 1  | -8.36318970 | -0.56996375 | 0.83802289  |
| 1  | 5.89771080  | -2.77486372 | -3.35067725 | 1  | 8.37121010  | -1.80996370 | 0.28622290  |
| 1  | 4.33451080  | -3.54446363 | -3.62667727 | 8  | 1.19021046  | 2.33393621  | 0.22612289  |
| 6  | 3.85551047  | -0.99316370 | -2.99797726 | 15 | -0.23178956 | 2.80253625  | -0.09297711 |
| 1  | 3.33201051  | -0.18406372 | -2.48517728 | 8  | -0.31308958 | 4.04283619  | 1.04792285  |
| 1  | 3.19811034  | -1.40286374 | -3.77537727 | 8  | -1.53658962 | 2.03883624  | 0.70112288  |
| 1  | 4.73241043  | -0.56226373 | -3.49277711 | 6  | -1.55978954 | 4.13223648  | 1.70732296  |
| 6  | 3.04421043  | -2.78826380 | -1.40857708 | 6  | -1.98488963 | 2.68753624  | 1.90572286  |
| 1  | 3.34191036  | -3.59306383 | -0.72767711 | 1  | -2.29528952 | 4.67903614  | 1.10042286  |
| 1  | 2.42411041  | -3.22846365 | -2.19937730 | 1  | -1.41858959 | 4.65503645  | 2.65542269  |
| 1  | 2.43161035  | -2.08286381 | -0.84547710 | 1  | -1.48088956 | 2.22813630  | 2.76002288  |
| 12 | -1.52888954 | 0.06923628  | -0.03017711 | 1  | -3.06358957 | 2.54503632  | 1.97562289  |
| 8  | 0.18191044  | -0.63746375 | 0.65862292  | 8  | -0.46798956 | 3.75763631  | -1.37417710 |
| 8  | -3.19758964 | -0.73576373 | -0.04947711 | 6  | -0.10918957 | 5.15203619  | -1.37267709 |
| 6  | 0.28071043  | -1.92456365 | 1.28712285  | 1  | -0.82418960 | 5.73713636  | -0.79257709 |
| 6  | 1.39791036  | -1.97996378 | 2.31382275  | 1  | 0.89571041  | 5.29903603  | -0.97387713 |
| 1  | -0.67258960 | -2.15796375 | 1.77362287  | 1  | -0.14268957 | 5.45683622  | -2.41947722 |
| 6  | -4.52058935 | -0.74016374 | 0.15292290  | 1  | 0.27571043  | -0.03946371 | -4.13047743 |
| 6  | -5.05068922 | -1.22246373 | 1.39112294  | 1  | 0.46191043  | -0.73376375 | -2.51967716 |
| 6  | -6.42988920 | -1.13516378 | 1.60562289  | 1  | -1.16118956 | -0.37426376 | -3.16047716 |
| 1  | -6.85288954 | -1.47616374 | 2.54432273  | 1  | 1.43261039  | -2.96886373 | 2.78332281  |

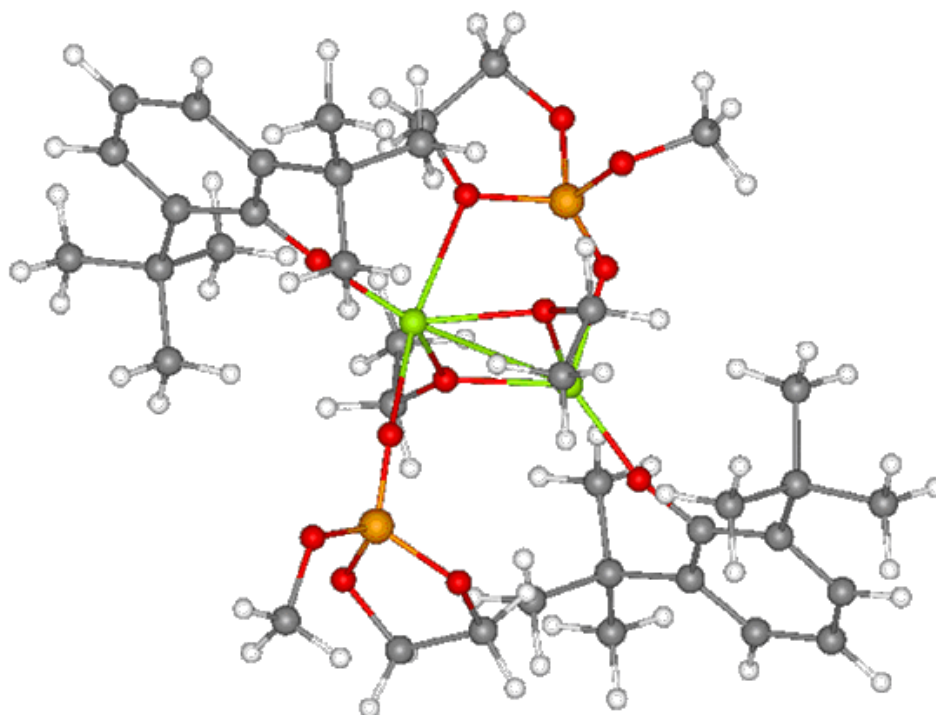
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|   |             |             |             |   |            |             |            |
|---|-------------|-------------|-------------|---|------------|-------------|------------|
| 6 | -7.29548931 | -0.63056374 | 0.64252287  | 1 | 2.37761045 | -1.80766368 | 1.85382295 |
| 6 | -6.78028917 | -0.23926373 | -0.58747709 | 1 | 1.24101043 | -1.23866379 | 3.10502267 |
| 1 | -7.47438955 | 0.11263628  | -1.34287715 |   |            |             |            |

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## DTS-12



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2677084.1 (Joules/Mol)      |
|                                              | 639.83845 (Kcal/Mol)        |
| Zero-point correction=                       | 1.019647 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.083697                    |
| Thermal correction to Enthalpy=              | 1.084641                    |
| Thermal correction to Gibbs Free Energy=     | 0.919498                    |
| Sum of electronic and zero-point Energies=   | -3471.846660                |
| Sum of electronic and thermal Energies=      | -3471.782610                |
| Sum of electronic and thermal Enthalpies=    | -3471.781666                |
| Sum of electronic and thermal Free Energies= | -3471.946809                |

| cartesian |             |             |             |   |             |             |             |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 12        | 1.60025001  | -0.71859998 | -0.50744498 | 6 | -3.55065012 | 0.71190000  | -3.06664491 |
| 8         | 0.07594994  | -1.36530006 | 0.74805504  | 1 | -2.80334997 | 0.22669999  | -2.43764496 |
| 8         | 3.35995007  | -0.15270001 | -0.17334498 | 1 | -4.11055040 | -0.06760000 | -3.59644508 |
| 6         | 0.19584994  | -1.76270008 | 2.12475514  | 1 | -3.02915001 | 1.31949997  | -3.81614494 |
| 1         | 1.15915000  | -2.26819992 | 2.26185513  | 6 | -5.46665049 | 2.25790000  | -3.21344495 |
| 1         | -0.58395004 | -2.49709988 | 2.34405494  | 1 | -6.02115011 | 1.53569996  | -3.82234502 |
| 6         | 4.69434977  | -0.09650001 | -0.14614499 | 1 | -6.18835020 | 2.90720010  | -2.70684505 |
| 6         | 5.42674971  | -0.69739997 | 0.92905504  | 1 | -4.88975048 | 2.88590002  | -3.90204501 |
| 6         | 6.82044983  | -0.58529997 | 0.94025505  | 6 | -5.65985012 | -1.68700004 | 3.20675492  |
| 1         | 7.38914967  | -1.03240001 | 1.74825501  | 1 | -6.38965034 | -0.93330002 | 3.51965499  |

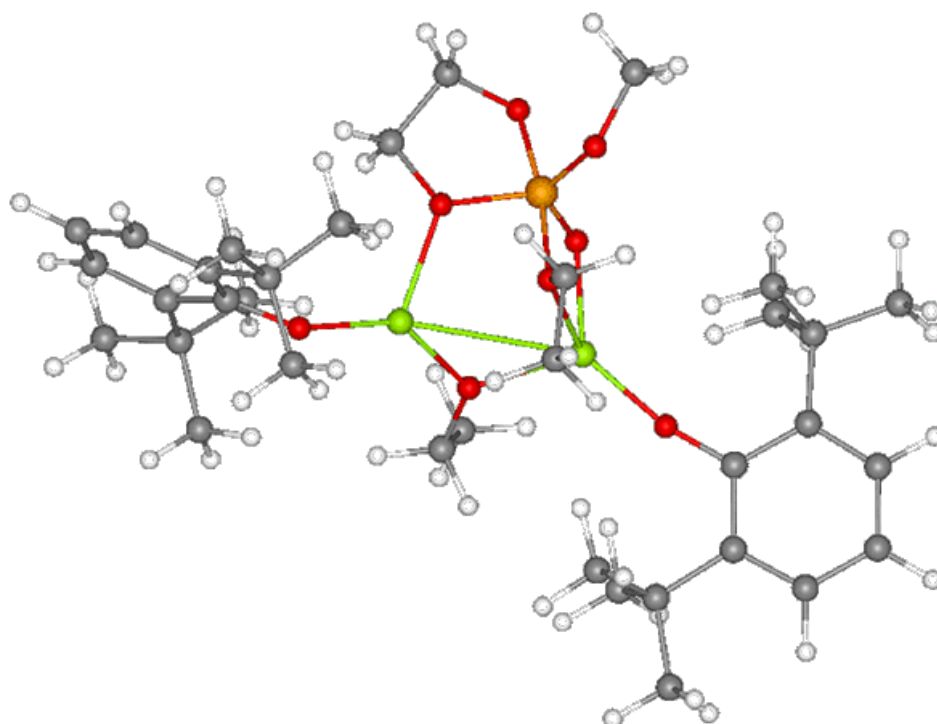
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 7.51794958  | 0.08250000  | -0.05854498 | 1  | -6.20415020 | -2.55110002 | 2.81055498  |
| 6  | 6.80624962  | 0.65079999  | -1.10754502 | 1  | -5.13015032 | -2.02279997 | 4.10585499  |
| 1  | 7.36424971  | 1.16049993  | -1.88524497 | 6  | -3.67175007 | -2.28189993 | 1.87965500  |
| 6  | 5.41174984  | 0.58039999  | -1.18564498 | 1  | -2.90055013 | -1.98420000 | 1.17025506  |
| 6  | 4.72814989  | -1.47210002 | 2.06015515  | 1  | -3.18304992 | -2.64339995 | 2.79335499  |
| 6  | 4.69504976  | 1.22049999  | -2.38774490 | 1  | -4.22045040 | -3.12500000 | 1.44295502  |
| 6  | 4.00664949  | -2.70609999 | 1.48305500  | 6  | -3.90195012 | 0.02209999  | 2.92015505  |
| 1  | 3.27985001  | -2.44039989 | 0.71365505  | 1  | -4.62135029 | 0.77990001  | 3.24965501  |
| 1  | 3.48804998  | -3.25689983 | 2.27835512  | 1  | -3.37844992 | -0.35189998 | 3.80935502  |
| 1  | 4.73064995  | -3.38569999 | 1.02075505  | 1  | -3.18155003 | 0.51709998  | 2.26745510  |
| 6  | 3.74705005  | -0.55199999 | 2.80945492  | 6  | 0.07944994  | -0.60600001 | 3.10105515  |
| 1  | 3.01075006  | -0.11850001 | 2.13235497  | 1  | 1.01424992  | 1.74909997  | -2.56304502 |
| 1  | 4.29064989  | 0.27130002  | 3.28665495  | 1  | -8.43485069 | -0.24110001 | -0.41294497 |
| 1  | 3.21784997  | -1.10340011 | 3.59605503  | 1  | 8.60225010  | 0.15329999  | -0.02334498 |
| 6  | 5.71364975  | -2.00440001 | 3.11635494  | 8  | -0.96205008 | 1.67379999  | 1.13375509  |
| 1  | 6.26694965  | -1.19860005 | 3.61005497  | 15 | -0.40345007 | 2.97900009  | 1.54045498  |
| 1  | 6.43604994  | -2.71169996 | 2.69575500  | 8  | 0.11664994  | 3.91720009  | 0.34365499  |
| 1  | 5.15274954  | -2.53679991 | 3.89265513  | 8  | 0.95424998  | 2.95609999  | 2.40485501  |
| 6  | 5.66644955  | 1.90950000  | -3.36384487 | 6  | 1.50335002  | 4.28749990  | 0.52535504  |
| 1  | 6.38634968  | 1.20919991  | -3.79964495 | 6  | 2.07404995  | 3.30719995  | 1.55575502  |
| 1  | 6.22274971  | 2.72560000  | -2.89044499 | 1  | 1.53304994  | 5.32189989  | 0.87885505  |
| 1  | 5.09444952  | 2.34179997  | -4.19244480 | 1  | 1.99994993  | 4.21049976  | -0.44114500 |
| 6  | 3.72304988  | 2.31380010  | -1.90524495 | 1  | 2.47014999  | 2.39960003  | 1.09425509  |
| 1  | 2.96495008  | 1.89879990  | -1.23904502 | 1  | 2.83704996  | 3.75850010  | 2.18945503  |
| 1  | 3.22215009  | 2.79150009  | -2.75644493 | 8  | -1.47654998 | 3.75890017  | 2.39595509  |
| 1  | 4.27784967  | 3.08850002  | -1.36194491 | 8  | 1.21504998  | -2.56130004 | -1.21224499 |
| 6  | 3.95724988  | 0.14139999  | -3.20244503 | 15 | -0.14275005 | -3.02810001 | -0.75194496 |
| 1  | 4.67324972  | -0.57639998 | -3.61574507 | 8  | -0.57755005 | -4.08440018 | -1.93964493 |
| 1  | 3.40695000  | 0.59000003  | -4.03794479 | 8  | -1.52645004 | -2.16689992 | -0.86344498 |
| 1  | 3.25274992  | -0.42510000 | -2.59164500 | 6  | -2.00075006 | -4.14800024 | -2.04164505 |
| 12 | -1.32365000 | -0.02120000 | -0.01514498 | 6  | -2.46165013 | -2.71239996 | -1.83414495 |
| 8  | 0.15784994  | 0.35280001  | -1.30584502 | 1  | -2.40884995 | -4.81830025 | -1.27614498 |
| 8  | -3.21475005 | 0.09269999  | -0.05604498 | 1  | -2.25565004 | -4.52730036 | -3.03224492 |
| 6  | 0.12834994  | 1.10289991  | -2.50764489 | 1  | -2.37755013 | -2.12019992 | -2.74634504 |
| 6  | 0.08144994  | 0.21859999  | -3.74694490 | 1  | -3.45915008 | -2.61229992 | -1.40774500 |
| 1  | -0.74135005 | 1.77379990  | -2.50254488 | 8  | -0.23415007 | -3.97399998 | 0.53405505  |
| 6  | -4.53945017 | 0.06999999  | -0.10574498 | 6  | 0.59934998  | -5.15230036 | 0.57365501  |
| 6  | -5.23845005 | 0.71450001  | -1.18134499 | 6  | -1.22375000 | 5.08220005  | 2.90525508  |
| 6  | -6.62695026 | 0.57270002  | -1.26354492 | 1  | -0.36085007 | 5.07340002  | 3.57525492  |
| 1  | -7.16755009 | 1.03450000  | -2.08294487 | 1  | -1.06895006 | 5.78160000  | 2.08005500  |
| 6  | -7.35635042 | -0.13990000 | -0.31854498 | 1  | 0.38074994  | -5.80250025 | -0.27664500 |

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|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -6.68655014 | -0.68650001 | 0.77035505  | 1 | 1.65474999  | -4.87170029 | 0.57055503  |
| 1 | -7.27325010 | -1.19850004 | 1.52585506  | 1 | -2.11855006 | 5.36179972  | 3.45875502  |
| 6 | -5.30025005 | -0.58520001 | 0.92105502  | 1 | 0.35124993  | -5.65660000 | 1.50705504  |
| 6 | -4.50395012 | 1.57690001  | -2.22394490 | 1 | 0.22894993  | -0.98610002 | 4.11835480  |
| 6 | -4.63755035 | -1.12690008 | 2.20115495  | 1 | 0.82964993  | 0.16710000  | 2.92055511  |
| 6 | -3.72815013 | 2.70880008  | -1.52004492 | 1 | -0.90935004 | -0.14330001 | 3.06115508  |
| 1 | -3.02815008 | 2.31980014  | -0.77964497 | 1 | 0.09354994  | 0.82999998  | -4.65684509 |
| 1 | -3.17135000 | 3.30739999  | -2.25204492 | 1 | 0.94004989  | -0.45879999 | -3.77934504 |
| 1 | -4.42445040 | 3.37680006  | -1.00084496 | 1 | -0.82835007 | -0.38859999 | -3.76204491 |

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# DTS-12r



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2366006.0 (Joules/Mol)      |
|                                              | 565.48901 (Kcal/Mol)        |
| Zero-point correction=                       | 0.901164 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.955850                    |
| Thermal correction to Enthalpy=              | 0.956794                    |
| Thermal correction to Gibbs Free Energy=     | 0.811183                    |
| Sum of electronic and zero-point Energies=   | -2711.256473                |
| Sum of electronic and thermal Energies=      | -2711.201787                |
| Sum of electronic and thermal Enthalpies=    | -2711.200843                |
| Sum of electronic and thermal Free Energies= | -2711.346454                |

| cartesian |             |             |             |   |             |             |             |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 12        | 1.69343948  | 0.25357798  | 0.67307812  | 6 | -5.18076038 | 0.03337798  | -1.42072177 |
| 8         | 0.52263939  | 1.48557806  | -0.56542188 | 6 | -4.67696047 | -1.81072187 | 1.97917819  |
| 8         | 3.37303948  | -0.43352205 | 0.31177813  | 6 | -4.40266037 | 0.42727798  | -2.69102192 |
| 6         | 0.51943940  | 1.84217799  | -1.96512175 | 6 | -3.95816064 | -3.05782199 | 1.42477822  |
| 1         | 1.34203947  | 2.53807807  | -2.14592171 | 1 | -3.20786047 | -2.79362202 | 0.67737812  |
| 1         | -0.41726062 | 2.35837793  | -2.19672179 | 1 | -3.47066045 | -3.61482191 | 2.23457813  |
| 6         | 4.62153959  | -0.64652205 | -0.10822188 | 1 | -4.67956066 | -3.72762203 | 0.94547814  |
| 6         | 5.59563923  | 0.40097797  | -0.06742188 | 6 | -3.70206046 | -0.94772202 | 2.80367827  |
| 6         | 6.87893963  | 0.13847798  | -0.55812186 | 1 | -2.82246065 | -0.64562201 | 2.22717810  |
| 1         | 7.63113928  | 0.91977793  | -0.54362190 | 1 | -4.19416046 | -0.03902203 | 3.16597819  |

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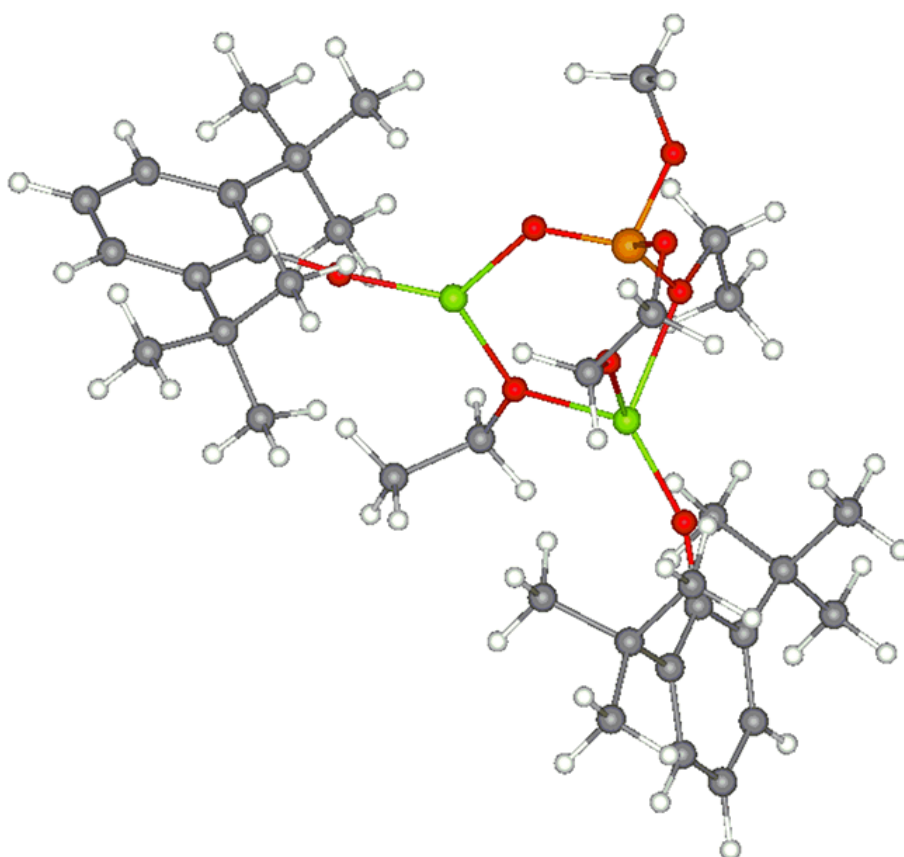
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 7.23513937  | -1.10372198 | -1.06912184 | 1  | -3.33296061 | -1.50312197 | 3.67327809  |
| 6  | 6.29383945  | -2.12662196 | -1.07222188 | 6  | -5.73236036 | -2.31812191 | 2.97937822  |
| 1  | 6.59323931  | -3.09552193 | -1.45682180 | 1  | -6.25816059 | -1.50052202 | 3.48377824  |
| 6  | 4.99353933  | -1.94022202 | -0.59382188 | 1  | -6.47546053 | -2.96212196 | 2.49927807  |
| 6  | 5.27243948  | 1.79557800  | 0.50057811  | 1  | -5.23766041 | -2.91422200 | 3.75387812  |
| 6  | 4.01563931  | -3.13002205 | -0.56302190 | 6  | -5.33596039 | 0.86857796  | -3.83362174 |
| 6  | 4.80793953  | 1.68847799  | 1.96737814  | 1  | -6.04676056 | 0.08277797  | -4.10862160 |
| 1  | 3.95423937  | 1.02127802  | 2.08707809  | 1  | -5.90046072 | 1.77477801  | -3.58962178 |
| 1  | 4.52583933  | 2.67327809  | 2.35777807  | 1  | -4.73536062 | 1.09177804  | -4.72232199 |
| 1  | 5.61983967  | 1.29667807  | 2.58957815  | 6  | -3.46676064 | 1.61797798  | -2.41222191 |
| 6  | 4.21343946  | 2.49377799  | -0.37402189 | 1  | -2.74386048 | 1.39517796  | -1.62512183 |
| 1  | 3.30323935  | 1.90117800  | -0.47492188 | 1  | -2.91036057 | 1.89227808  | -3.31682181 |
| 1  | 4.60583925  | 2.65877795  | -1.38352180 | 1  | -4.04116058 | 2.49477792  | -2.09302187 |
| 1  | 3.93873954  | 3.46717811  | 0.04917812  | 6  | -3.60166049 | -0.77822202 | -3.22542191 |
| 6  | 6.49823952  | 2.72767806  | 0.50967813  | 1  | -4.28026056 | -1.58832192 | -3.51272178 |
| 1  | 6.88163948  | 2.92487812  | -0.49692190 | 1  | -3.02866054 | -0.49042207 | -4.11542177 |
| 1  | 7.31583929  | 2.32817793  | 1.11837816  | 1  | -2.91266060 | -1.17532194 | -2.47842193 |
| 1  | 6.21173954  | 3.69307804  | 0.94237810  | 6  | 0.67763937  | 0.59157795  | -2.80572176 |
| 6  | 4.64203930  | -4.42122221 | -1.11982179 | 1  | 0.75353938  | -2.86182189 | 1.08127820  |
| 1  | 5.52213955  | -4.73532200 | -0.54932189 | 1  | -8.39946079 | -0.02602203 | -0.26322189 |
| 1  | 4.92943954  | -4.32302237 | -2.17222190 | 1  | 8.23923969  | -1.27672195 | -1.44872177 |
| 1  | 3.90813947  | -5.23272228 | -1.05712187 | 8  | 1.13673949  | 1.88747799  | 1.69637823  |
| 6  | 2.76663947  | -2.84902191 | -1.42032182 | 15 | 0.14763939  | 2.64077806  | 0.81797814  |
| 1  | 2.21653938  | -1.98012209 | -1.05742180 | 8  | -0.48556060 | 3.67177796  | 1.98897815  |
| 1  | 2.09063935  | -3.71332192 | -1.40942180 | 8  | -1.43946052 | 1.95747805  | 0.63547814  |
| 1  | 3.05153942  | -2.66032195 | -2.46132183 | 6  | -1.86256051 | 3.93087792  | 1.80977821  |
| 6  | 3.62113953  | -3.42522192 | 0.89767814  | 6  | -2.45546055 | 2.57757807  | 1.46387815  |
| 1  | 4.50283957  | -3.72112203 | 1.47637820  | 1  | -2.03736067 | 4.65437794  | 1.00027812  |
| 1  | 2.89683938  | -4.24852228 | 0.94547814  | 1  | -2.26866055 | 4.33247757  | 2.74017811  |
| 1  | 3.18813944  | -2.54582191 | 1.37677813  | 1  | -2.59666061 | 1.96777797  | 2.35957813  |
| 12 | -1.51766050 | -0.08782203 | 0.24177814  | 1  | -3.37786055 | 2.62147808  | 0.88337809  |
| 8  | 0.08103940  | -0.91682202 | 0.89937812  | 8  | 0.58963937  | 3.82197809  | -0.19562188 |
| 8  | -3.19836044 | -0.63302207 | -0.25052190 | 6  | 0.89163941  | 5.15867758  | 0.24507812  |
| 6  | 0.09713940  | -2.16142201 | 1.60897815  | 1  | -0.02036061 | 5.71437788  | 0.47057810  |
| 6  | 0.56303936  | -1.98652196 | 3.04507828  | 1  | 1.54043949  | 5.14647770  | 1.12147820  |
| 1  | -0.90856063 | -2.60202193 | 1.60147822  | 1  | 1.40863943  | 5.62537766  | -0.59422189 |
| 6  | -4.53376055 | -0.53282201 | -0.28012189 | 1  | 0.70553941  | 0.86647797  | -3.86502171 |
| 6  | -5.30926037 | -1.01792192 | 0.81717813  | 1  | 1.60943949  | 0.06927797  | -2.57132173 |
| 6  | -6.69186068 | -0.80672204 | 0.79387814  | 1  | -0.15646061 | -0.10522203 | -2.67032194 |
| 1  | -7.30406046 | -1.14322197 | 1.62317812  | 1  | 0.55073941  | -2.94812202 | 3.56927824  |
| 6  | -7.32366037 | -0.18152203 | -0.27482188 | 1  | 1.58933949  | -1.60492194 | 3.08867812  |

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|   |             |            |             |   |             |             |            |
|---|-------------|------------|-------------|---|-------------|-------------|------------|
| 6 | -6.56796074 | 0.20687798 | -1.37492180 | 1 | -0.08376060 | -1.28902197 | 3.58617806 |
| 1 | -7.08386040 | 0.65197796 | -2.21872187 |   |             |             |            |

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|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2368512.0 (Joules/Mol)      |
|                                              | 566.08796 (Kcal/Mol)        |
| Zero-point correction=                       | 0.902119 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.956579                    |
| Thermal correction to Enthalpy=              | 0.957524                    |
| Thermal correction to Gibbs Free Energy=     | 0.812642                    |
| Sum of electronic and zero-point Energies=   | -2711.267556                |
| Sum of electronic and thermal Energies=      | -2711.213095                |
| Sum of electronic and thermal Enthalpies=    | -2711.212151                |
| Sum of electronic and thermal Free Energies= | -2711.357032                |

| cartesian |             |             |             |   |             |             |             |  |  |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|--|--|
| 12        | 1.67499804  | -0.51287043 | -0.19634765 | 6 | -5.29080200 | 0.27622956  | 1.35405231  |  |  |
| 8         | -1.02200186 | -2.62527037 | -1.12104762 | 6 | -3.66490197 | 2.52142954  | -1.38864768 |  |  |
| 8         | 3.30439806  | 0.21922956  | 0.19255234  | 6 | -5.24330187 | -1.15347040 | 1.92045224  |  |  |
| 6         | -1.04810190 | -3.90587044 | -0.40454766 | 6 | -2.19680190 | 2.69772959  | -0.95614767 |  |  |
| 1         | -0.02390195 | -4.18797064 | -0.16254766 | 1 | -1.76220191 | 1.78602958  | -0.54074764 |  |  |
| 1         | -1.46280193 | -4.65077066 | -1.08384764 | 1 | -1.57360196 | 3.01812959  | -1.80014765 |  |  |
| 6         | 4.52779818  | 0.60812956  | 0.54775232  | 1 | -2.11990190 | 3.46272945  | -0.17664766 |  |  |

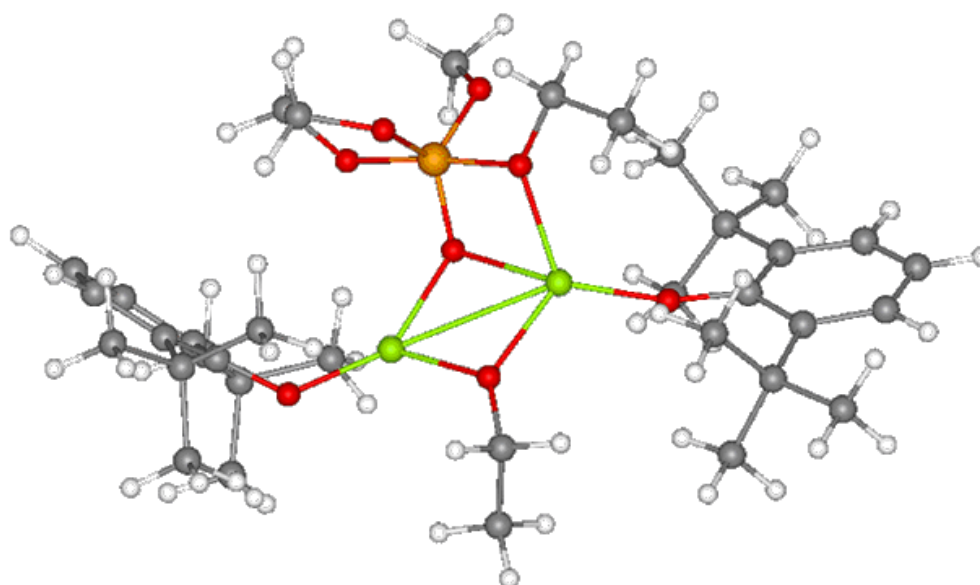
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 5.08319807  | 1.79632950  | -0.01854765 | 6  | -3.79390192 | 1.54562950  | -2.57594752 |
| 6  | 6.34649801  | 2.20782948  | 0.41665232  | 1  | -3.46130180 | 0.53732955  | -2.32134748 |
| 1  | 6.78929806  | 3.11282945  | 0.01445234  | 1  | -4.84070206 | 1.47362959  | -2.88934755 |
| 6  | 7.07179785  | 1.48872960  | 1.36055231  | 1  | -3.21800184 | 1.90882945  | -3.43694758 |
| 6  | 6.53889799  | 0.31142956  | 1.87345231  | 6  | -4.11440182 | 3.89642954  | -1.91704762 |
| 1  | 7.12899828  | -0.24587044 | 2.59315252  | 1  | -5.14900208 | 3.88272953  | -2.27424765 |
| 6  | 5.28149796  | -0.16217044 | 1.48595238  | 1  | -4.01930189 | 4.68492937  | -1.16374767 |
| 6  | 4.33689785  | 2.60452962  | -1.09724760 | 1  | -3.48030186 | 4.18212938  | -2.76404762 |
| 6  | 4.75329828  | -1.49427044 | 2.05225253  | 6  | -6.39050198 | -1.44227040 | 2.90485239  |
| 6  | 3.00459814  | 3.15532947  | -0.55184764 | 1  | -6.34800196 | -0.80477047 | 3.79415250  |
| 1  | 2.34289813  | 2.35582948  | -0.21564767 | 1  | -7.37500191 | -1.32317042 | 2.44075251  |
| 1  | 2.48449802  | 3.73502946  | -1.32474768 | 1  | -6.31540203 | -2.48047042 | 3.24765253  |
| 1  | 3.18069816  | 3.81732965  | 0.30285233  | 6  | -5.39370203 | -2.16877055 | 0.76905233  |
| 6  | 4.08539820  | 1.72602952  | -2.34054756 | 1  | -4.64100170 | -2.01727033 | -0.00644766 |
| 1  | 3.52129817  | 0.82372957  | -2.09654760 | 1  | -5.31860209 | -3.19627047 | 1.14715230  |
| 1  | 5.03499794  | 1.40892959  | -2.78484750 | 1  | -6.37700176 | -2.06007028 | 0.29855233  |
| 1  | 3.53159809  | 2.29122949  | -3.10124755 | 6  | -3.93650198 | -1.37837040 | 2.70335245  |
| 6  | 5.14709806  | 3.82112956  | -1.57874763 | 1  | -3.88340187 | -0.69627047 | 3.55875254  |
| 1  | 6.10729790  | 3.53142953  | -2.01784754 | 1  | -3.88200188 | -2.40467048 | 3.08715248  |
| 1  | 5.33869791  | 4.53752947  | -0.77294767 | 1  | -3.06010199 | -1.19647050 | 2.08065248  |
| 1  | 4.58039808  | 4.34902954  | -2.35414767 | 6  | -1.88130188 | -3.74227047 | 0.84255230  |
| 6  | 5.75319815  | -2.16137052 | 3.01415253  | 1  | 0.17199805  | -0.48157042 | 2.75805235  |
| 1  | 5.95649815  | -1.54447043 | 3.89555240  | 1  | -7.19010210 | 3.10692954  | 1.64845228  |
| 1  | 6.70569801  | -2.39047050 | 2.52565241  | 1  | 8.04979801  | 1.83642960  | 1.68395233  |
| 1  | 5.33399820  | -3.10917044 | 3.37075233  | 8  | 1.46489811  | -1.74247050 | -1.67824769 |
| 6  | 4.51669788  | -2.50327039 | 0.90895236  | 15 | 0.15659803  | -2.28977036 | -2.27494764 |
| 1  | 3.85479808  | -2.11167049 | 0.13385235  | 8  | -0.10290196 | -2.14037037 | -3.88074756 |
| 1  | 4.08589792  | -3.43417048 | 1.29835236  | 8  | -0.68770200 | -0.61697042 | -2.14054751 |
| 1  | 5.46489811  | -2.75177050 | 0.42065233  | 6  | -0.55960196 | -0.89927047 | -4.42314768 |
| 6  | 3.46109819  | -1.27497041 | 2.86395240  | 6  | -0.42800194 | 0.12992956  | -3.31174755 |
| 1  | 3.65179801  | -0.62027043 | 3.72095251  | 1  | -1.60090196 | -1.03177047 | -4.73054790 |
| 1  | 3.07699800  | -2.22867036 | 3.24695253  | 1  | 0.05639805  | -0.66567045 | -5.29374790 |
| 1  | 2.67729807  | -0.80017048 | 2.26985240  | 1  | 0.58509803  | 0.55002958  | -3.27454758 |
| 12 | -1.64040196 | -0.66017044 | -0.39464766 | 1  | -1.15310192 | 0.93782949  | -3.40954757 |
| 8  | -0.04410195 | -0.28587043 | 0.70425230  | 8  | 0.49389806  | -3.88217044 | -2.44884753 |
| 8  | -3.35870194 | -0.06597044 | -0.02754766 | 6  | 1.63049805  | -4.28267050 | -3.22044754 |
| 6  | -0.20570195 | 0.24852957  | 2.02985239  | 1  | 1.45199811  | -4.10807037 | -4.28474760 |
| 6  | 0.50109804  | 1.57962954  | 2.21535254  | 1  | 2.52589798  | -3.74537039 | -2.89584756 |
| 1  | -1.27660191 | 0.37602955  | 2.23235250  | 1  | 1.76159811  | -5.35147047 | -3.04264760 |
| 6  | -4.36170197 | 0.72992957  | 0.36435235  | 1  | -1.92720187 | -4.70407057 | 1.36355233  |
| 6  | -4.53260183 | 2.02642965  | -0.21664765 | 1  | -1.43450189 | -3.01947045 | 1.53195238  |

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|   |             |            |             |   |             |             |            |
|---|-------------|------------|-------------|---|-------------|-------------|------------|
| 6 | -5.54990196 | 2.85192966 | 0.27405232  | 1 | -2.90540195 | -3.44007039 | 0.61595231 |
| 1 | -5.68680191 | 3.84472966 | -0.14014766 | 1 | 0.34569806  | 1.94562960  | 3.23615241 |
| 6 | -6.41260195 | 2.44132948 | 1.28205228  | 1 | 1.57989812  | 1.48932958  | 2.05375242 |
| 6 | -6.28440189 | 1.15592957 | 1.79375231  | 1 | 0.10799804  | 2.33012962  | 1.52325237 |
| 1 | -6.98860168 | 0.83712953 | 2.55455256  |   |             |             |            |

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## DI-2r



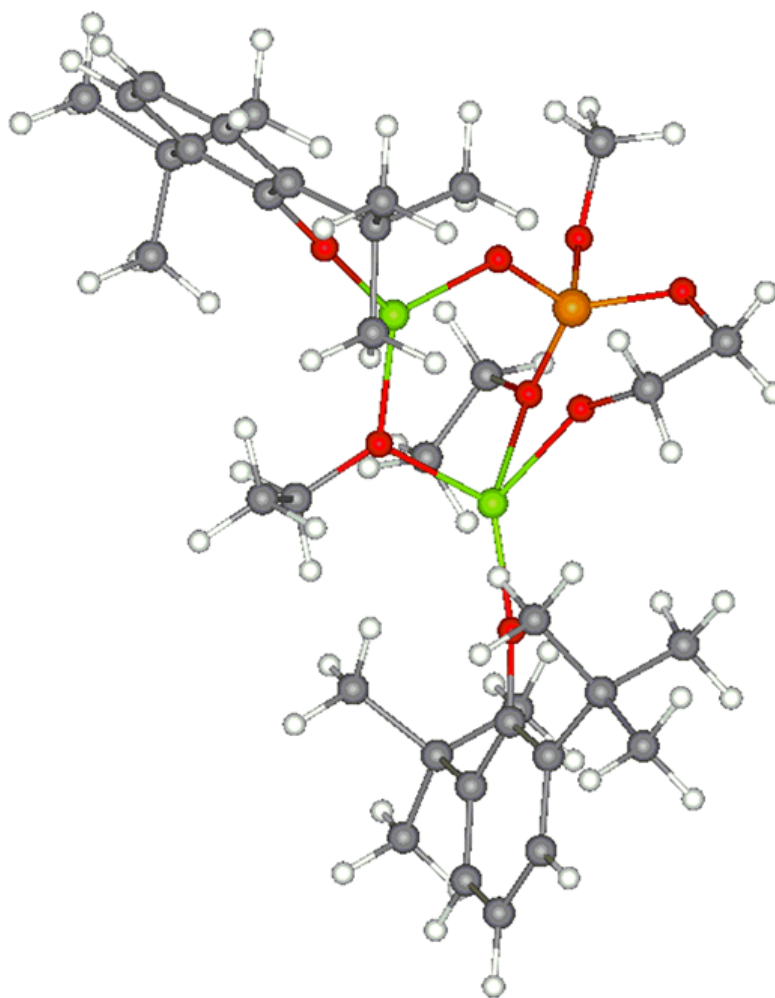
|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2369398.6 (Joules/Mol)      |
|                                              | 566.29986 (Kcal/Mol)        |
| Zero-point correction=                       | 0.902456 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.957493                    |
| Thermal correction to Enthalpy=              | 0.958438                    |
| Thermal correction to Gibbs Free Energy=     | 0.809607                    |
| Sum of electronic and zero-point Energies=   | -2711.266067                |
| Sum of electronic and thermal Energies=      | -2711.211030                |
| Sum of electronic and thermal Enthalpies=    | -2711.210086                |
| Sum of electronic and thermal Free Energies= | -2711.358916                |

| cartesian |            |             |             |   |             |             |             |  |  |  |  |
|-----------|------------|-------------|-------------|---|-------------|-------------|-------------|--|--|--|--|
| 12        | 0.96483839 | 0.02281040  | 0.50933141  | 6 | -5.57366133 | 0.80051023  | 0.66733158  |  |  |  |  |
| 8         | 0.46853828 | -1.07198989 | 2.20163035  | 6 | -4.45956135 | -1.17289007 | -2.48956966 |  |  |  |  |
| 8         | 2.73793840 | 0.08961041  | -0.02976881 | 6 | -5.29746151 | 2.16231060  | 1.33503032  |  |  |  |  |
| 6         | 1.09273827 | -1.38839006 | 3.46463037  | 6 | -4.70396137 | -0.03008961 | -3.49746966 |  |  |  |  |
| 1         | 1.46683836 | -2.41448951 | 3.41163039  | 1 | -4.33646154 | 0.92161006  | -3.10526967 |  |  |  |  |
| 1         | 0.32983828 | -1.32879007 | 4.24563026  | 1 | -4.19446182 | -0.23638959 | -4.44726944 |  |  |  |  |
| 6         | 4.05763865 | -0.07248962 | -0.13176875 | 1 | -5.77336121 | 0.07631044  | -3.70426965 |  |  |  |  |
| 6         | 4.60623884 | -1.32869005 | -0.54256845 | 6 | -2.93296146 | -1.39389002 | -2.33776975 |  |  |  |  |
| 6         | 5.99693871 | -1.47749007 | -0.55256844 | 1 | -2.38236189 | -0.45438975 | -2.50446963 |  |  |  |  |
| 1         | 6.43523884 | -2.42588949 | -0.84456867 | 1 | -2.67156172 | -1.85989010 | -1.37976968 |  |  |  |  |
| 6         | 6.85373878 | -0.44098973 | -0.20196867 | 1 | -2.55366182 | -2.06388974 | -3.11716962 |  |  |  |  |
| 6         | 6.31403875 | 0.79921025  | 0.11933121  | 6 | -5.02536154 | -2.46488953 | -3.10516953 |  |  |  |  |
| 1         | 6.99723864 | 1.60980999  | 0.34843129  | 1 | -4.86506128 | -3.33568954 | -2.45976973 |  |  |  |  |

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|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 4.93463850  | 1.02570999  | 0.14073120  | 1  | -6.09566116 | -2.38388944 | -3.31546974 |
| 6  | 3.71443892  | -2.50618958 | -0.97806954 | 1  | -4.52586126 | -2.66318941 | -4.05956984 |
| 6  | 4.40243864  | 2.45321059  | 0.37213132  | 6  | -6.38006115 | 2.52631044  | 2.36573029  |
| 6  | 2.76843834  | -2.08068967 | -2.12036967 | 1  | -7.37766123 | 2.56911063  | 1.91673040  |
| 1  | 2.14693832  | -1.22719014 | -1.84486961 | 1  | -6.41086149 | 1.82450998  | 3.20683026  |
| 1  | 2.11313820  | -2.91368937 | -2.40386963 | 1  | -6.16626120 | 3.51781058  | 2.77953029  |
| 1  | 3.34653854  | -1.79259002 | -3.00496960 | 6  | -3.94946146 | 2.18441057  | 2.08133054  |
| 6  | 2.91643810  | -3.04498959 | 0.22223118  | 1  | -3.11016178 | 2.01491046  | 1.40403032  |
| 1  | 2.29413843  | -2.28088951 | 0.68933153  | 1  | -3.79596186 | 3.16081047  | 2.55623031  |
| 1  | 3.59663868  | -3.42508936 | 0.99243158  | 1  | -3.92116165 | 1.42860997  | 2.87383032  |
| 1  | 2.26243830  | -3.86908937 | -0.08716880 | 6  | -5.30716133 | 3.26691055  | 0.25723121  |
| 6  | 4.53173876  | -3.69228935 | -1.52296960 | 1  | -6.28296137 | 3.31061053  | -0.23846860 |
| 1  | 5.18153858  | -4.13778830 | -0.76246846 | 1  | -5.11886120 | 4.24571228  | 0.71523154  |
| 1  | 5.14993858  | -3.40828943 | -2.38086963 | 1  | -4.54486132 | 3.08731055  | -0.50276846 |
| 1  | 3.84533882  | -4.47778749 | -1.85936952 | 6  | 2.21833849  | -0.41148975 | 3.72773027  |
| 6  | 5.53523874  | 3.47521043  | 0.58173144  | 1  | 0.84133828  | 3.11661053  | -0.11106877 |
| 1  | 6.21103859  | 3.52501059  | -0.27786863 | 1  | -7.86576128 | -1.74009001 | 0.71353155  |
| 1  | 6.12973881  | 3.26041055  | 1.47633040  | 1  | 7.93073559  | -0.58978975 | -0.20676866 |
| 1  | 5.10033846  | 4.47271252  | 0.71113157  | 8  | -0.75616169 | -1.12629008 | 0.26863119  |
| 6  | 3.50833845  | 2.54291058  | 1.62253034  | 15 | -0.95616174 | -1.93169010 | 1.61073041  |
| 1  | 2.62643814  | 1.90690994  | 1.53363037  | 8  | -2.40926170 | -2.60908937 | 1.03453124  |
| 1  | 3.16933823  | 3.57421064  | 1.77973032  | 8  | -1.72976172 | -1.37459004 | 2.94473028  |
| 1  | 4.05693865  | 2.22811055  | 2.51663041  | 6  | -3.33836174 | -2.86498952 | 2.07263041  |
| 6  | 3.62683868  | 2.90131044  | -0.88306880 | 6  | -3.11476183 | -1.73309004 | 3.06793046  |
| 1  | 4.29783869  | 2.93831062  | -1.74796963 | 1  | -3.15056181 | -3.84518957 | 2.53353047  |
| 1  | 3.20583820  | 3.90501165  | -0.74206841 | 1  | -4.34536171 | -2.85158944 | 1.65163040  |
| 1  | 2.81713820  | 2.20831060  | -1.11766958 | 1  | -3.71906185 | -0.85718977 | 2.82143044  |
| 12 | -1.88266170 | 0.32251024  | -0.47046849 | 1  | -3.29286146 | -2.02478981 | 4.10483027  |
| 8  | -0.28846177 | 1.39060998  | -0.19816867 | 8  | -0.14886180 | -3.32128954 | 1.76693034  |
| 8  | -3.62086153 | 0.95631003  | -0.71096843 | 6  | -0.54666173 | -4.55328751 | 1.14763057  |
| 6  | -0.14346179 | 2.78561044  | -0.45736849 | 1  | -1.44016171 | -4.96658754 | 1.62003040  |
| 6  | -0.30086178 | 3.10601044  | -1.93486953 | 1  | -0.72746170 | -4.41608763 | 0.08073123  |
| 1  | -0.89216173 | 3.34021044  | 0.12493120  | 1  | 0.29223830  | -5.23388767 | 1.29733038  |
| 6  | -4.76066113 | 0.32021022  | -0.40276855 | 1  | 2.70433855  | -0.66188973 | 4.67633057  |
| 6  | -5.16246128 | -0.81638974 | -1.16366959 | 1  | 2.97643852  | -0.45398974 | 2.94083047  |
| 6  | -6.27276134 | -1.54579008 | -0.72576845 | 1  | 1.84343803  | 0.61371022  | 3.80503035  |
| 1  | -6.58666134 | -2.43598938 | -1.26086962 | 1  | -0.17406181 | 4.17961264  | -2.11146975 |
| 6  | -7.00976133 | -1.15389013 | 0.38833135  | 1  | 0.44593829  | 2.57181048  | -2.52996969 |
| 6  | -6.67536116 | 0.02661041  | 1.04793119  | 1  | -1.29926169 | 2.82951045  | -2.29446959 |
| 1  | -7.30326128 | 0.34841025  | 1.87253034  |    |             |             |             |

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|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2368509.7 (Joules/Mol)      |
|                                              | 566.08739 (Kcal/Mol)        |
| Zero-point correction=                       | 0.902118 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.956579                    |
| Thermal correction to Enthalpy=              | 0.957523                    |
| Thermal correction to Gibbs Free Energy=     | 0.812635                    |
| Sum of electronic and zero-point Energies=   | -2711.267557                |
| Sum of electronic and thermal Energies=      | -2711.213096                |
| Sum of electronic and thermal Enthalpies=    | -2711.212152                |
| Sum of electronic and thermal Free Energies= | -2711.357039                |

cartesian

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 12 | 1.67498267  | -0.51273811 | -0.19668184 | 6 | -5.29091740 | 0.27596188  | 1.35421813  |
| 8  | -1.02201724 | -2.62503815 | -1.12118185 | 6 | -3.66491723 | 2.52196193  | -1.38788188 |
| 8  | 3.30448294  | 0.21916185  | 0.19251816  | 6 | -5.24321699 | -1.15383816 | 1.92021823  |
| 6  | -1.04781735 | -3.90573812 | -0.40478185 | 6 | -2.19681716 | 2.69846201  | -0.95528185 |

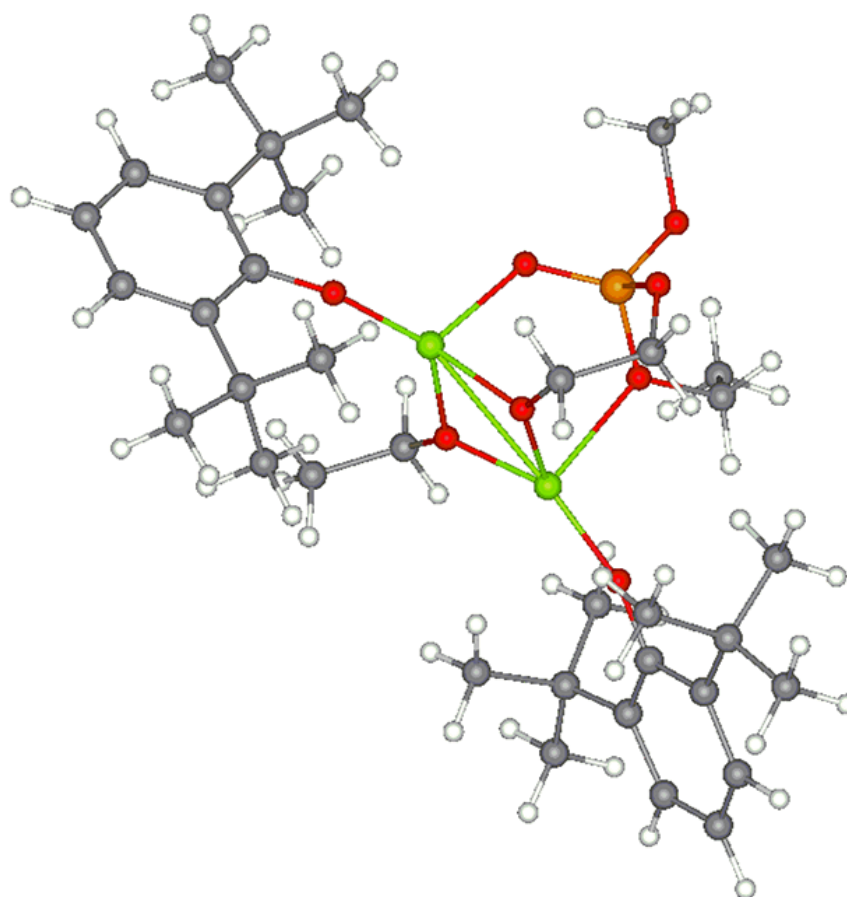
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1  | -0.02361726 | -4.18783808 | -0.16288184 | 1  | -1.76221728 | 1.78676188  | -0.53968185 |
| 1  | -1.46261728 | -4.65063810 | -1.08408189 | 1  | -1.57361734 | 3.01896191  | -1.79918194 |
| 6  | 4.52788305  | 0.60806185  | 0.54751819  | 1  | -2.12011719 | 3.46346188  | -0.17568184 |
| 6  | 5.08328295  | 1.79626191  | -0.01898184 | 6  | -3.79361725 | 1.54626191  | -2.57528186 |
| 6  | 6.34658289  | 2.20776200  | 0.41611814  | 1  | -3.46081710 | 0.53796184  | -2.32078195 |
| 1  | 6.78928280  | 3.11266208  | 0.01381816  | 1  | -4.84031725 | 1.47406185  | -2.88888192 |
| 6  | 7.07198286  | 1.48856187  | 1.35991812  | 1  | -3.21771717 | 1.90966189  | -3.43618178 |
| 6  | 6.53918266  | 0.31136185  | 1.87291813  | 6  | -4.11461735 | 3.89686203  | -1.91618192 |
| 1  | 7.12928295  | -0.24593812 | 2.59251809  | 1  | -5.14911699 | 3.88306189  | -2.27348185 |
| 6  | 5.28158283  | -0.16223814 | 1.48571813  | 1  | -4.01981735 | 4.68526220  | -1.16268182 |
| 6  | 4.33678293  | 2.60456204  | -1.09748185 | 1  | -3.48041725 | 4.18286180  | -2.76298189 |
| 6  | 4.75348282  | -1.49433815 | 2.05211806  | 6  | -6.39051723 | -1.44303811 | 2.90441823  |
| 6  | 3.00468278  | 3.15536189  | -0.55178183 | 1  | -6.34831715 | -0.80563813 | 3.79381800  |
| 1  | 2.34298277  | 2.35596204  | -0.21548185 | 1  | -7.37501717 | -1.32403815 | 2.44031811  |
| 1  | 2.48448277  | 3.73516202  | -1.32458186 | 1  | -6.31531715 | -2.48123813 | 3.24701810  |
| 1  | 3.18098283  | 3.81746197  | 0.30281818  | 6  | -5.39341736 | -2.16893792 | 0.76871818  |
| 6  | 4.08498287  | 1.72606182  | -2.34068179 | 1  | -4.64051723 | -2.01713800 | -0.00678185 |
| 1  | 3.52068281  | 0.82376188  | -2.09658194 | 1  | -5.31811714 | -3.19653797 | 1.14651811  |
| 1  | 5.03438282  | 1.40876186  | -2.78518200 | 1  | -6.37661695 | -2.06023812 | 0.29811817  |
| 1  | 3.53108287  | 2.29126191  | -3.10128188 | 6  | -3.93651724 | -1.37873816 | 2.70331812  |
| 6  | 5.14698267  | 3.82096195  | -1.57918191 | 1  | -3.88351727 | -0.69673812 | 3.55871820  |
| 1  | 6.10708284  | 3.53116202  | -2.01858187 | 1  | -3.88201714 | -2.40503812 | 3.08711815  |
| 1  | 5.33888292  | 4.53736210  | -0.77348185 | 1  | -3.06001711 | -1.19673812 | 2.08071804  |
| 1  | 4.58018303  | 4.34896183  | -2.35438180 | 6  | -1.88091731 | -3.74223804 | 0.84241813  |
| 6  | 5.75328302  | -2.16133809 | 3.01401806  | 1  | 0.17268273  | -0.48263812 | 2.75791812  |
| 1  | 5.95658302  | -1.54423809 | 3.89531827  | 1  | -7.19051695 | 3.10636187  | 1.64891815  |
| 1  | 6.70578289  | -2.39053798 | 2.52561808  | 1  | 8.04998207  | 1.83626187  | 1.68321812  |
| 1  | 5.33398294  | -3.10893798 | 3.37081814  | 8  | 1.46488273  | -1.74223816 | -1.67878187 |
| 6  | 4.51678276  | -2.50333810 | 0.90881819  | 15 | 0.15648274  | -2.28943801 | -2.27528191 |
| 1  | 3.85478282  | -2.11193800 | 0.13371815  | 8  | -0.10341725 | -2.13993812 | -3.88098192 |
| 1  | 4.08618259  | -3.43433809 | 1.29831815  | 8  | -0.68781722 | -0.61663812 | -2.14048171 |
| 1  | 5.46508265  | -2.75173807 | 0.42041814  | 6  | -0.56011724 | -0.89873815 | -4.42308187 |
| 6  | 3.46118283  | -1.27493811 | 2.86371803  | 6  | -0.42831728 | 0.13036187  | -3.31158185 |
| 1  | 3.65188289  | -0.62003815 | 3.72051811  | 1  | -1.60151732 | -1.03113806 | -4.73028183 |
| 1  | 3.07718277  | -2.22863793 | 3.24681807  | 1  | 0.05568274  | -0.66503817 | -5.29388142 |
| 1  | 2.67738271  | -0.80033815 | 2.26941800  | 1  | 0.58478278  | 0.55046183  | -3.27448177 |
| 12 | -1.64041734 | -0.66023815 | -0.39448184 | 1  | -1.15331733 | 0.93826187  | -3.40928197 |
| 8  | -0.04401726 | -0.28603813 | 0.70421815  | 8  | 0.49368274  | -3.88183808 | -2.44938183 |
| 8  | -3.35861707 | -0.06573813 | -0.02728184 | 6  | 1.63018274  | -4.28223801 | -3.22108197 |
| 6  | -0.20531726 | 0.24776186  | 2.03001809  | 1  | 1.45168269  | -4.10753822 | -4.28528166 |
| 6  | 0.50128275  | 1.57896185  | 2.21601820  | 1  | 2.52568293  | -3.74503803 | -2.89658189 |

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|   |             |            |             |   |             |             |             |
|---|-------------|------------|-------------|---|-------------|-------------|-------------|
| 1 | -1.27621734 | 0.37506187 | 2.23291802  | 1 | 1.76138270  | -5.35113811 | -3.04348183 |
| 6 | -4.36171722 | 0.72996187 | 0.36461818  | 1 | -1.92661726 | -4.70403814 | 1.36341810  |
| 6 | -4.53271723 | 2.02656198 | -0.21608184 | 1 | -1.43411732 | -3.01943803 | 1.53181815  |
| 6 | -5.55011702 | 2.85186195 | 0.27471817  | 1 | -2.90511727 | -3.44013810 | 0.61611819  |
| 1 | -5.68711710 | 3.84466195 | -0.13938184 | 1 | 0.34598273  | 1.94446194  | 3.23701811  |
| 6 | -6.41291714 | 2.44086194 | 1.28241813  | 1 | 1.58008265  | 1.48876190  | 2.05421805  |
| 6 | -6.28461695 | 1.15546191 | 1.79391813  | 1 | 0.10798274  | 2.32956195  | 1.52421808  |
| 1 | -6.98891735 | 0.83636183 | 2.55451822  |   |             |             |             |

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## DI-3i



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2366479.9 (Joules/Mol)      |
|                                              | 565.60227 (Kcal/Mol)        |
| Zero-point correction=                       | 0.901345 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.957150                    |
| Thermal correction to Enthalpy=              | 0.958094                    |
| Thermal correction to Gibbs Free Energy=     | 0.809885                    |
| Sum of electronic and zero-point Energies=   | -2711.292350                |
| Sum of electronic and thermal Energies=      | -2711.236545                |
| Sum of electronic and thermal Enthalpies=    | -2711.235601                |
| Sum of electronic and thermal Free Energies= | -2711.383810                |

| cartesian |             |             |             |   |             |            |             |  |  |  |  |
|-----------|-------------|-------------|-------------|---|-------------|------------|-------------|--|--|--|--|
| 12        | 1.61461520  | -0.36706188 | -0.07907338 | 6 | -4.84858465 | 1.19083810 | 1.37392652  |  |  |  |  |
| 8         | -1.22338474 | -2.45706201 | 0.05442663  | 6 | -4.65568447 | 0.42493814 | -2.44847322 |  |  |  |  |
| 8         | 3.35091519  | 0.22053812  | -0.31317338 | 6 | -4.00308466 | 1.15523803 | 2.66052675  |  |  |  |  |
| 6         | -2.44038486 | -3.27376199 | 0.28832662  | 6 | -3.38218474 | 1.19933808 | -2.84067321 |  |  |  |  |
| 1         | -2.52978468 | -3.99146199 | -0.52937341 | 1 | -2.57638478 | 1.05343807 | -2.11997342 |  |  |  |  |
| 1         | -3.25188470 | -2.54916191 | 0.21852662  | 1 | -3.02798486 | 0.88103813 | -3.82947326 |  |  |  |  |

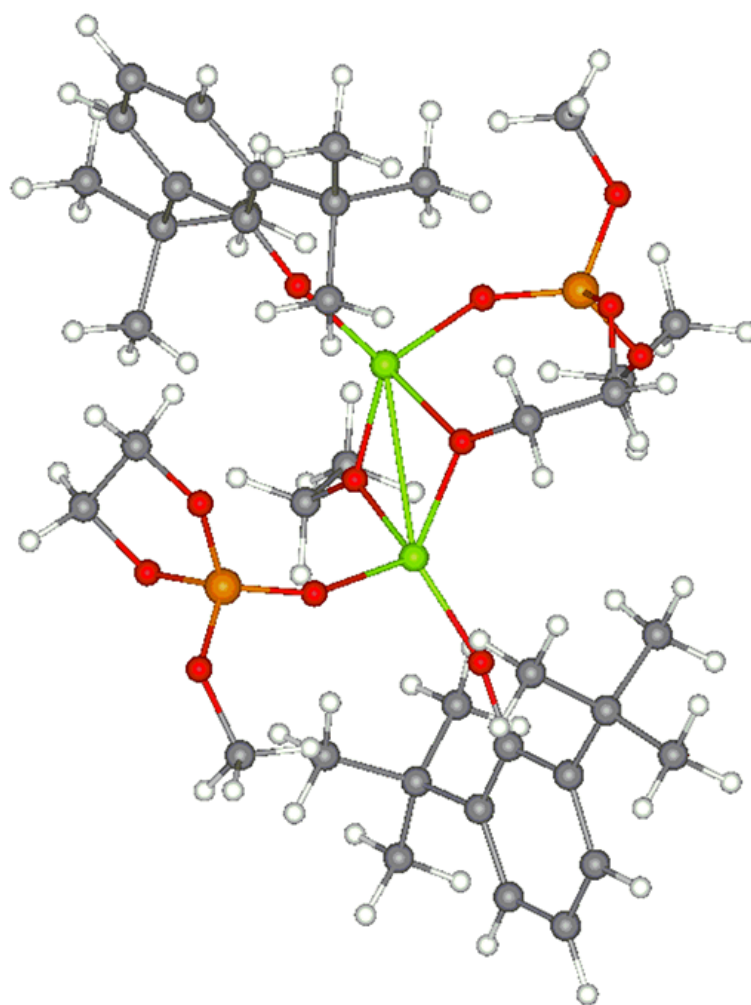
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 4.53621531  | 0.81893814  | -0.22097339 | 1  | -3.58948469 | 2.27333808  | -2.89137340 |
| 6  | 4.73921537  | 2.10923815  | -0.80527335 | 6  | -4.39958429 | -1.09366190 | -2.45347333 |
| 6  | 5.99331570  | 2.71213818  | -0.66837335 | 1  | -3.66208482 | -1.36666191 | -1.69697344 |
| 1  | 6.17031527  | 3.69323802  | -1.09637344 | 1  | -5.32428455 | -1.63826191 | -2.23337340 |
| 6  | 7.04101563  | 2.09273815  | 0.00402662  | 1  | -4.04288435 | -1.42506194 | -3.43747330 |
| 6  | 6.84261560  | 0.82823813  | 0.54702663  | 6  | -5.68598461 | 0.69663817  | -3.55937338 |
| 1  | 7.67491531  | 0.35493815  | 1.05692661  | 1  | -6.61968470 | 0.14593811  | -3.40527320 |
| 6  | 5.61631536  | 0.16363813  | 0.45032662  | 1  | -5.92418432 | 1.76113808  | -3.65247321 |
| 6  | 3.62351537  | 2.83103800  | -1.58467340 | 1  | -5.27238464 | 0.37073815  | -4.52047348 |
| 6  | 5.46011543  | -1.24646187 | 1.05032659  | 6  | -4.77428436 | 1.66663814  | 3.89142680  |
| 6  | 2.43041515  | 3.14893818  | -0.66197336 | 1  | -5.07978439 | 2.71243811  | 3.78642678  |
| 1  | 2.02311540  | 2.25413799  | -0.18937337 | 1  | -5.66488457 | 1.06553805  | 4.10242653  |
| 1  | 1.62401521  | 3.63333797  | -1.22637343 | 1  | -4.12478447 | 1.60713804  | 4.77172661  |
| 1  | 2.73791528  | 3.82903814  | 0.13942662  | 6  | -3.56968474 | -0.28406188 | 2.99982667  |
| 6  | 3.17371535  | 1.97143817  | -2.78357339 | 1  | -2.99098468 | -0.73626184 | 2.19252658  |
| 1  | 2.84851527  | 0.98033816  | -2.46437335 | 1  | -2.96518469 | -0.30206186 | 3.91452670  |
| 1  | 4.00191545  | 1.83953810  | -3.48837328 | 1  | -4.44928455 | -0.91566187 | 3.16642666  |
| 1  | 2.34801531  | 2.45803809  | -3.31777334 | 6  | -2.78458476 | 2.08633804  | 2.50242662  |
| 6  | 4.08871555  | 4.17793846  | -2.16637325 | 1  | -3.11688471 | 3.11493802  | 2.32822680  |
| 1  | 4.92661572  | 4.06133842  | -2.86157322 | 1  | -2.16608477 | 2.08133817  | 3.40732670  |
| 1  | 4.38411570  | 4.88833809  | -1.38707340 | 1  | -2.14978480 | 1.80963802  | 1.65742660  |
| 1  | 3.26241517  | 4.63323832  | -2.72417331 | 6  | -2.39118481 | -3.94196200 | 1.64172661  |
| 6  | 6.76481533  | -1.76256192 | 1.68442655  | 1  | 0.99191523  | -0.64816189 | 3.04002666  |
| 1  | 7.09921551  | -1.13706183 | 2.51892662  | 1  | -7.94618464 | 2.23523808  | 0.36282665  |
| 1  | 7.58001566  | -1.83076191 | 0.95642668  | 1  | 8.00471497  | 2.58753800  | 0.09712662  |
| 1  | 6.59731531  | -2.77036190 | 2.08142662  | 8  | 1.35541523  | -2.41036201 | -0.14297338 |
| 6  | 5.07991552  | -2.25656199 | -0.05147338 | 15 | 0.10311527  | -3.04556203 | -0.65357339 |
| 1  | 4.15501547  | -1.97696197 | -0.55627340 | 8  | -0.12138474 | -3.01386189 | -2.22037339 |
| 1  | 4.95401525  | -3.25906181 | 0.37772661  | 8  | 0.04091527  | -0.25606188 | -1.34727347 |
| 1  | 5.87381554  | -2.31026196 | -0.80457336 | 6  | -0.63688475 | -1.88536191 | -2.98697329 |
| 6  | 4.40731525  | -1.24476194 | 2.17622662  | 6  | 0.10091527  | -0.59226185 | -2.70717335 |
| 1  | 4.71601534  | -0.57806188 | 2.98852658  | 1  | -1.69948471 | -1.79016197 | -2.75307322 |
| 1  | 4.28221560  | -2.25206184 | 2.59232664  | 1  | -0.52628475 | -2.19066191 | -4.02937365 |
| 1  | 3.43391514  | -0.90166187 | 1.82212663  | 1  | 1.14491522  | -0.69216186 | -3.03557324 |
| 12 | -1.29728472 | -0.13366188 | 0.09642662  | 1  | -0.35898474 | 0.18423812  | -3.33497334 |
| 8  | 0.23681527  | 0.08953811  | 1.26382661  | 8  | 0.03351526  | -4.59446192 | -0.32687336 |
| 8  | -3.12338471 | 0.19233812  | 0.02692662  | 6  | 1.20321524  | -5.42626190 | -0.52757341 |
| 6  | 0.42971525  | 0.22023813  | 2.66512680  | 1  | 1.37811530  | -5.56396151 | -1.59627342 |
| 6  | 1.16941524  | 1.50003803  | 3.02182674  | 1  | 2.07191515  | -4.97166157 | -0.04937338 |
| 1  | -0.54288477 | 0.20473813  | 3.17262673  | 1  | 0.96911526  | -6.38176155 | -0.06127338 |
| 6  | -4.34198427 | 0.73953813  | 0.11442661  | 1  | -3.34008479 | -4.46286154 | 1.80562663  |

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|   |             |            |             |   |             |             |            |
|---|-------------|------------|-------------|---|-------------|-------------|------------|
| 6 | -5.15178442 | 0.86613816 | -1.05877340 | 1 | -1.58208477 | -4.67186165 | 1.69822657 |
| 6 | -6.43538427 | 1.40573812 | -0.93127334 | 1 | -2.26858473 | -3.20476198 | 2.43802667 |
| 1 | -7.06718445 | 1.50923812 | -1.80657339 | 1 | 1.30771530  | 1.57293808  | 4.10652685 |
| 6 | -6.94258451 | 1.82343805 | 0.29272664  | 1 | 2.15801525  | 1.52693808  | 2.55302668 |
| 6 | -6.14418459 | 1.71533811 | 1.42412663  | 1 | 0.60931528  | 2.37763810  | 2.68562675 |
| 1 | -6.55098438 | 2.05683804 | 2.36932659  |   |             |             |            |

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## DI-3



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2674867.4 (Joules/Mol)      |
|                                              | 639.30865 (Kcal/Mol)        |
| Zero-point correction=                       | 1.018803 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.084629                    |
| Thermal correction to Enthalpy=              | 1.085573                    |
| Thermal correction to Gibbs Free Energy=     | 0.911889                    |
| Sum of electronic and zero-point Energies=   | -3471.884180                |
| Sum of electronic and thermal Energies=      | -3471.818355                |
| Sum of electronic and thermal Enthalpies=    | -3471.817411                |
| Sum of electronic and thermal Free Energies= | -3471.991094                |

cartesian

|    |             |             |             |   |             |            |            |
|----|-------------|-------------|-------------|---|-------------|------------|------------|
| 12 | 1.39179766  | 0.57710826  | -0.25066918 | 6 | -3.80180240 | 2.07320833 | 2.36733079 |
| 8  | 0.09679771  | 4.50490808  | -0.26006916 | 1 | -3.11060238 | 1.97310817 | 1.52943087 |
| 8  | 2.98979759  | -0.39779174 | 0.02983083  | 1 | -4.50360250 | 2.87960839 | 2.12753081 |
| 6  | -0.16790231 | 4.64860821  | -1.68766928 | 1 | -3.24320245 | 2.37220836 | 3.26393080 |

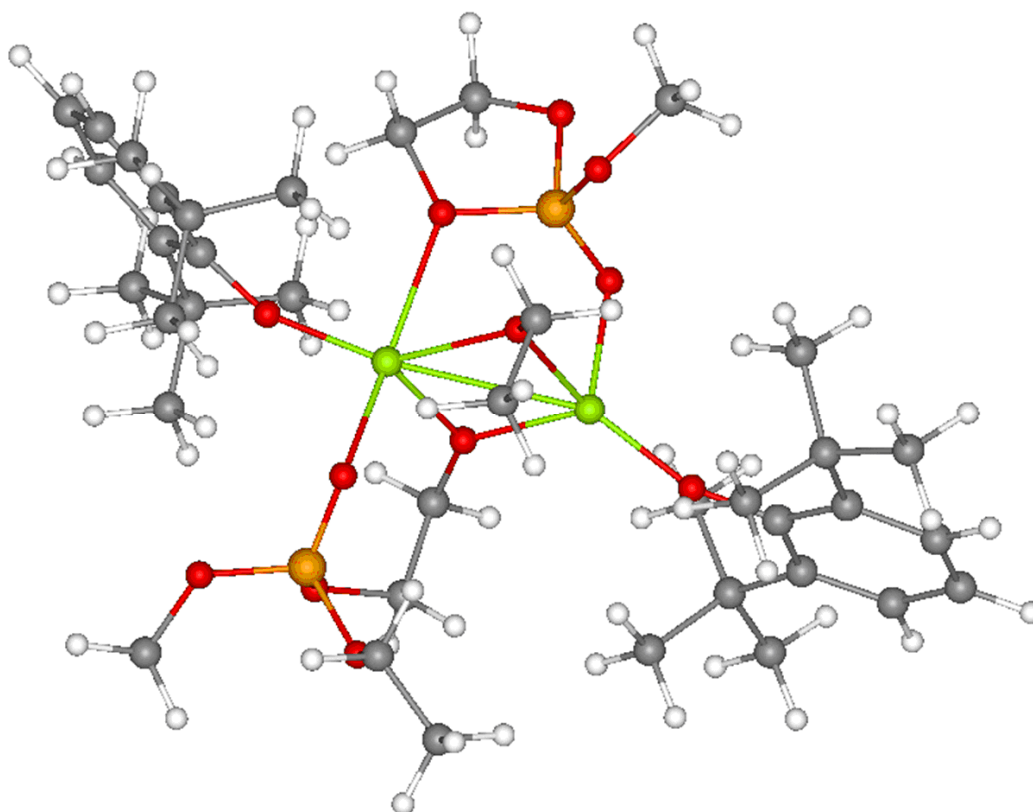
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1  | -1.24830234 | 4.52560806  | -1.77776909 | 6  | -5.52230215 | 1.03390825  | 3.79713082  |
| 1  | 0.31869772  | 3.82960844  | -2.22216916 | 1  | -6.23220253 | 1.83750820  | 3.57523084  |
| 6  | 4.22669744  | -0.85729170 | 0.19313082  | 1  | -6.08930254 | 0.14430827  | 4.09133101  |
| 6  | 5.01029778  | -1.25959182 | -0.93976921 | 1  | -4.93690252 | 1.34740818  | 4.66933107  |
| 6  | 6.28569746  | -1.79129171 | -0.72456914 | 6  | -5.69490242 | -0.71369171 | -3.56096911 |
| 1  | 6.88849783  | -2.10319161 | -1.57056928 | 1  | -6.30160236 | -1.61109173 | -3.40016913 |
| 6  | 6.82209778  | -1.93549180 | 0.54933083  | 1  | -6.36930227 | 0.13780826  | -3.70056915 |
| 6  | 6.07359743  | -1.51639175 | 1.64303088  | 1  | -5.14950228 | -0.85649168 | -4.50086927 |
| 1  | 6.51259756  | -1.61879182 | 2.62953091  | 6  | -3.85150242 | 0.75510830  | -2.84016919 |
| 6  | 4.79399776  | -0.96899170 | 1.50673079  | 1  | -3.09920239 | 1.00830829  | -2.09236908 |
| 6  | 4.48429775  | -1.12319171 | -2.37976909 | 1  | -3.35030246 | 0.57290828  | -3.79896903 |
| 6  | 4.05269766  | -0.46679175 | 2.75973082  | 1  | -4.50490236 | 1.62610829  | -2.96406913 |
| 6  | 4.17169762  | 0.35140827  | -2.70316911 | 6  | -3.81280231 | -1.74159181 | -2.34456921 |
| 1  | 3.47419763  | 0.79160827  | -1.98986912 | 1  | -4.44170237 | -2.61649156 | -2.14306903 |
| 1  | 3.74539757  | 0.44440827  | -3.70946908 | 1  | -3.28870225 | -1.91889179 | -3.29176903 |
| 1  | 5.09019756  | 0.94770831  | -2.67156911 | 1  | -3.07240224 | -1.68169177 | -1.54456925 |
| 6  | 3.23679757  | -2.00619173 | -2.56746912 | 6  | 0.28459772  | 6.00600815  | -2.18086910 |
| 1  | 2.45659757  | -1.75489175 | -1.84716916 | 1  | -1.17360234 | -0.79989171 | -2.98006916 |
| 1  | 3.50799775  | -3.06029153 | -2.43216920 | 1  | -8.51640224 | -0.21449172 | 0.27673084  |
| 1  | 2.82869768  | -1.89569175 | -3.57966900 | 1  | 7.81499767  | -2.35639167 | 0.68723083  |
| 6  | 5.50659752  | -1.58499181 | -3.43406916 | 8  | 1.77759767  | 2.54530835  | -0.50296915 |
| 1  | 5.76489782  | -2.64409161 | -3.32956910 | 15 | 1.36529768  | 3.74910831  | 0.29643083  |
| 1  | 6.43149757  | -0.99989170 | -3.39926910 | 8  | 1.03799760  | 3.49020839  | 1.81553078  |
| 1  | 5.07549763  | -1.45349181 | -4.43306923 | 8  | -0.06530229 | 0.74820828  | 1.10433078  |
| 6  | 4.86249781  | -0.67829168 | 4.05183077  | 6  | -0.18420230 | 2.85880828  | 2.31163096  |
| 1  | 5.81919765  | -0.14559174 | 4.03803062  | 6  | -0.07840229 | 1.34680820  | 2.37053084  |
| 1  | 5.06039762  | -1.73739171 | 4.24933100  | 1  | -1.02030230 | 3.17810845  | 1.68613076  |
| 1  | 4.28839779  | -0.29189172 | 4.90163088  | 1  | -0.30850229 | 3.27430844  | 3.31413078  |
| 6  | 2.72099757  | -1.21459174 | 2.95723081  | 1  | 0.81979769  | 1.07940829  | 2.94313097  |
| 1  | 2.04709768  | -1.08709180 | 2.10993099  | 1  | -0.94200230 | 1.00620818  | 2.96023083  |
| 1  | 2.20999765  | -0.85849172 | 3.86043096  | 8  | 2.50839758  | 4.84750795  | 0.32813084  |
| 1  | 2.90439773  | -2.28669167 | 3.08873081  | 6  | 3.88119769  | 4.47290802  | 0.58343083  |
| 6  | 3.81819773  | 1.05120826  | 2.63783097  | 1  | 4.00609779  | 4.22620821  | 1.63923073  |
| 1  | 4.77939749  | 1.57590818  | 2.59463096  | 1  | 4.16879749  | 3.62680840  | -0.04316917 |
| 1  | 3.26509762  | 1.43370819  | 3.50443077  | 1  | 4.47899771  | 5.34790802  | 0.33203083  |
| 1  | 3.26229763  | 1.30080819  | 1.73283076  | 1  | 0.01069771  | 6.11540794  | -3.23506904 |
| 12 | -1.44970238 | -0.22009173 | 0.04933083  | 1  | -0.19860230 | 6.80610800  | -1.61476922 |
| 8  | -0.08650229 | -0.08029173 | -1.38176918 | 1  | 1.36749768  | 6.12190819  | -2.09306908 |
| 8  | -3.28820229 | 0.18330827  | 0.05823083  | 1  | 0.01799771  | 0.52510828  | -4.70756912 |
| 6  | -0.17640230 | -0.40039173 | -2.75766921 | 1  | -0.65910226 | 1.58970821  | -3.46086907 |
| 6  | 0.08149771  | 0.80620831  | -3.64976907 | 1  | 1.07899761  | 1.22220826  | -3.47126913 |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1 | 0.53769773  | -1.19659173 | -3.00496912 | 8  | -1.38730240 | -2.17519164 | 0.62283081  |
| 6 | -4.61310244 | 0.09440827  | 0.10953083  | 15 | -0.78270227 | -3.53289175 | 0.66303080  |
| 6 | -5.31000233 | 0.33920828  | 1.33903074  | 8  | 0.53459769  | -3.75829172 | 1.53243089  |
| 6 | -6.70210218 | 0.21220827  | 1.36223078  | 8  | -0.22020230 | -4.01799154 | -0.76026917 |
| 1 | -7.24370241 | 0.38610825  | 2.28583097  | 6  | 1.66689765  | -4.03399181 | 0.66473085  |
| 6 | -7.43370247 | -0.12579173 | 0.22963083  | 6  | 1.05839765  | -4.67309189 | -0.58336920 |
| 6 | -6.75860214 | -0.33209175 | -0.96766919 | 1  | 2.33359766  | -4.70629168 | 1.20373082  |
| 1 | -7.34390211 | -0.57849169 | -1.84726906 | 1  | 2.17669773  | -3.09289169 | 0.44833082  |
| 6 | -5.36780214 | -0.22849172 | -1.06626916 | 1  | 1.64899766  | -4.49019194 | -1.47976923 |
| 6 | -4.56860256 | 0.76030827  | 2.62043095  | 1  | 0.88449770  | -5.74549198 | -0.45646918 |
| 6 | -4.68550253 | -0.47339174 | -2.42376900 | 8  | -1.78460228 | -4.60879183 | 1.24303079  |
| 6 | -3.61410236 | -0.35609174 | 3.08703089  | 6  | -3.22160244 | -4.44269180 | 1.13483071  |
| 1 | -2.89510226 | -0.63219172 | 2.31483078  | 1  | -3.49940228 | -3.39979172 | 1.28753090  |
| 1 | -3.06150246 | -0.04729173 | 3.98363090  | 1  | -3.55110240 | -4.78529167 | 0.15243083  |
| 1 | -4.18310213 | -1.25669181 | 3.34473085  | 1  | -3.64950228 | -5.07029200 | 1.91473079  |

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## DTS-34a



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2677556.9 (Joules/Mol)      |
|                                              | 639.95145 (Kcal/Mol)        |
| Zero-point correction=                       | 1.019828 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.084439                    |
| Thermal correction to Enthalpy=              | 1.085384                    |
| Thermal correction to Gibbs Free Energy=     | 0.918929                    |
| Sum of electronic and zero-point Energies=   | -3471.860748                |
| Sum of electronic and thermal Energies=      | -3471.796136                |
| Sum of electronic and thermal Enthalpies=    | -3471.795192                |
| Sum of electronic and thermal Free Energies= | -3471.961647                |

cartesian

|    |             |             |             |   |            |            |             |
|----|-------------|-------------|-------------|---|------------|------------|-------------|
| 12 | -1.28265727 | -0.03242502 | 0.23479581  | 6 | 3.82534266 | 2.26117492 | -2.16570401 |
| 8  | -0.02175735 | 4.04617500  | 1.40289581  | 1 | 3.20124269 | 1.97767508 | -1.31700420 |
| 8  | -3.14255738 | 0.00317498  | -0.16950417 | 1 | 4.54464293 | 3.00957489 | -1.81520414 |
| 6  | 0.25744265  | 3.97557497  | 2.83069587  | 1 | 3.19954252 | 2.73347497 | -2.93430400 |
| 1  | 0.35414264  | 2.92527485  | 3.11419582  | 6 | 5.43534279 | 1.57067502 | -3.90140414 |
| 1  | -0.59315735 | 4.40747499  | 3.36759591  | 1 | 6.16084290 | 2.31877494 | -3.56560397 |
| 6  | -4.37325716 | -0.43862504 | -0.38270417 | 1 | 5.97764301 | 0.77097499 | -4.41650391 |
| 6  | -5.17485714 | -0.93472499 | 0.70109582  | 1 | 4.78894281 | 2.05317497 | -4.64360428 |

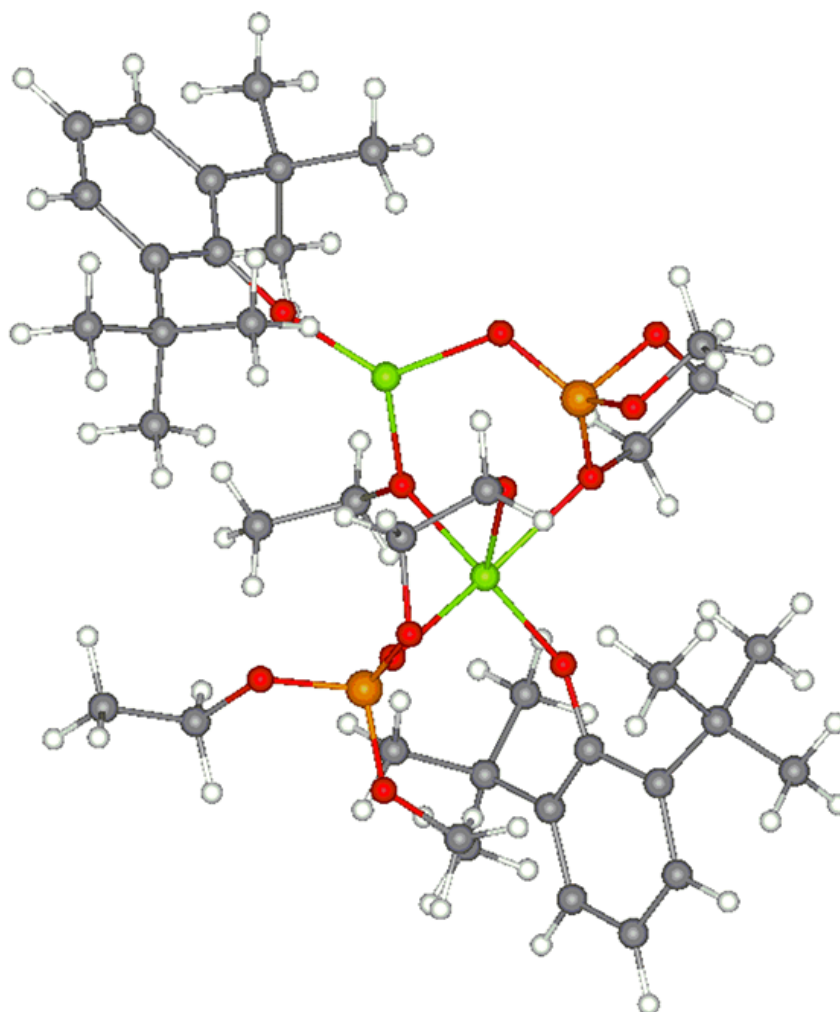
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | -6.41485739 | -1.51042497 | 0.40719581  | 6  | 6.13624287  | -1.73722494 | 2.86529589  |
| 1  | -7.02525711 | -1.91222501 | 1.20909584  | 1  | 6.71434259  | -2.57652521 | 2.46489596  |
| 6  | -6.91295719 | -1.58002496 | -0.88950419 | 1  | 6.83264303  | -0.93702501 | 3.13699603  |
| 6  | -6.17815733 | -1.00742507 | -1.92190421 | 1  | 5.66094303  | -2.08392501 | 3.79039598  |
| 1  | -6.60475731 | -1.02112508 | -2.91950417 | 6  | 4.26764297  | -0.14702502 | 2.62379599  |
| 6  | -4.92965698 | -0.41422501 | -1.70750415 | 1  | 3.48854256  | 0.27857497  | 1.99059570  |
| 6  | -4.72695732 | -0.80962497 | 2.17099595  | 1  | 3.80824256  | -0.53992504 | 3.53949594  |
| 6  | -4.21045732 | 0.28447497  | -2.87860417 | 1  | 4.94514275  | 0.66517502  | 2.90999603  |
| 6  | -4.41285706 | 0.66347498  | 2.50219584  | 6  | 4.15094280  | -2.47402501 | 1.60409582  |
| 1  | -3.63775730 | 1.07557499  | 1.85689580  | 1  | 4.74034262  | -3.27772522 | 1.14919579  |
| 1  | -4.08395720 | 0.75667500  | 3.54519582  | 1  | 3.71604252  | -2.85972500 | 2.53489590  |
| 1  | -5.31295729 | 1.27607501  | 2.37969589  | 1  | 3.33864260  | -2.24032521 | 0.91359580  |
| 6  | -3.50545740 | -1.70152497 | 2.45989585  | 6  | 1.53014266  | 4.74627495  | 3.09619594  |
| 1  | -2.67515731 | -1.49682498 | 1.78299582  | 1  | 1.40164268  | -1.92992496 | 2.60949588  |
| 1  | -3.76435733 | -2.75992513 | 2.34099603  | 1  | 8.67454243  | -0.35982502 | -0.95410419 |
| 1  | -3.15325737 | -1.55722499 | 3.48869586  | 1  | -7.87755728 | -2.04102516 | -1.08710420 |
| 6  | -5.82245731 | -1.25292504 | 3.15809584  | 8  | -1.21375728 | 1.76137495  | 1.27319586  |
| 1  | -6.07405710 | -2.31462502 | 3.06069589  | 15 | -1.18075728 | 3.16127491  | 0.75749582  |
| 1  | -6.74115705 | -0.66902500 | 3.04079604  | 8  | -0.96235734 | 3.36557484  | -0.79110420 |
| 1  | -5.46525717 | -1.09942496 | 4.18279600  | 8  | 0.17734265  | 0.56427503  | -1.01190412 |
| 6  | -5.06595707 | 0.31657496  | -4.15790415 | 6  | 0.24614263  | 2.95247483  | -1.49930418 |
| 1  | -6.02145720 | 0.82797498  | -4.00230408 | 6  | 0.12904266  | 1.53447497  | -2.02480412 |
| 1  | -5.27145720 | -0.68502498 | -4.55080414 | 1  | 1.10764265  | 3.06897497  | -0.83770418 |
| 1  | -4.52455711 | 0.86347502  | -4.93820429 | 1  | 0.33394265  | 3.66207480  | -2.32500410 |
| 6  | -2.90335751 | -0.44112504 | -3.24980402 | 1  | -0.80455738 | 1.45667505  | -2.59670401 |
| 1  | -2.21285748 | -0.49842504 | -2.40650415 | 1  | 0.95264262  | 1.39997506  | -2.74050403 |
| 1  | -2.39315748 | 0.07687498  | -4.07170391 | 8  | -2.56415749 | 3.87527490  | 1.04269576  |
| 1  | -3.11575747 | -1.46062505 | -3.59380412 | 6  | -2.84245753 | 5.20097494  | 0.54939580  |
| 6  | -3.92255735 | 1.75297499  | -2.50730395 | 1  | -2.06245732 | 5.90057468  | 0.86069584  |
| 1  | -4.86215734 | 2.28777480  | -2.32920408 | 1  | -2.92155743 | 5.18217468  | -0.53860420 |
| 1  | -3.39765739 | 2.26047492  | -3.32700396 | 1  | -3.79645753 | 5.48757505  | 0.98969579  |
| 1  | -3.31695747 | 1.82767498  | -1.60420418 | 1  | 1.75574267  | 4.71587467  | 4.16619587  |
| 12 | 1.67284274  | -0.55152500 | -0.35960418 | 1  | 2.37184262  | 4.30787468  | 2.55469584  |
| 8  | 0.27704263  | -1.18282497 | 1.04519582  | 1  | 1.42634273  | 5.79207468  | 2.79569602  |
| 8  | 3.47754264  | -0.07852502 | -0.27670416 | 1  | 0.67944264  | -0.32902503 | 4.30319595  |
| 6  | 0.46154267  | -1.39182496 | 2.45529604  | 1  | 1.26074266  | 0.57497501  | 2.89729595  |
| 6  | 0.47504264  | -0.09882502 | 3.25139594  | 1  | -0.48175737 | 0.42547497  | 3.19549584  |
| 1  | -0.34115735 | -2.04182506 | 2.82149601  | 8  | 1.21214271  | -2.38492513 | -1.02110410 |
| 6  | 4.79894304  | -0.14412501 | -0.44540417 | 15 | 0.09014264  | -3.02082515 | -0.23900416 |
| 6  | 5.40224266  | 0.37087497  | -1.63780415 | 8  | -0.37725735 | -4.33052492 | -1.12060416 |
| 6  | 6.78884268  | 0.27297497  | -1.78650415 | 8  | -1.39045727 | -2.32422519 | -0.27530417 |

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|   |            |             |             |   |             |             |             |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 7.26254272 | 0.65117502  | -2.68610406 | 6 | -1.59535730 | -4.07292509 | -1.82540417 |
| 6 | 7.59864283 | -0.29602501 | -0.81090420 | 6 | -2.39305735 | -3.18122506 | -0.89090419 |
| 6 | 7.01154280 | -0.77252501 | 0.35499582  | 1 | -2.08915734 | -5.02712488 | -2.01590419 |
| 1 | 7.65734291 | -1.20282495 | 1.11279583  | 1 | -1.37465727 | -3.57622504 | -2.77620411 |
| 6 | 5.63184261 | -0.71072501 | 0.57229584  | 1 | -3.11925745 | -2.53622508 | -1.38140416 |
| 6 | 4.56864262 | 1.04137504  | -2.74450397 | 1 | -2.87645745 | -3.74742508 | -0.09180418 |
| 6 | 5.04834270 | -1.25412500 | 1.88859582  | 8 | 0.43254265  | -3.75332522 | 1.13329577  |
| 6 | 3.58544254 | 0.03427498  | -3.37210417 | 6 | 1.00444269  | -5.08052492 | 1.14839578  |
| 1 | 2.91464257 | -0.41012502 | -2.63520408 | 1 | 0.29754263  | -5.80312490 | 0.73939580  |
| 1 | 2.97594261 | 0.51677501  | -4.14650393 | 1 | 1.93714273  | -5.10142517 | 0.58139580  |
| 1 | 4.13154268 | -0.79062498 | -3.84130406 | 1 | 1.20604265  | -5.29342508 | 2.19769597  |

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# DTS-34b



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2675402.3 (Joules/Mol)      |
|                                              | 639.43649 (Kcal/Mol)        |
| Zero-point correction=                       | 1.019007 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.083277                    |
| Thermal correction to Enthalpy=              | 1.084221                    |
| Thermal correction to Gibbs Free Energy=     | 0.918416                    |
| Sum of electronic and zero-point Energies=   | -3471.853723                |
| Sum of electronic and thermal Energies=      | -3471.789452                |
| Sum of electronic and thermal Enthalpies=    | -3471.788508                |
| Sum of electronic and thermal Free Energies= | -3471.954313                |

| cartesian |            |             |             |   |             |            |            |
|-----------|------------|-------------|-------------|---|-------------|------------|------------|
| 12        | 1.29129159 | -0.34226170 | -0.08221585 | 6 | -3.59640837 | 2.72733831 | 0.77288413 |
| 8         | 0.35969162 | 3.82743835  | 1.27178407  | 1 | -2.96420836 | 2.02323842 | 0.22948414 |
| 8         | 3.10579157 | -0.68396175 | -0.59791589 | 1 | -4.02400827 | 3.42003846 | 0.03948414 |

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|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 0.39459160  | 4.69233799  | 0.09858415  | 1  | -2.96940827 | 3.30873847  | 1.46068406  |
| 1  | 0.17149162  | 4.08373833  | -0.78131580 | 6  | -5.53350830 | 3.10563850  | 2.25438428  |
| 1  | 1.40479159  | 5.10153818  | 0.00438415  | 1  | -5.97570801 | 3.81373835  | 1.54568410  |
| 6  | 4.36579180  | -0.27166170 | -0.68541586 | 1  | -6.33610821 | 2.69263840  | 2.87408423  |
| 6  | 4.83299208  | 0.42013830  | -1.85401595 | 1  | -4.87240791 | 3.67693830  | 2.91618419  |
| 6  | 6.12199163  | 0.96313822  | -1.84371579 | 6  | -6.39640808 | -2.62756157 | -2.61391568 |
| 1  | 6.47889185  | 1.51523829  | -2.70651579 | 1  | -7.19890833 | -3.03406167 | -1.98971593 |
| 6  | 6.98129177  | 0.81353831  | -0.76111591 | 1  | -6.84230804 | -1.96096170 | -3.35941577 |
| 6  | 6.56899166  | 0.03703830  | 0.31688416  | 1  | -5.94890833 | -3.46906161 | -3.15491581 |
| 1  | 7.27499199  | -0.12886170 | 1.12368417  | 6  | -4.23070812 | -1.47176170 | -2.78601575 |
| 6  | 5.29669189  | -0.54076171 | 0.37808415  | 1  | -3.43290830 | -0.90526175 | -2.30241585 |
| 6  | 3.96579170  | 0.57053828  | -3.11951566 | 1  | -3.78890848 | -2.33436155 | -3.30031586 |
| 6  | 4.96389198  | -1.49926174 | 1.54058409  | 1  | -4.66850805 | -0.81556165 | -3.54601574 |
| 6  | 2.82599163  | 1.57563829  | -2.87391567 | 6  | -4.75210810 | -2.99276161 | -0.81601584 |
| 1  | 2.20719171  | 1.30053830  | -2.01991582 | 1  | -5.55690813 | -3.38786173 | -0.18721586 |
| 1  | 2.18139172  | 1.65833831  | -3.75801587 | 1  | -4.32120800 | -3.83286166 | -1.37441587 |
| 1  | 3.23679161  | 2.57033849  | -2.66561580 | 1  | -3.98870826 | -2.60636163 | -0.13881585 |
| 6  | 3.40609169  | -0.79856169 | -3.55701566 | 6  | -0.62590837 | 5.78913832  | 0.29508415  |
| 1  | 2.82039165  | -1.26726174 | -2.76551580 | 1  | -1.17560840 | -0.82816172 | -3.00491571 |
| 1  | 4.22649193  | -1.47796178 | -3.81421590 | 1  | -8.82320881 | 0.88993835  | -0.44741586 |
| 1  | 2.77489161  | -0.68476176 | -4.44721603 | 1  | 7.97469187  | 1.25523829  | -0.77711582 |
| 6  | 4.76819181  | 1.10573828  | -4.32051611 | 8  | 1.39069164  | 1.66773832  | 0.28188413  |
| 1  | 5.63019180  | 0.47213832  | -4.55461597 | 15 | 1.40019166  | 2.64243841  | 1.41748416  |
| 1  | 5.12499189  | 2.12973833  | -4.16781616 | 8  | 1.01759160  | 1.97533834  | 2.80178428  |
| 1  | 4.12099171  | 1.12233829  | -5.20471621 | 8  | 0.24859163  | -0.85226166 | 1.67818415  |
| 6  | 6.17499208  | -1.75896168 | 2.45518422  | 6  | -0.23010837 | 1.23373830  | 2.90758419  |
| 1  | 6.51069164  | -0.85566175 | 2.97628427  | 6  | -0.02470837 | -0.26436171 | 2.94988418  |
| 1  | 7.02549171  | -2.17586160 | 1.90618408  | 1  | -0.91790837 | 1.53343832  | 2.11188412  |
| 1  | 5.89299202  | -2.48726153 | 3.22388434  | 1  | -0.66230839 | 1.54823828  | 3.86008430  |
| 6  | 4.54909182  | -2.86496162 | 0.96028411  | 1  | 0.78219163  | -0.50006169 | 3.65028429  |
| 1  | 3.68309164  | -2.75106168 | 0.30988413  | 1  | -0.95230836 | -0.68956172 | 3.35188413  |
| 1  | 4.29889202  | -3.56626153 | 1.76668417  | 8  | 2.77019167  | 3.38123846  | 1.65738416  |
| 1  | 5.36869192  | -3.29686165 | 0.37588415  | 6  | 4.06389189  | 2.78033829  | 1.38138413  |
| 6  | 3.84549165  | -0.95596170 | 2.44778419  | 1  | 4.74879169  | 3.61393833  | 1.23618412  |
| 1  | 4.15289164  | -0.02266170 | 2.93118429  | 1  | 4.37099171  | 2.18593836  | 2.24098420  |
| 1  | 3.61259151  | -1.67666173 | 3.24108434  | 1  | 4.02369165  | 2.16273832  | 0.48428416  |
| 1  | 2.92459154  | -0.77206171 | 1.89528418  | 1  | -0.61380839 | 6.45223808  | -0.57511580 |
| 12 | -2.00660849 | -0.87316167 | -0.01961586 | 1  | -1.63090837 | 5.37453794  | 0.39798415  |
| 8  | -0.45520839 | -0.41006172 | -1.10321593 | 1  | -0.39470840 | 6.38123798  | 1.18398416  |
| 8  | -3.70660830 | -0.16716170 | -0.07151586 | 1  | -1.16420841 | 1.52553833  | -3.79821587 |
| 6  | -0.54910839 | -0.08486170 | -2.49121571 | 1  | -2.12610841 | 1.39563823  | -2.31511569 |

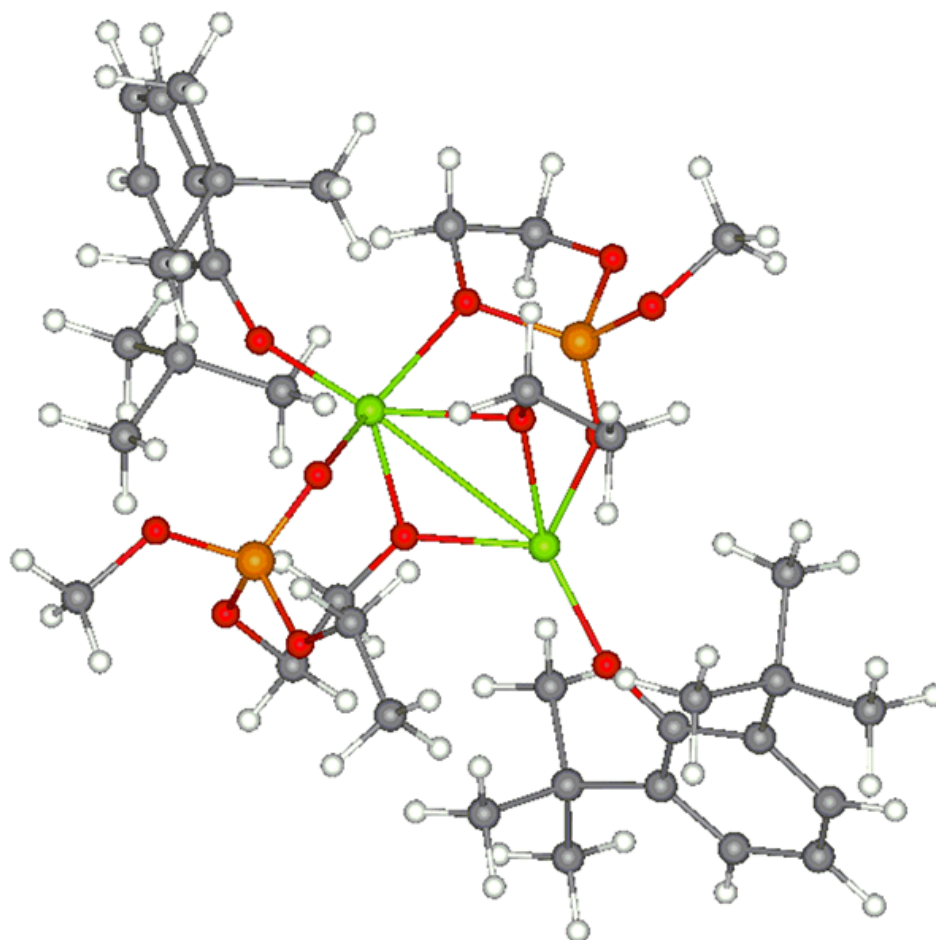
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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -1.11490834 | 1.30673826  | -2.72551584 | 1  | -0.48070836 | 2.05993843  | -2.24901581 |
| 1 | 0.44589162  | -0.15866169 | -2.94741583 | 8  | -1.60670841 | -2.38366151 | 1.13678420  |
| 6 | -5.01350832 | 0.07973829  | -0.15601584 | 15 | -0.14330837 | -2.69836164 | 1.45758414  |
| 6 | -5.57710838 | 1.15743828  | 0.59518415  | 8  | 1.02079165  | -2.47496152 | 0.28608415  |
| 6 | -6.94360828 | 1.42083824  | 0.46498415  | 8  | -0.17690837 | -4.35046196 | 1.12438416  |
| 1 | -7.39200830 | 2.23703837  | 1.02128410  | 6  | 1.16889167  | -3.59306169 | -0.60841584 |
| 6 | -7.76350832 | 0.66193831  | -0.36221585 | 6  | 0.86419159  | -4.79116201 | 0.27148414  |
| 6 | -7.21220827 | -0.39896169 | -1.07131588 | 1  | 2.18519163  | -3.56656170 | -0.99971592 |
| 1 | -7.86960793 | -0.98806167 | -1.70161593 | 1  | 0.44569162  | -3.48376155 | -1.42191589 |
| 6 | -5.85370827 | -0.72156167 | -0.99101591 | 1  | 0.50889164  | -5.64926195 | -0.30391586 |
| 6 | -4.71830797 | 2.00823832  | 1.54748416  | 1  | 1.74819160  | -5.08566189 | 0.85248411  |
| 6 | -5.30770826 | -1.92606175 | -1.78121591 | 8  | 0.29939163  | -2.85316157 | 2.99998426  |
| 6 | -4.12740803 | 1.11713827  | 2.65928435  | 6  | 0.10539162  | -4.06696177 | 3.74948430  |
| 1 | -3.52330828 | 0.30523831  | 2.24858427  | 1  | -0.91800839 | -4.43176174 | 3.65138435  |
| 1 | -3.50820827 | 1.71363831  | 3.34178424  | 1  | 0.80389160  | -4.83866167 | 3.42378426  |
| 1 | -4.92900801 | 0.66013825  | 3.24918413  | 1  | 0.30739161  | -3.79606152 | 4.78688383  |

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# DI-4a



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2675654.7 (Joules/Mol)      |
|                                              | 639.49683 (Kcal/Mol)        |
| Zero-point correction=                       | 1.019103 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.083295                    |
| Thermal correction to Enthalpy=              | 1.084239                    |
| Thermal correction to Gibbs Free Energy=     | 0.918799                    |
| Sum of electronic and zero-point Energies=   | -3471.863012                |
| Sum of electronic and thermal Energies=      | -3471.798820                |
| Sum of electronic and thermal Enthalpies=    | -3471.797876                |
| Sum of electronic and thermal Free Energies= | -3471.963316                |

| cartesian |             |            |             |   |            |            |             |  |  |
|-----------|-------------|------------|-------------|---|------------|------------|-------------|--|--|
| 12        | -1.40637171 | 0.01214166 | 0.29771671  | 6 | 3.64512825 | 1.60164165 | -2.90508342 |  |  |
| 8         | 0.17102832  | 3.98694158 | 1.16441679  | 1 | 3.15262818 | 1.65724158 | -1.93298328 |  |  |
| 8         | -3.19937181 | 0.07704166 | -0.34208328 | 1 | 4.46172810 | 2.33194160 | -2.90658331 |  |  |
| 6         | 0.48162836  | 3.96464181 | 2.58651662  | 1 | 2.93572831 | 1.89354169 | -3.69048333 |  |  |
| 1         | 0.56272835  | 2.92264175 | 2.90531659  | 6 | 4.90692806 | 0.24804164 | -4.53638315 |  |  |

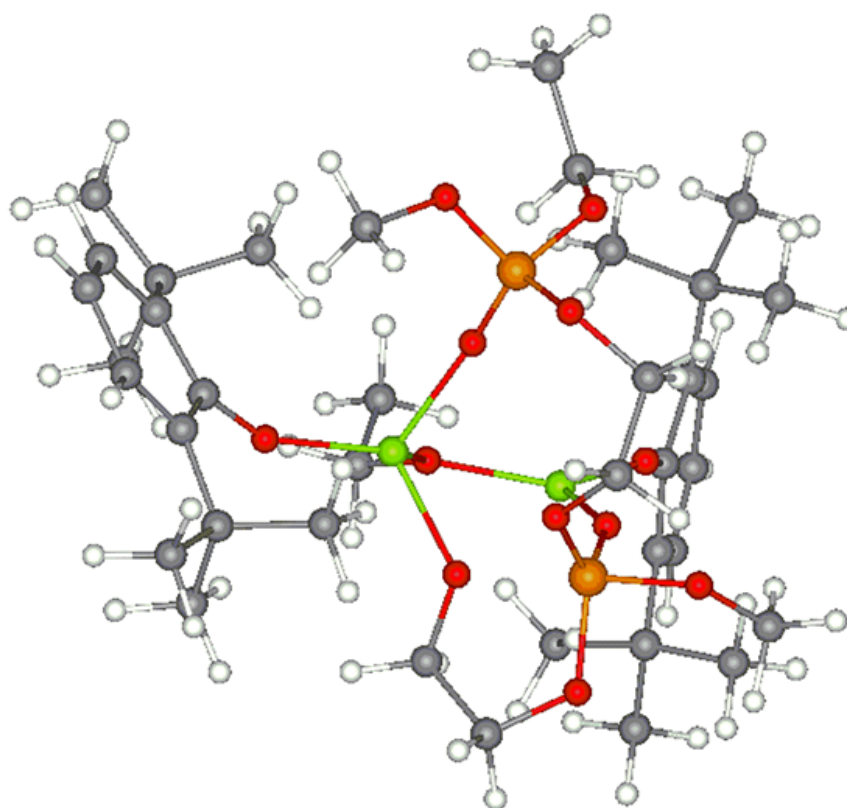
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1  | -0.34517166 | 4.43374205  | 3.12901664  | 1  | 5.71992826  | 0.98104167  | -4.55278349 |
| 6  | -4.38757181 | -0.45495832 | -0.60608327 | 1  | 5.31072807  | -0.72355837 | -4.83988333 |
| 6  | -4.73387194 | -0.81805837 | -1.95178330 | 1  | 4.18112850  | 0.54984164  | -5.30028343 |
| 6  | -5.92967176 | -1.50825834 | -2.17508340 | 6  | 6.54142809  | -0.69805837 | 2.77701664  |
| 1  | -6.19477177 | -1.81555831 | -3.18128347 | 1  | 7.04202843  | -1.66025841 | 2.62711668  |
| 6  | -6.81177187 | -1.81115842 | -1.14388323 | 1  | 7.27972841  | 0.09954165  | 2.64241672  |
| 6  | -6.52557182 | -1.35525835 | 0.13841671  | 1  | 6.21242809  | -0.66615838 | 3.82211661  |
| 1  | -7.25327158 | -1.54555833 | 0.92011672  | 6  | 4.67272806  | 0.82054162  | 2.26311660  |
| 6  | -5.35117149 | -0.65765834 | 0.43911672  | 1  | 3.78762817  | 1.03994167  | 1.66351676  |
| 6  | -3.85027170 | -0.42385834 | -3.15178347 | 1  | 4.39512825  | 0.80834162  | 3.32461667  |
| 6  | -5.15437174 | -0.08535834 | 1.85771680  | 1  | 5.38542843  | 1.63964164  | 2.11451674  |
| 6  | -2.49917173 | -1.16335833 | -3.12538338 | 6  | 4.38512850  | -1.71005833 | 2.15211654  |
| 1  | -1.93497169 | -0.96465838 | -2.21288347 | 1  | 4.88622808  | -2.65105844 | 1.90181673  |
| 1  | -1.87537169 | -0.86245835 | -3.97628355 | 1  | 4.11742830  | -1.74135840 | 3.21491671  |
| 1  | -2.65347171 | -2.24605846 | -3.20398331 | 1  | 3.46342826  | -1.67405832 | 1.56901670  |
| 6  | -3.63677168 | 1.10344160  | -3.14908338 | 6  | 1.77722824  | 4.71504211  | 2.79291654  |
| 1  | -3.19427180 | 1.44554162  | -2.21268344 | 1  | -0.72287166 | -1.18415833 | 3.35421658  |
| 1  | -4.59617186 | 1.61764169  | -3.27428341 | 1  | 8.46752834  | -0.94995838 | -1.58868325 |
| 1  | -2.98717165 | 1.40224159  | -3.98208332 | 1  | -7.72917175 | -2.35945845 | -1.34378326 |
| 6  | -4.50317192 | -0.77115834 | -4.50188351 | 8  | -1.29177177 | 1.86094165  | 1.22371674  |
| 1  | -5.47637177 | -0.28545833 | -4.62698317 | 15 | -1.09497178 | 3.20234156  | 0.59491676  |
| 1  | -4.63627195 | -1.84975839 | -4.63858318 | 8  | -0.88037169 | 3.26134157  | -0.96508324 |
| 1  | -3.85547185 | -0.42165834 | -5.31388330 | 8  | 0.15462831  | 0.41874167  | -0.88438326 |
| 6  | -6.40737152 | -0.25505835 | 2.73711658  | 6  | 0.29312834  | 2.72604156  | -1.65468323 |
| 1  | -6.64747190 | -1.30595839 | 2.93201661  | 6  | 0.11412831  | 1.26324165  | -2.00838327 |
| 1  | -7.28727150 | 0.22284167  | 2.29431653  | 1  | 1.17642832  | 2.89024162  | -1.03248322 |
| 1  | -6.22997189 | 0.22014166  | 3.70861673  | 1  | 0.37562832  | 3.33354163  | -2.55828333 |
| 6  | -4.87747192 | 1.42864168  | 1.77571678  | 1  | -0.83677167 | 1.15224159  | -2.54298329 |
| 1  | -3.99637175 | 1.64604163  | 1.17401671  | 1  | 0.91152835  | 1.01214159  | -2.71878338 |
| 1  | -4.72337151 | 1.84374166  | 2.77971673  | 8  | -2.38077164 | 4.09194183  | 0.83601671  |
| 1  | -5.73387194 | 1.94384170  | 1.32671678  | 6  | -2.52297163 | 5.39294195  | 0.23001671  |
| 6  | -4.01087141 | -0.79975837 | 2.60071659  | 1  | -1.67287171 | 6.03144169  | 0.48331672  |
| 1  | -4.23937178 | -1.86325836 | 2.73471665  | 1  | -2.61017179 | 5.29004192  | -0.85268325 |
| 1  | -3.85777164 | -0.35965833 | 3.59371662  | 1  | -3.43957162 | 5.81274176  | 0.64161676  |
| 1  | -3.06777167 | -0.73555839 | 2.05721664  | 1  | 2.03092837  | 4.71414185  | 3.85701656  |
| 12 | 1.66492832  | -0.57485837 | -0.08638328 | 1  | 2.59452820  | 4.24114180  | 2.24441671  |
| 8  | 0.20272832  | -0.88795835 | 1.52131677  | 1  | 1.68652833  | 5.75244188  | 2.46121669  |
| 8  | 3.44372821  | -0.04205834 | -0.34238330 | 1  | 1.04252827  | -0.12045834 | 4.73381662  |
| 6  | -0.00417168 | -0.49465832 | 2.90281653  | 1  | 1.73982823  | -1.43645835 | 3.76821661  |
| 6  | 1.27312827  | -0.45265833 | 3.71481657  | 1  | 1.99292827  | 0.25044167  | 3.28721666  |
| 1  | -0.46267167 | 0.49814168  | 2.88261652  | 8  | 1.13192832  | -2.47965837 | -0.07898328 |

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|   |            |             |             |    |             |             |             |
|---|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 4.72692823 | -0.25085834 | -0.65778327 | 15 | 0.03622832  | -2.75825834 | 0.94091672  |
| 6 | 5.15812826 | -0.19375835 | -2.02318335 | 8  | -0.44387168 | -4.30405807 | 0.55241674  |
| 6 | 6.49932814 | -0.45645833 | -2.31798339 | 8  | -1.48917174 | -2.16555834 | 0.55591673  |
| 1 | 6.83882809 | -0.43285832 | -3.34758329 | 6  | -1.47697175 | -4.29025793 | -0.42458329 |
| 6 | 7.43152809 | -0.74585837 | -1.32978320 | 8  | 0.42512834  | -3.11675835 | 2.45781660  |
| 6 | 7.01982832 | -0.75175834 | -0.00318328 | 6  | 0.53982830  | -4.46145821 | 2.96451664  |
| 1 | 7.76312828 | -0.95645839 | 0.75941676  | 1  | -0.43337166 | -4.95255804 | 2.97981668  |
| 6 | 5.69432831 | -0.50425833 | 0.36701670  | 1  | 1.23932827  | -5.04415798 | 2.36401653  |
| 6 | 4.20262814 | 0.18884166  | -3.16818333 | 1  | 0.92212832  | -4.34885836 | 3.97981668  |
| 6 | 5.31772804 | -0.51995832 | 1.85861671  | 6  | -2.39527178 | -3.16735840 | 0.02581672  |
| 6 | 3.07322836 | -0.84765834 | -3.32138348 | 1  | -2.97607183 | -2.70785832 | -0.77168328 |
| 1 | 2.47182822 | -0.95215833 | -2.41788340 | 1  | -3.05867171 | -3.47465825 | 0.83741677  |
| 1 | 2.40152836 | -0.57365835 | -4.14428329 | 1  | -1.97327173 | -5.26235819 | -0.41778329 |
| 1 | 3.48872828 | -1.83605838 | -3.54268336 | 1  | -1.05567169 | -4.10035801 | -1.41858327 |

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# DI-4b



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2676526.6 (Joules/Mol)      |
|                                              | 639.70521 (Kcal/Mol)        |
| Zero-point correction=                       | 1.019435 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.084350                    |
| Thermal correction to Enthalpy=              | 1.085294                    |
| Thermal correction to Gibbs Free Energy=     | 0.916106                    |
| Sum of electronic and zero-point Energies=   | -3471.853971                |
| Sum of electronic and thermal Energies=      | -3471.789056                |
| Sum of electronic and thermal Enthalpies=    | -3471.788112                |
| Sum of electronic and thermal Free Energies= | -3471.957300                |

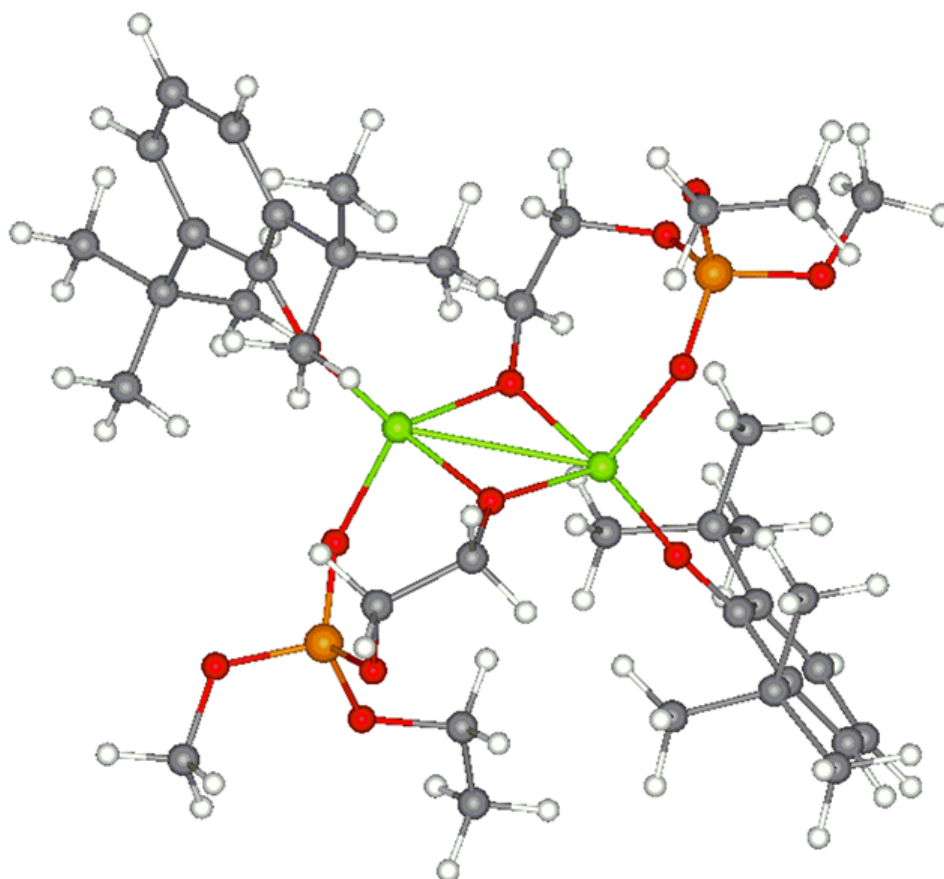
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|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 12        | 1.36022258  | 0.42852250  | 0.37905079  | 6 | -3.39377737 | -2.91677737 | -0.98374921 |
| 8         | 0.61102259  | -1.42517757 | -3.68844914 | 1 | -2.68607736 | -2.12297750 | -0.73714918 |
| 8         | 2.96222258  | -0.01157750 | 1.29305077  | 1 | -3.47877741 | -3.57467747 | -0.11234919 |
| 6         | -0.17447741 | -2.51357746 | -3.11484909 | 1 | -2.97797751 | -3.50767732 | -1.80994916 |
| 1         | -1.18347740 | -2.35227752 | -3.49584913 | 6 | -5.64167738 | -3.54427743 | -1.79254913 |
| 1         | -0.19657741 | -2.40557742 | -2.02784920 | 1 | -5.73207712 | -4.29457760 | -0.99984920 |
| 6         | 4.20472288  | -0.48467749 | 1.20245075  | 1 | -6.64857721 | -3.23517752 | -2.09154916 |
| 6         | 4.46082258  | -1.88857758 | 1.35965085  | 1 | -5.18237734 | -4.03957748 | -2.65554905 |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 5.74572277  | -2.37057734 | 1.08985090  | 6  | -5.76807737 | 2.41482258  | 2.83885098  |
| 1  | 5.94882298  | -3.43327737 | 1.16715074  | 1  | -6.83067703 | 2.51762247  | 2.60075092  |
| 6  | 6.79232264  | -1.52717757 | 0.73395079  | 1  | -5.67497730 | 1.81462240  | 3.75065088  |
| 6  | 6.56882286  | -0.15497752 | 0.71665078  | 1  | -5.39127731 | 3.41932249  | 3.06125093  |
| 1  | 7.40992260  | 0.49662250  | 0.50555080  | 6  | -3.47207737 | 1.83262241  | 2.09355092  |
| 6  | 5.30972290  | 0.40052250  | 0.97085077  | 1  | -3.11007738 | 0.83642250  | 2.36895084  |
| 6  | 3.38412261  | -2.86137748 | 1.87795091  | 1  | -2.84247732 | 2.27802253  | 1.30915070  |
| 6  | 5.16082287  | 1.93432248  | 1.01115084  | 1  | -3.31287742 | 2.47122264  | 2.96945095  |
| 6  | 2.21182251  | -3.00857735 | 0.89015085  | 6  | -5.16777706 | 2.74762249  | 0.45265079  |
| 1  | 1.66192257  | -2.07767749 | 0.75495082  | 1  | -6.23017740 | 2.81762266  | 0.19855082  |
| 1  | 1.50062263  | -3.76147747 | 1.25185084  | 1  | -4.80447721 | 3.75962257  | 0.67305082  |
| 1  | 2.57222247  | -3.33277750 | -0.09234919 | 1  | -4.63427734 | 2.36872268  | -0.42264920 |
| 6  | 2.88552260  | -2.36567736 | 3.25075078  | 6  | 0.37902260  | -3.85497761 | -3.54404902 |
| 1  | 2.54072261  | -1.33167756 | 3.20085096  | 1  | -0.93837738 | -0.05397750 | 3.11015081  |
| 1  | 3.69712257  | -2.41197753 | 3.98505092  | 1  | -8.05577755 | -1.72257757 | 1.93565083  |
| 1  | 2.06582260  | -2.99687743 | 3.61665082  | 1  | 7.77962303  | -1.92977750 | 0.52065080  |
| 6  | 3.93602252  | -4.28187752 | 2.09895086  | 8  | 1.31552255  | -0.32927752 | -1.48084927 |
| 1  | 4.77892303  | -4.29347754 | 2.79725099  | 15 | 1.73352253  | -0.66767746 | -2.87924910 |
| 1  | 4.25412273  | -4.75857735 | 1.16515088  | 8  | 2.09982252  | 0.56562251  | -3.79754925 |
| 1  | 3.14752269  | -4.90897751 | 2.52965093  | 8  | 1.33572257  | 2.77262259  | -1.93104911 |
| 6  | 6.52422285  | 2.65152264  | 0.98215085  | 6  | 1.18472254  | 1.65582240  | -4.08844948 |
| 1  | 7.05512285  | 2.51272249  | 0.03415081  | 6  | 1.58362257  | 2.90012264  | -3.33304906 |
| 1  | 7.18002272  | 2.32432246  | 1.79565096  | 1  | 0.15562259  | 1.36742246  | -3.86274910 |
| 1  | 6.36342287  | 3.72882247  | 1.10215092  | 1  | 1.27422261  | 1.82612240  | -5.16394949 |
| 6  | 4.47542286  | 2.36672258  | 2.32295084  | 1  | 2.66252255  | 3.05302262  | -3.41914916 |
| 1  | 3.51002264  | 1.87592244  | 2.45035076  | 1  | 1.06052256  | 3.76082253  | -3.75054908 |
| 1  | 4.32892275  | 3.45432258  | 2.33405089  | 8  | 3.00282264  | -1.59707749 | -2.98574924 |
| 1  | 5.10092258  | 2.10562253  | 3.18365097  | 6  | 4.28952265  | -1.20797753 | -2.43334913 |
| 6  | 4.37282276  | 2.44702268  | -0.20734920 | 1  | 4.64682293  | -0.30997747 | -2.94044924 |
| 1  | 4.86222267  | 2.13592243  | -1.13734913 | 1  | 4.21522284  | -1.04807758 | -1.35734916 |
| 1  | 4.33172274  | 3.54352260  | -0.20514919 | 1  | 4.95732260  | -2.04277754 | -2.63564920 |
| 1  | 3.34282255  | 2.09352255  | -0.22604918 | 1  | -0.26797742 | -4.64927721 | -3.15894914 |
| 12 | -1.89937747 | 0.61232251  | 0.08005080  | 1  | 0.40822262  | -3.93217754 | -4.63374949 |
| 8  | -0.42137742 | -0.12107749 | 1.10285091  | 1  | 1.38722253  | -4.01387739 | -3.15494919 |
| 8  | -3.65207744 | 0.08602250  | -0.23404919 | 1  | -1.58707738 | -2.44347739 | 3.28435087  |
| 6  | -0.56967741 | -0.77567750 | 2.36525083  | 1  | -2.51977754 | -1.67777753 | 1.99205089  |
| 6  | -1.50907743 | -1.96857750 | 2.29995084  | 1  | -1.13827741 | -2.71287751 | 1.58935070  |
| 1  | 0.41372257  | -1.10667753 | 2.71495080  | 8  | -1.12507749 | 1.98962247  | -1.01094913 |
| 6  | -4.79997730 | -0.35347748 | 0.28175080  | 15 | -0.06557742 | 3.09872246  | -1.17054915 |
| 6  | -5.38367701 | -1.56607759 | -0.19584920 | 8  | 0.91562259  | 2.41072249  | 0.29535079  |
| 6  | -6.54927731 | -2.02687740 | 0.42365080  | 8  | -0.18747742 | 4.47352266  | -0.29184920 |

---

|   |             |             |             |   |             |            |             |
|---|-------------|-------------|-------------|---|-------------|------------|-------------|
| 1 | -7.00597715 | -2.95367742 | 0.09285080  | 6 | 0.60952258  | 3.13032246 | 1.47125077  |
| 6 | -7.15767717 | -1.33157754 | 1.46395087  | 6 | 0.43692261  | 4.55752277 | 0.98805076  |
| 6 | -6.62047720 | -0.11607750 | 1.87405086  | 1 | 1.42812252  | 3.04142261 | 2.19075084  |
| 1 | -7.12887716 | 0.42942250  | 2.66215086  | 1 | -0.31367743 | 2.75302267 | 1.93595076  |
| 6 | -5.46147728 | 0.40732250  | 1.29255080  | 1 | -0.20817740 | 5.15502262 | 1.63585091  |
| 6 | -4.77087736 | -2.34737754 | -1.37284923 | 1 | 1.40292263  | 5.05782270 | 0.86795086  |
| 6 | -4.96827698 | 1.81672251  | 1.66765070  | 8 | -0.70247746 | 3.86142254 | -2.49744916 |
| 6 | -4.64147711 | -1.43557751 | -2.61034918 | 6 | -2.05717754 | 4.30182266 | -2.48664904 |
| 1 | -4.01787710 | -0.56467748 | -2.40394902 | 1 | -2.73707747 | 3.46512246 | -2.30134916 |
| 1 | -4.20527697 | -1.99347746 | -3.44914913 | 1 | -2.20937753 | 5.07882261 | -1.73094916 |
| 1 | -5.62757730 | -1.07867754 | -2.92704916 | 1 | -2.25897741 | 4.72082281 | -3.47514915 |

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|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2673282.3 (Joules/Mol)      |
|                                              | 638.92981 (Kcal/Mol)        |
| Zero-point correction=                       | 1.018199 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.084123                    |
| Thermal correction to Enthalpy=              | 1.085067                    |
| Thermal correction to Gibbs Free Energy=     | 0.910990                    |
| Sum of electronic and zero-point Energies=   | -3471.894056                |
| Sum of electronic and thermal Energies=      | -3471.828132                |
| Sum of electronic and thermal Enthalpies=    | -3471.827188                |
| Sum of electronic and thermal Free Energies= | -3472.001265                |

| cartesian |             |             |             |   |            |             |             |
|-----------|-------------|-------------|-------------|---|------------|-------------|-------------|
| 12        | -1.14802015 | -0.51941490 | -0.23583333 | 6 | 6.03008032 | 1.88918507  | 3.18096662  |
| 8         | 1.77637982  | 4.94498539  | -0.74133331 | 1 | 6.17727995 | 1.09858501  | 3.92486668  |
| 8         | -2.90602016 | 0.06898512  | 0.06866667  | 1 | 6.99658012 | 2.10808516  | 2.71546674  |
| 6         | 1.53067982  | 6.15018511  | -1.49263334 | 1 | 5.71748018 | 2.78908515  | 3.72246671  |
| 1         | 2.47347975  | 6.69538498  | -1.49593329 | 6 | 5.08898020 | -2.63271475 | -2.77283335 |
| 1         | 0.75467992  | 6.74288511  | -1.00483334 | 1 | 6.08428001 | -2.27841473 | -3.05983329 |

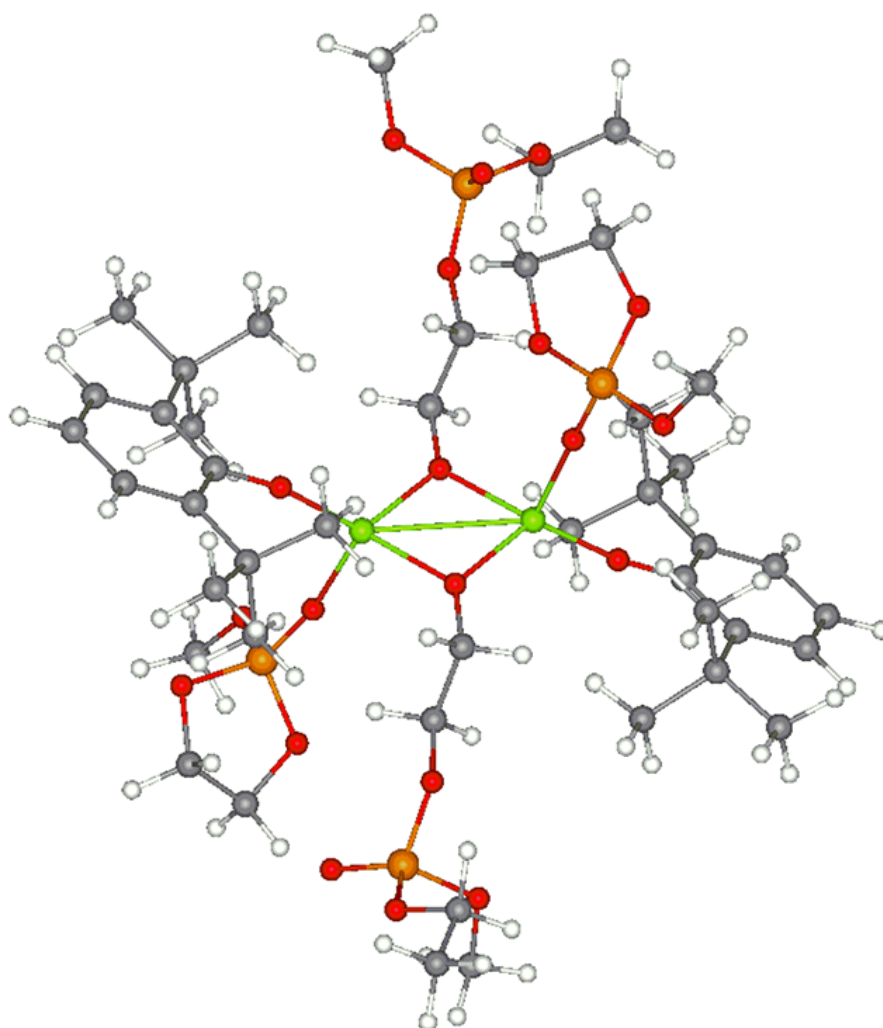
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | -4.19051981 | 0.34038511  | 0.26756668  | 1  | 5.20348024  | -3.57931471 | -2.23333335 |
| 6  | -5.08262014 | 0.49518511  | -0.84533334 | 1  | 4.54067993  | -2.84951472 | -3.69703341 |
| 6  | -6.41411972 | 0.84238511  | -0.59833336 | 6  | 2.93887997  | -2.20481491 | -1.64513338 |
| 1  | -7.09982014 | 0.97218513  | -1.42883337 | 1  | 2.28517985  | -1.50971496 | -1.11783338 |
| 6  | -6.90341997 | 1.02848506  | 0.68936670  | 1  | 2.43367982  | -2.50211477 | -2.57303333 |
| 6  | -6.04642010 | 0.83708513  | 1.76706672  | 1  | 3.06027985  | -3.09871483 | -1.02273333 |
| 1  | -6.44961977 | 0.96388513  | 2.76616669  | 6  | 4.14788008  | -0.35251489 | -2.87263322 |
| 6  | -4.70351982 | 0.48478511  | 1.59946668  | 1  | 5.12847996  | 0.02658512  | -3.18033338 |
| 6  | -4.61261988 | 0.28668511  | -2.29643345 | 1  | 3.58867979  | -0.61731488 | -3.77953339 |
| 6  | -3.83132005 | 0.22018512  | 2.84166670  | 1  | 3.62457991  | 0.45258513  | -2.35523343 |
| 6  | -4.07401991 | -1.14551497 | -2.48823333 | 1  | 7.91578007  | -1.94671500 | 1.03216672  |
| 1  | -3.28042006 | -1.38981497 | -1.78213334 | 1  | -7.94242001 | 1.30498505  | 0.85176665  |
| 1  | -3.68792009 | -1.27851498 | -3.50703335 | 8  | 1.18747985  | 2.72988510  | 0.27366668  |
| 1  | -4.87771988 | -1.87421489 | -2.33683324 | 15 | 0.66847992  | 3.82228518  | -0.60273331 |
| 6  | -3.54062009 | 1.33098507  | -2.65703344 | 8  | 0.23957989  | 3.34558511  | -2.06083322 |
| 1  | -2.70482016 | 1.29898500  | -1.95683336 | 8  | 0.16097988  | 0.48568511  | -1.33853328 |
| 1  | -3.96882010 | 2.33948517  | -2.62503338 | 6  | 0.96067989  | 2.29038525  | -2.75953341 |
| 1  | -3.16092014 | 1.16278505  | -3.67313337 | 6  | 0.23457989  | 0.96078509  | -2.65213323 |
| 6  | -5.74921989 | 0.45898512  | -3.32063341 | 1  | 1.98277986  | 2.22158527  | -2.37113333 |
| 1  | -6.17251968 | 1.46898508  | -3.30913329 | 1  | 1.01327991  | 2.61338520  | -3.80253339 |
| 1  | -6.56201982 | -0.25761488 | -3.16273332 | 1  | -0.76602006 | 1.08038509  | -3.08593345 |
| 1  | -5.35311985 | 0.28478512  | -4.32783318 | 1  | 0.78707993  | 0.25968510  | -3.29943323 |
| 6  | -4.60542011 | 0.41528511  | 4.15826702  | 8  | -0.59592009 | 4.61288500  | -0.09053333 |
| 1  | -5.46201992 | -0.26161489 | 4.24276686  | 6  | -1.89592016 | 3.95488524  | 0.07206667  |
| 1  | -4.96532011 | 1.44268501  | 4.28006697  | 1  | -2.20882010 | 3.58278513  | -0.90513331 |
| 1  | -3.93872023 | 0.20268512  | 5.00166702  | 1  | -1.77052009 | 3.11158514  | 0.75276667  |
| 6  | -2.62882018 | 1.18118501  | 2.89986658  | 6  | -2.86452007 | 4.97328520  | 0.62246668  |
| 1  | -1.97942019 | 1.07188511  | 2.03096676  | 8  | 0.18207988  | -4.70161486 | -0.22113334 |
| 1  | -2.02962017 | 0.99288511  | 3.79956675  | 6  | 0.32537988  | -4.95681477 | -1.65043330 |
| 1  | -2.97542024 | 2.21988511  | 2.94616675  | 1  | 1.36167991  | -5.27791500 | -1.76063335 |
| 6  | -3.35322022 | -1.24451494 | 2.82966661  | 1  | 0.19457988  | -4.01341486 | -2.18473339 |
| 1  | -4.21072006 | -1.92451489 | 2.87516665  | 6  | -0.64112008 | -6.01991463 | -2.12983322 |
| 1  | -2.71142006 | -1.45081496 | 3.69536662  | 8  | -1.11972010 | -2.51501489 | -0.58413333 |
| 1  | -2.79692006 | -1.47771490 | 1.92116666  | 15 | -0.89272010 | -3.67171478 | 0.33606666  |
| 12 | 1.52427983  | 0.74278510  | 0.10676667  | 8  | -0.39302012 | -3.34421492 | 1.79366672  |
| 8  | 3.36427975  | 0.41008511  | -0.05273333 | 8  | 0.30637988  | -0.42391488 | 1.13766670  |
| 6  | 4.54697990  | -0.14561488 | 0.19166666  | 6  | 0.83457989  | -2.60691476 | 2.09986663  |
| 6  | 5.34798002  | 0.30308512  | 1.29206669  | 6  | 0.55667990  | -1.13121498 | 2.32146668  |
| 6  | 6.54048014  | -0.37391487 | 1.56716669  | 1  | 1.56337988  | -2.75901484 | 1.29996669  |
| 1  | 7.15307999  | -0.06701488 | 2.40826678  | 1  | 1.20697987  | -3.07071471 | 3.01586676  |
| 6  | 6.98758030  | -1.43561494 | 0.78806669  | 1  | -0.28422013 | -1.03521490 | 3.02176666  |

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|   |            |             |             |   |             |             |             |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 6.24898005 | -1.80791497 | -0.32933334 | 1 | 1.44497991  | -0.73411489 | 2.83436656  |
| 1 | 6.63407993 | -2.60841489 | -0.95233333 | 8 | -2.25552011 | -4.43831491 | 0.57806665  |
| 6 | 5.04648018 | -1.17921495 | -0.66603333 | 6 | -2.35072017 | -5.53331470 | 1.51166666  |
| 6 | 4.95458031 | 1.52848506  | 2.13986659  | 1 | -1.61892009 | -6.30841494 | 1.27106667  |
| 6 | 4.31207991 | -1.58321500 | -1.95813334 | 1 | -2.19652009 | -5.16821480 | 2.52836657  |
| 6 | 4.78957987 | 2.76378512  | 1.23146665  | 1 | -3.35982013 | -5.92811489 | 1.40416670  |
| 1 | 4.03808022 | 2.60088515  | 0.45916668  | 1 | -0.44592011 | -6.23091459 | -3.18603325 |
| 1 | 4.48988008 | 3.63758516  | 1.82266665  | 1 | -0.51192009 | -6.94921494 | -1.56853330 |
| 1 | 5.74007988 | 2.99838519  | 0.73936665  | 1 | -1.67972016 | -5.69171476 | -2.03833342 |
| 6 | 3.66047978 | 1.26958501  | 2.93326664  | 1 | 1.23677981  | 5.91058540  | -2.51753330 |
| 1 | 2.81467986 | 1.07168508  | 2.27316666  | 1 | -3.84042025 | 4.49778509  | 0.75256670  |
| 1 | 3.77997994 | 0.40678513  | 3.59796667  | 1 | -2.52902007 | 5.34848499  | 1.59256673  |
| 1 | 3.39987993 | 2.13978529  | 3.54696655  | 1 | -2.97872019 | 5.81788540  | -0.06243333 |

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## DI-1m2



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 3285193.1 (Joules/Mol)      |
|                                              | 785.17999 (Kcal/Mol)        |
| Zero-point correction=                       | 1.251264 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.338420                    |
| Thermal correction to Enthalpy=              | 1.339365                    |
| Thermal correction to Gibbs Free Energy=     | 1.111674                    |
| Sum of electronic and zero-point Energies=   | -4993.015820                |
| Sum of electronic and thermal Energies=      | -4992.928663                |
| Sum of electronic and thermal Enthalpies=    | -4992.927719                |
| Sum of electronic and thermal Free Energies= | -4993.155410                |

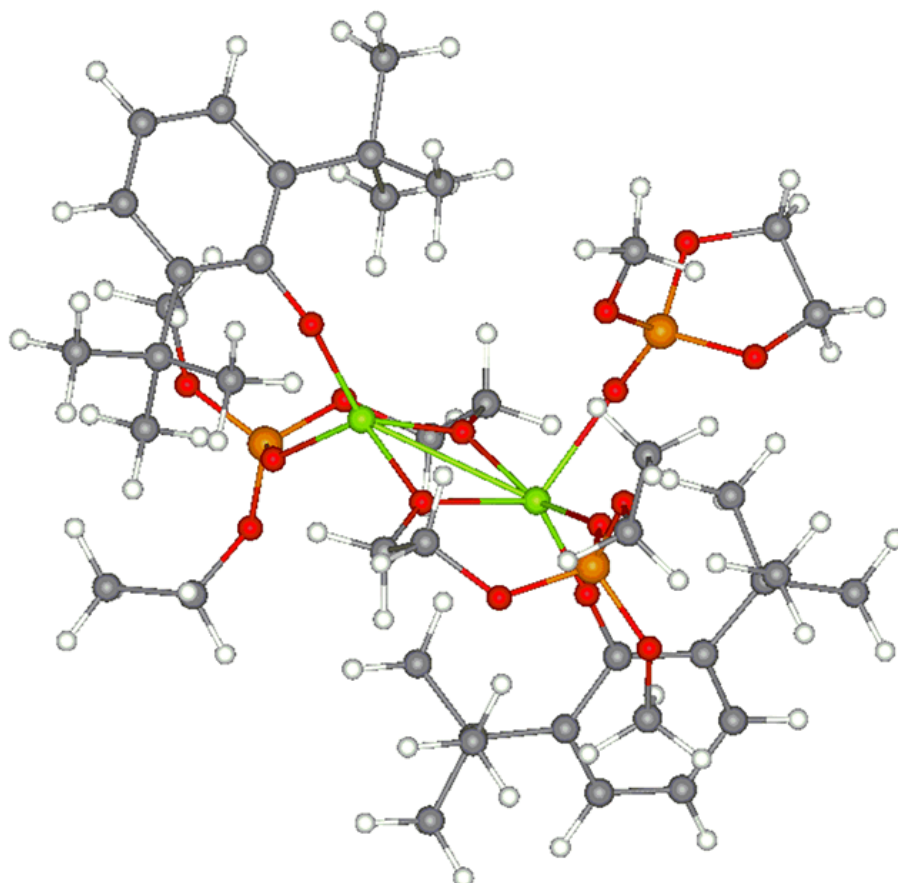
| cartesian |             |            |             |   |            |             |
|-----------|-------------|------------|-------------|---|------------|-------------|
| 12        | -0.48869064 | 1.40340960 | -0.17518666 | 1 | 0.94410932 | -2.98419046 |
| 8         | 1.12910938  | 0.32810956 | -0.56008667 | 6 | 3.34910941 | -2.95539045 |
| 8         | -0.46909064 | 3.13330936 | 0.56261337  | 1 | 4.02230930 | -3.71549058 |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 2.33440948  | 0.64530957  | -1.20878661 | 1  | 3.96490932  | -2.16109061 | -1.98898661 |
| 6  | 3.46970940  | 0.65710956  | -0.19498666 | 1  | 2.77940941  | -2.53819060 | -0.71808666 |
| 1  | 2.27500939  | 1.62730956  | -1.69598663 | 1  | 2.56780934  | -0.08979043 | -1.98908663 |
| 6  | -0.61229068 | 4.39600992  | 0.94651335  | 1  | -2.48599052 | 0.04910957  | 2.19191337  |
| 6  | 0.16620934  | 5.43570948  | 0.33801335  | 1  | 1.03940940  | -8.04549026 | -2.10438657 |
| 6  | -0.03509066 | 6.75670958  | 0.74781334  | 1  | -1.08629060 | 8.13060951  | 2.03691339  |
| 1  | 0.53950930  | 7.55560970  | 0.29081336  | 8  | -1.63209057 | 1.45420957  | -1.86588669 |
| 6  | -0.95089066 | 7.09380960  | 1.73811328  | 15 | -2.41709065 | 1.49280953  | -3.11988664 |
| 6  | -1.68069065 | 6.08060980  | 2.34911323  | 8  | -3.98029065 | 1.77970958  | -2.91578674 |
| 1  | -2.37999058 | 6.35570955  | 3.13181329  | 8  | -2.53929067 | 0.13110957  | -3.95708656 |
| 6  | -1.53719068 | 4.73810959  | 1.98711336  | 6  | -4.79549074 | 0.75080961  | -3.53938675 |
| 6  | 1.23640943  | 5.12490988  | -0.72288668 | 6  | -3.86179066 | -0.43979043 | -3.76638675 |
| 6  | -2.37429070 | 3.66490936  | 2.70471334  | 1  | -5.18849087 | 1.16040957  | -4.47408676 |
| 6  | 0.59920931  | 4.49680948  | -1.97658670 | 1  | -5.60089064 | 0.49410957  | -2.85278654 |
| 1  | 0.01980934  | 3.60430956  | -1.74208665 | 1  | -3.84659052 | -1.10369039 | -2.90148664 |
| 1  | 1.37070942  | 4.22790956  | -2.70958662 | 1  | -4.10379076 | -1.00449049 | -4.66628647 |
| 1  | -0.08289066 | 5.20940971  | -2.45348668 | 8  | -1.78949058 | 2.57420945  | -4.08648682 |
| 6  | 2.29790950  | 4.18920994  | -0.11418665 | 6  | -2.37989068 | 2.86760950  | -5.36678648 |
| 1  | 1.84210944  | 3.27460957  | 0.26761335  | 1  | -2.38119054 | 1.97620952  | -5.99848652 |
| 1  | 2.80260944  | 4.68440962  | 0.72271335  | 1  | -3.39409065 | 3.25250936  | -5.23598671 |
| 1  | 3.06070948  | 3.92620945  | -0.85748667 | 1  | -1.75149059 | 3.63650942  | -5.81328678 |
| 6  | 1.98420942  | 6.38240957  | -1.20038664 | 8  | 4.72470903  | 0.81310958  | -0.91178668 |
| 1  | 2.50870943  | 6.88930988  | -0.38338667 | 1  | 3.35300946  | 1.47870958  | 0.51631331  |
| 1  | 1.31800938  | 7.10560989  | -1.68328667 | 1  | 3.49570942  | -0.28879043 | 0.35021335  |
| 1  | 2.73840928  | 6.09060955  | -1.94048667 | 8  | -4.64599085 | -1.00879049 | 1.03501332  |
| 6  | -3.25699067 | 4.25000954  | 3.82191324  | 1  | -3.56839061 | 0.43330956  | -0.01558665 |
| 1  | -3.99029040 | 4.97010994  | 3.44341326  | 1  | -3.22839069 | -1.25539041 | -0.47268665 |
| 1  | -2.66419053 | 4.73940992  | 4.60201311  | 8  | 1.67660940  | -1.58589041 | 1.91791332  |
| 1  | -3.81629062 | 3.43680954  | 4.29931355  | 15 | 2.50650930  | -2.04089046 | 3.05671334  |
| 6  | -1.45539057 | 2.62640953  | 3.37941337  | 8  | 3.63360929  | -0.99399042 | 3.50651336  |
| 1  | -0.80069065 | 2.13060951  | 2.66211343  | 8  | 3.45450950  | -3.31229043 | 2.82291341  |
| 1  | -2.05129051 | 1.86300957  | 3.89591336  | 6  | 4.95800924  | -1.59129047 | 3.46291327  |
| 1  | -0.82089067 | 3.11590958  | 4.12671328  | 6  | 4.81520891  | -2.85139060 | 2.60791326  |
| 6  | -3.32959056 | 2.99250937  | 1.70031333  | 1  | 5.25390911  | -1.81559038 | 4.49161339  |
| 1  | -4.03879070 | 3.72550941  | 1.30021334  | 1  | 5.63480902  | -0.87459040 | 3.00011325  |
| 1  | -3.90449071 | 2.19280958  | 2.18451333  | 1  | 4.95610905  | -2.63489056 | 1.54751337  |
| 1  | -2.78639054 | 2.57130957  | 0.85291332  | 1  | 5.48260927  | -3.65509057 | 2.91761327  |
| 12 | 0.50590932  | -1.37449038 | 0.26481333  | 8  | 1.56510937  | -2.37469053 | 4.28031349  |
| 8  | -1.08939064 | -0.28169042 | 0.69971335  | 6  | 2.10450935  | -2.80959058 | 5.54351330  |
| 8  | 0.42260936  | -3.07279062 | -0.54688668 | 1  | 2.69960928  | -3.71589065 | 5.41121340  |
| 6  | -2.28009057 | -0.63359040 | 1.35751331  | 1  | 2.70330930  | -2.01269054 | 5.99101353  |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -3.43009067 | -0.58289039 | 0.36321333  | 1  | 1.24390936  | -3.02219057 | 6.17551327  |
| 1 | -2.22019053 | -1.64739037 | 1.77401340  | 15 | 6.08540916  | 0.83190960  | -0.08788665 |
| 6 | 0.56770933  | -4.32889032 | -0.95248663 | 8  | 7.19360924  | 0.75440961  | -1.22988665 |
| 6 | -0.25649065 | -5.36929035 | -0.40828666 | 8  | 6.10490894  | 2.34350944  | 0.46641335  |
| 6 | -0.05509066 | -6.68389034 | -0.83858663 | 8  | 6.27810907  | -0.20129043 | 0.95481336  |
| 1 | -0.66419065 | -7.48329020 | -0.42998666 | 15 | -5.97419071 | -1.22029042 | 0.18221334  |
| 6 | 0.90480930  | -7.01359034 | -1.78868663 | 8  | -6.99079084 | -0.07019043 | 0.64101332  |
| 6 | 1.67980933  | -5.99899054 | -2.33848667 | 8  | -5.83739090 | -1.24179041 | -1.29218662 |
| 1 | 2.41340947  | -6.26749039 | -3.09138656 | 8  | -6.51309109 | -2.57019043 | 0.86141336  |
| 6 | 1.53830934  | -4.66249037 | -1.95378661 | 6  | 7.00820923  | 2.69380951  | 1.52701330  |
| 6 | -1.37059057 | -5.06769037 | 0.60921335  | 6  | 7.15950918  | 1.64240956  | -2.37598658 |
| 6 | 2.42370939  | -3.58809042 | -2.60888672 | 6  | -7.21969080 | 0.20870958  | 2.04471326  |
| 6 | -0.78069067 | -4.48449039 | 1.90721333  | 6  | -7.62649107 | -3.24099064 | 0.24571334  |
| 1 | -0.19009066 | -3.58789063 | 1.71851337  | 1  | -6.26769066 | 0.48700958  | 2.50571322  |
| 1 | -1.57799065 | -4.23139048 | 2.61731339  | 6  | -8.22839069 | 1.33180964  | 2.13961339  |
| 1 | -0.12169066 | -5.21679020 | 2.38711333  | 1  | -7.58629084 | -0.70129043 | 2.53121328  |
| 6 | -2.38869071 | -4.09609032 | -0.01808665 | 1  | -7.77479076 | -4.16099024 | 0.81061333  |
| 1 | -1.89889061 | -3.18109059 | -0.35448664 | 1  | -8.52969074 | -2.62589049 | 0.30061334  |
| 1 | -2.86519051 | -4.56029034 | -0.88888663 | 1  | -7.40009069 | -3.47539043 | -0.79678667 |
| 1 | -3.17689061 | -3.83879066 | 0.70011336  | 1  | 6.76300907  | 3.71770954  | 1.80891335  |
| 6 | -2.15929055 | -6.32419014 | 1.01921332  | 1  | 6.87190914  | 2.02830935  | 2.38221335  |
| 1 | -2.65259051 | -6.80139017 | 0.16571334  | 1  | 8.04580975  | 2.64480948  | 1.18391335  |
| 1 | -1.52719057 | -7.07009029 | 1.51301336  | 6  | 8.41121006  | 1.39850962  | -3.18948674 |
| 1 | -2.94269061 | -6.03879023 | 1.73081338  | 1  | 6.25660896  | 1.42560959  | -2.95308661 |
| 6 | 3.34450936  | -4.16219044 | -3.70068669 | 1  | 7.10690928  | 2.67680955  | -2.02168655 |
| 1 | 4.05010891  | -4.90209007 | -3.30788660 | 1  | 8.41030979  | 2.05030942  | -4.06848669 |
| 1 | 2.77790928  | -4.62439013 | -4.51608658 | 1  | 9.30780983  | 1.61180961  | -2.60158658 |
| 1 | 3.93650937  | -3.34789062 | -4.13398647 | 1  | 8.45710945  | 0.36060959  | -3.52868676 |
| 6 | 1.55030942  | -2.52059054 | -3.29828668 | 1  | -8.41709042 | 1.56750953  | 3.19131327  |
| 1 | 0.86960930  | -2.03359056 | -2.59938669 | 1  | -7.85329103 | 2.23200941  | 1.64641333  |
| 1 | 2.17870927  | -1.75419044 | -3.76988673 | 1  | -9.17559052 | 1.04810953  | 1.67331338  |

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|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2980843.5 (Joules/Mol)      |
|                                              | 712.43870 (Kcal/Mol)        |
| Zero-point correction=                       | 1.135343 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.211051                    |
| Thermal correction to Enthalpy=              | 1.211996                    |
| Thermal correction to Gibbs Free Energy=     | 1.016741                    |
| Sum of electronic and zero-point Energies=   | -4232.457906                |
| Sum of electronic and thermal Energies=      | -4232.382198                |
| Sum of electronic and thermal Enthalpies=    | -4232.381254                |
| Sum of electronic and thermal Free Energies= | -4232.576508                |

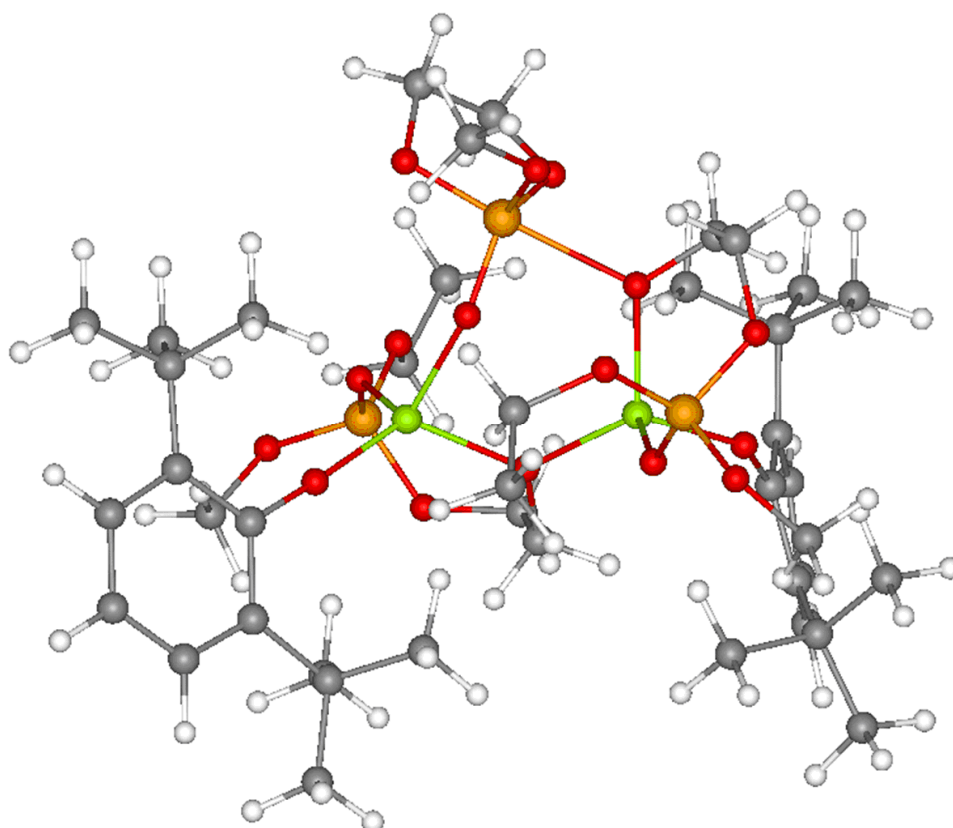
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|-----------|------------|-------------|-------------|---|-------------|------------|-------------|--|--|
| 12        | 1.63710141 | 0.42053843  | -0.10244668 | 6 | -2.64319873 | 5.09163809 | -2.13104677 |  |  |
| 8         | 2.24240136 | 4.69813824  | 0.73785335  | 1 | -3.57459879 | 5.18583822 | -2.69964671 |  |  |
| 8         | 3.09280133 | -0.80566156 | -0.15304667 | 1 | -2.58329868 | 5.92993832 | -1.42844665 |  |  |
| 6         | 2.42190123 | 5.32613802  | -0.56374669 | 1 | -1.81629860 | 5.20273829 | -2.84244680 |  |  |
| 1         | 1.49970138 | 5.88543844  | -0.72834665 | 6 | -1.14649856 | 3.71553850 | -0.73364669 |  |  |
| 1         | 2.49260139 | 4.54913807  | -1.32924664 | 1 | -0.96519858 | 2.77483845 | -0.21464667 |  |  |
| 6         | 4.32870150 | -1.26776159 | -0.02244667 | 1 | -0.34369859 | 3.85963845 | -1.46754658 |  |  |

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|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 5.25450134  | -1.20086169 | -1.11874664 | 1  | -1.08789861 | 4.52983809  | -0.00174667 |
| 6  | 6.58340168  | -1.57746160 | -0.90044665 | 6  | -2.56889868 | 2.66053843  | -2.53384662 |
| 1  | 7.30300140  | -1.50456166 | -1.70934665 | 1  | -3.52279878 | 2.71773839  | -3.07064676 |
| 6  | 7.02470160  | -2.06106162 | 0.32655331  | 1  | -1.76389861 | 2.81953859  | -3.26264668 |
| 6  | 6.09910154  | -2.23256159 | 1.35035336  | 1  | -2.46829867 | 1.65783834  | -2.11684680 |
| 1  | 6.44380140  | -2.66756153 | 2.28285336  | 6  | 3.63300133  | 6.23543835  | -0.55754668 |
| 6  | 4.75460148  | -1.87576163 | 1.20685339  | 1  | 1.22550142  | 0.08363841  | -3.04324675 |
| 6  | 4.80770159  | -0.78316158 | -2.53244662 | 1  | -6.43269825 | 5.08113813  | 0.77915335  |
| 6  | 3.76330137  | -2.17956161 | 2.34595323  | 1  | 8.06640148  | -2.33806157 | 0.47005332  |
| 6  | 4.39310169  | 0.69873840  | -2.57554674 | 8  | 2.48790121  | 2.26493859  | -0.09404667 |
| 1  | 3.61370134  | 0.93333840  | -1.85204661 | 15 | 2.74110126  | 3.22703838  | 1.03075337  |
| 1  | 4.03170156  | 0.97143847  | -3.57574677 | 8  | 2.08430123  | 2.84783840  | 2.41145325  |
| 1  | 5.25140142  | 1.34113836  | -2.34734678 | 8  | 0.21370140  | 0.77543843  | 1.19785345  |
| 6  | 3.64650130  | -1.69106162 | -2.98714662 | 6  | 0.63500142  | 2.71973848  | 2.60755324  |
| 1  | 2.81460118  | -1.65536165 | -2.28224683 | 6  | 0.16350138  | 1.28083837  | 2.49645329  |
| 1  | 3.98600125  | -2.73086143 | -3.05524683 | 1  | 0.11760139  | 3.36133838  | 1.89205337  |
| 1  | 3.28950119  | -1.38886166 | -3.98054695 | 1  | 0.46810138  | 3.10223842  | 3.61745334  |
| 6  | 5.92510176  | -0.95056158 | -3.57854676 | 1  | 0.75110137  | 0.66723841  | 3.19585323  |
| 1  | 6.28890133  | -1.98196161 | -3.63494682 | 1  | -0.86889857 | 1.28753841  | 2.87845325  |
| 1  | 6.78010130  | -0.29346159 | -3.38634682 | 8  | 4.28160143  | 3.39883852  | 1.35885334  |
| 1  | 5.53220129  | -0.68646157 | -4.56724691 | 6  | 5.15550137  | 2.24733853  | 1.46335340  |
| 6  | 4.40410137  | -2.99996161 | 3.47975326  | 1  | 5.02480173  | 1.78053832  | 2.44035316  |
| 1  | 5.20640135  | -2.45756149 | 3.99145317  | 1  | 4.95250130  | 1.52873838  | 0.66775334  |
| 1  | 4.80860138  | -3.95196152 | 3.11995316  | 1  | 6.16890144  | 2.63443851  | 1.36705339  |
| 1  | 3.64030123  | -3.22856140 | 4.23195314  | 1  | 3.70330119  | 6.74953842  | -1.52164662 |
| 6  | 2.58870125  | -3.02236152 | 1.80945337  | 1  | 3.54740119  | 6.98913813  | 0.22925334  |
| 1  | 2.06430125  | -2.51676154 | 0.99875331  | 1  | 4.55470133  | 5.67053843  | -0.39964667 |
| 1  | 1.87330139  | -3.23006153 | 2.61515331  | 8  | -1.75189865 | -1.37356162 | -3.50494671 |
| 1  | 2.95970130  | -3.98106146 | 1.42815340  | 1  | 0.09280140  | -1.43346167 | -4.33214664 |
| 6  | 3.24150133  | -0.88126159 | 2.98545337  | 1  | 0.02200139  | -2.18606162 | -2.72014666 |
| 1  | 4.06210136  | -0.32346159 | 3.44995332  | 8  | -1.47079861 | -1.48736167 | 1.57415342  |
| 1  | 2.50360131  | -1.10306168 | 3.76615334  | 15 | -1.58269858 | -2.94306159 | 1.78645337  |
| 1  | 2.76610136  | -0.23266158 | 2.24915338  | 8  | -3.05029869 | -3.61506152 | 1.77345335  |
| 12 | -1.36489856 | 0.04703841  | 0.10465333  | 8  | -1.16469860 | -3.40896153 | 3.27715325  |
| 8  | 0.11960139  | 0.02493841  | -1.30474663 | 6  | -3.49999881 | -3.80186152 | 3.12905335  |
| 8  | -2.80889869 | 1.32053840  | 0.22705333  | 6  | -2.23359871 | -4.11816168 | 3.93175316  |
| 6  | 0.18500140  | -0.02796159 | -2.69984674 | 1  | -4.21889830 | -4.62146187 | 3.13045335  |
| 6  | -0.30109861 | -1.32926166 | -3.31854677 | 1  | -3.98489881 | -2.88416147 | 3.47185326  |
| 1  | -0.38179860 | 0.79453844  | -3.16144681 | 1  | -2.29209876 | -3.76616144 | 4.96265316  |
| 6  | -3.72729874 | 2.26193857  | 0.35565332  | 1  | -1.99729860 | -5.18616199 | 3.92075324  |
| 6  | -4.84019852 | 2.08573842  | 1.25145340  | 8  | -0.71519858 | -3.73726153 | 0.73465335  |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -5.77989864 | 3.11313844  | 1.37685335  | 6  | -0.58469862 | -5.16856194 | 0.78715330  |
| 1 | -6.61859846 | 2.99623847  | 2.05495334  | 1  | -0.11939861 | -5.47106171 | 1.72825336  |
| 6 | -5.68729830 | 4.29883814  | 0.65735334  | 1  | -1.56119859 | -5.64256191 | 0.66275334  |
| 6 | -4.62759829 | 4.46063805  | -0.22724667 | 1  | 0.06650140  | -5.43766165 | -0.04254666 |
| 1 | -4.57439852 | 5.38613844  | -0.79104668 | 15 | -2.70959878 | -1.93806159 | -2.36844683 |
| 6 | -3.64719868 | 3.48033857  | -0.40734667 | 8  | -2.44209862 | -1.40686166 | -1.00844657 |
| 6 | -5.02839851 | 0.79743844  | 2.07535338  | 8  | -4.15929842 | -1.67416167 | -2.95344663 |
| 6 | -2.52019882 | 3.72863841  | -1.42644656 | 8  | -2.60549879 | -3.52496147 | -2.38534665 |
| 6 | -5.15489864 | -0.41976157 | 1.13995337  | 6  | -4.71889830 | -0.33796158 | -2.96234679 |
| 1 | -4.27339840 | -0.54276156 | 0.51175332  | 6  | -2.92949867 | -4.27326155 | -3.58694673 |
| 1 | -5.29359865 | -1.34156168 | 1.72045338  | 1  | -5.77759838 | -0.46276158 | -3.18574667 |
| 1 | -6.03149843 | -0.30656159 | 0.49105334  | 1  | -4.59419870 | 0.13563842  | -1.98764670 |
| 6 | -3.85169864 | 0.61143839  | 3.04995322  | 1  | -4.23679829 | 0.25433841  | -3.74164677 |
| 1 | -2.90749860 | 0.50583839  | 2.51885319  | 6  | -2.54889870 | -5.71836185 | -3.35604668 |
| 1 | -3.77649879 | 1.47073841  | 3.72585320  | 1  | -4.00049877 | -4.16516161 | -3.77754664 |
| 1 | -3.99799871 | -0.28596160 | 3.66685319  | 1  | -2.37899876 | -3.84646153 | -4.43114662 |
| 6 | -6.30629826 | 0.82553840  | 2.93385339  | 1  | -2.79789877 | -6.30786180 | -4.24344683 |
| 1 | -6.29209852 | 1.62773836  | 3.67945337  | 1  | -1.47659862 | -5.81616163 | -3.16794682 |
| 1 | -7.21259832 | 0.93303841  | 2.32825327  | 1  | -3.09499860 | -6.13206196 | -2.50424671 |
| 1 | -6.39159870 | -0.12176158 | 3.47975326  |    |             |             |             |



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2980126.7 (Joules/Mol)      |
|                                              | 712.26739 (Kcal/Mol)        |
| Zero-point correction=                       | 1.135070 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.209745                    |
| Thermal correction to Enthalpy=              | 1.210690                    |
| Thermal correction to Gibbs Free Energy=     | 1.018171                    |
| Sum of electronic and zero-point Energies=   | -4232.447059                |
| Sum of electronic and thermal Energies=      | -4232.372384                |
| Sum of electronic and thermal Enthalpies=    | -4232.371440                |
| Sum of electronic and thermal Free Energies= | -4232.563958                |

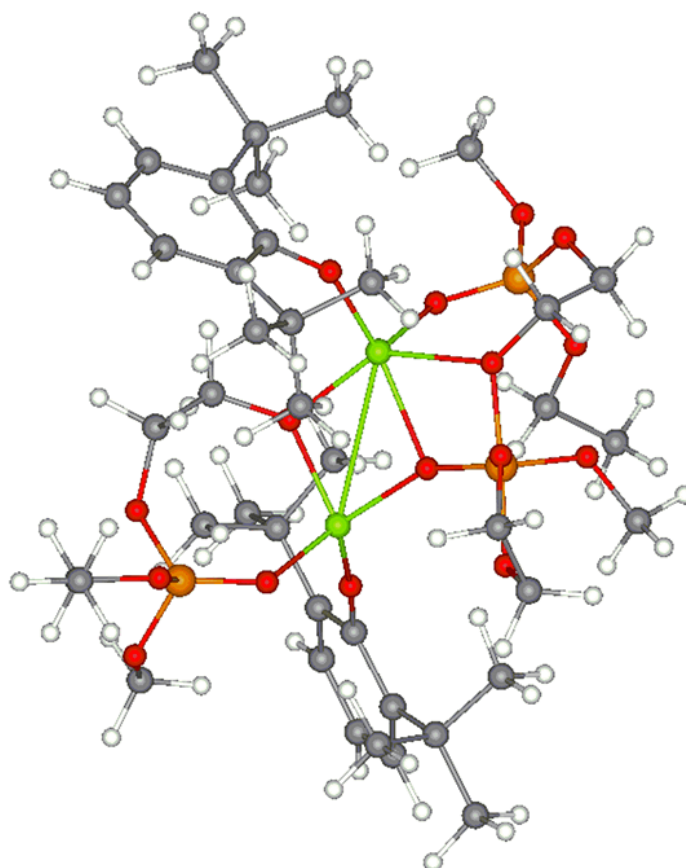
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|-----------|-------------|-------------|-------------|---|-------------|-------------|------------|--|--|
| 12        | 1.48326170  | -0.91144741 | -0.38568908 | 6 | -3.44833827 | -0.97094738 | 4.92311096 |  |  |
| 8         | -0.48183829 | -4.32634783 | -1.44908917 | 1 | -4.18983793 | -0.32524741 | 5.40541124 |  |  |
| 8         | 3.31576157  | -0.59634739 | 0.13391091  | 1 | -3.80933833 | -2.00394750 | 4.96841097 |  |  |
| 6         | -1.74533820 | -3.95264745 | -0.81818908 | 1 | -2.53333831 | -0.91994739 | 5.52411127 |  |  |
| 1         | -2.43703842 | -3.84944725 | -1.65468907 | 6 | -2.03593826 | -1.47934747 | 2.96621084 |  |  |
| 1         | -1.62563825 | -2.97534728 | -0.34798908 | 1 | -1.71163821 | -1.22154737 | 1.95821095 |  |  |
| 6         | 4.09836197  | 0.22475258  | 0.82331091  | 1 | -1.15843821 | -1.45284748 | 3.62351084 |  |  |
| 6         | 4.42346191  | -0.05354741 | 2.19471097  | 1 | -2.40903831 | -2.50944734 | 2.94871092 |  |  |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6  | 5.03416204  | 0.95315260  | 2.95081091  | 6  | -2.59873843 | 0.91635257  | 3.58101082  |
| 1  | 5.24156189  | 0.78605258  | 4.00281096  | 1  | -3.35773849 | 1.56955266  | 4.02691126  |
| 6  | 5.41106176  | 2.17225266  | 2.39541078  | 1  | -1.70423830 | 0.95995259  | 4.21511126  |
| 6  | 5.27296209  | 2.35015273  | 1.02181089  | 1  | -2.34903836 | 1.31375265  | 2.59581089  |
| 1  | 5.66776180  | 3.26075268  | 0.58201092  | 6  | -2.21733832 | -5.00534773 | 0.16131093  |
| 6  | 4.66896200  | 1.38915253  | 0.20431091  | 1  | 1.75036180  | 0.64195257  | 1.99671078  |
| 6  | 4.19666195  | -1.44534731 | 2.82201099  | 1  | -7.70753813 | -1.28094745 | 2.75681090  |
| 6  | 4.71676207  | 1.55095267  | -1.32848907 | 1  | 5.87016201  | 2.94235253  | 3.01061082  |
| 6  | 4.81716204  | -2.51974726 | 1.90581083  | 8  | 0.95346177  | -2.81744742 | 0.10841091  |
| 1  | 4.35986185  | -2.50704741 | 0.91511089  | 15 | 0.91036177  | -4.04244757 | -0.75968909 |
| 1  | 4.68566179  | -3.51614738 | 2.34711099  | 8  | 1.97566164  | -4.12494755 | -1.92298913 |
| 1  | 5.89276171  | -2.34774733 | 1.78861094  | 8  | 1.26191235  | -1.27968788 | -2.32824111 |
| 6  | 2.70766163  | -1.75654745 | 3.05711079  | 6  | 1.89026177  | -3.44714737 | -3.21088910 |
| 1  | 2.14396167  | -1.80834746 | 2.12541080  | 6  | 2.20676160  | -1.96654749 | -3.10918903 |
| 1  | 2.24626160  | -1.00254738 | 3.70421076  | 1  | 0.89106172  | -3.60834742 | -3.61608911 |
| 1  | 2.59836173  | -2.72624731 | 3.56041098  | 1  | 2.62766171  | -3.96214724 | -3.83168912 |
| 6  | 4.89346170  | -1.57694745 | 4.18941116  | 1  | 3.21446157  | -1.84284735 | -2.68918920 |
| 1  | 4.45136166  | -0.92554742 | 4.95111132  | 1  | 2.23676157  | -1.56934738 | -4.13498878 |
| 1  | 5.96446180  | -1.35794735 | 4.12771130  | 8  | 1.19926178  | -5.36054754 | 0.08031093  |
| 1  | 4.78686190  | -2.60664725 | 4.54891109  | 6  | 2.33076167  | -5.41584778 | 0.97321099  |
| 6  | 5.58886194  | 2.74555254  | -1.75658917 | 1  | 3.25946164  | -5.44554758 | 0.39901096  |
| 1  | 6.60806179  | 2.67565274  | -1.36288917 | 1  | 2.32786155  | -4.55554771 | 1.64401090  |
| 1  | 5.16576195  | 3.70715261  | -1.44428909 | 1  | 2.21676159  | -6.33774757 | 1.54251087  |
| 1  | 5.65906191  | 2.76465273  | -2.85018921 | 1  | -3.20513844 | -4.72084761 | 0.53621095  |
| 6  | 3.32806158  | 1.78105259  | -1.94668913 | 1  | -2.29493833 | -5.98274755 | -0.32188907 |
| 1  | 2.65736151  | 0.93675256  | -1.79418910 | 1  | -1.54173827 | -5.09074736 | 1.01561093  |
| 1  | 3.41366172  | 1.92525268  | -3.03088903 | 8  | -0.03663829 | 3.43135262  | 1.42621088  |
| 1  | 2.86036158  | 2.68125272  | -1.53108907 | 1  | 1.76846170  | 2.93585277  | 2.21611094  |
| 6  | 5.36236191  | 0.29105258  | -1.94158912 | 1  | 1.67126179  | 2.66745257  | 0.46281093  |
| 1  | 6.39846182  | 0.18935259  | -1.60028911 | 8  | -1.03193831 | -0.38634741 | -1.82488906 |
| 1  | 5.37136173  | 0.35835260  | -3.03688908 | 15 | -0.49643829 | -0.33214742 | -3.23598909 |
| 1  | 4.82006168  | -0.60944742 | -1.64978909 | 8  | 0.68796176  | 0.64705259  | -3.75308919 |
| 12 | -1.52193820 | 0.61995256  | -0.20358908 | 8  | -1.69853830 | 0.52985257  | -3.99788904 |
| 8  | 0.29756171  | 0.40865257  | 0.53941095  | 6  | 0.19806170  | 1.77745247  | -4.50128889 |
| 8  | -3.12943840 | 0.17675258  | 0.65261096  | 6  | -1.16453826 | 1.35045266  | -5.02908897 |
| 6  | 0.80746174  | 1.09315252  | 1.66511083  | 1  | 0.92366177  | 1.98805261  | -5.28838873 |
| 6  | 1.14196169  | 2.54945254  | 1.41061091  | 1  | 0.12296171  | 2.62985253  | -3.82128906 |
| 1  | 0.11046171  | 1.03205252  | 2.51161098  | 1  | -1.84023821 | 2.19355273  | -5.18558884 |
| 6  | -4.29153824 | -0.18664742 | 1.18391085  | 1  | -1.07143831 | 0.78155261  | -5.96378899 |
| 6  | -5.48363829 | -0.20424742 | 0.38701093  | 8  | -0.54723823 | -1.69174743 | -4.09378910 |
| 6  | -6.68453836 | -0.60004741 | 0.98461097  | 6  | -1.80353820 | -2.16994739 | -4.61358881 |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1 | -7.59643793 | -0.62114739 | 0.39741093  | 1  | -2.57873845 | -2.15624738 | -3.84548903 |
| 6 | -6.75943804 | -0.97504741 | 2.32091093  | 1  | -2.12543845 | -1.56864738 | -5.46648884 |
| 6 | -5.60303831 | -0.94864744 | 3.09191084  | 1  | -1.61693823 | -3.19654727 | -4.93068886 |
| 1 | -5.67723799 | -1.24014735 | 4.13411093  | 15 | -0.88483828 | 3.78055263  | 0.13721092  |
| 6 | -4.36693811 | -0.56094742 | 2.56621099  | 8  | -1.45563829 | 2.59875274  | -0.57828909 |
| 6 | -5.47313833 | 0.18195258  | -1.10358906 | 8  | -1.95723832 | 4.81285238  | 0.67811096  |
| 6 | -3.13103843 | -0.52654743 | 3.48351097  | 8  | -0.00343828 | 4.63745260  | -0.85938907 |
| 6 | -4.98293829 | 1.63135266  | -1.29248917 | 6  | -3.00843835 | 4.37825251  | 1.57591093  |
| 1 | -3.98753834 | 1.78965259  | -0.87838906 | 6  | 0.60226172  | 5.89525223  | -0.44068909 |
| 1 | -4.95213795 | 1.89005256  | -2.35788918 | 1  | -3.68543839 | 5.22605228  | 1.66921091  |
| 1 | -5.66893816 | 2.32845259  | -0.79718906 | 1  | -3.53723836 | 3.52165270  | 1.15531087  |
| 6 | -4.58973837 | -0.80254740 | -1.89488912 | 1  | -2.58203840 | 4.12755251  | 2.54851079  |
| 1 | -3.57193828 | -0.83984739 | -1.50608909 | 6  | 1.46176171  | 6.39735222  | -1.57778907 |
| 1 | -5.01343822 | -1.81214738 | -1.83728909 | 1  | -0.20243829 | 6.59505224  | -0.20138907 |
| 1 | -4.54083824 | -0.51034743 | -2.95098901 | 1  | 1.19506168  | 5.71605253  | 0.46111095  |
| 6 | -6.87313795 | 0.11785258  | -1.74098909 | 1  | 1.92546177  | 7.34535217  | -1.28968906 |
| 1 | -7.29983807 | -0.89044744 | -1.71288908 | 1  | 2.25426173  | 5.68355227  | -1.81448913 |
| 1 | -7.57953835 | 0.80425256  | -1.26178908 | 1  | 0.86056173  | 6.56635237  | -2.47458911 |
| 1 | -6.79993820 | 0.40905258  | -2.79518914 |    |             |             |             |

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|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2984866.0 (Joules/Mol)      |
|                                              | 713.40010 (Kcal/Mol)        |
| Zero-point correction=                       | 1.136875 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.211505                    |
| Thermal correction to Enthalpy=              | 1.212449                    |
| Thermal correction to Gibbs Free Energy=     | 1.022206                    |
| Sum of electronic and zero-point Energies=   | -4232.462257                |
| Sum of electronic and thermal Energies=      | -4232.387627                |
| Sum of electronic and thermal Enthalpies=    | -4232.386683                |
| Sum of electronic and thermal Free Energies= | -4232.576926                |

cartesian

|    |             |             |             |   |             |             |            |
|----|-------------|-------------|-------------|---|-------------|-------------|------------|
| 12 | 1.42370617  | -0.85265636 | -0.10319195 | 6 | -3.78189373 | -0.68795633 | 4.79710770 |
| 8  | -0.21909384 | -4.62775612 | -0.28969195 | 1 | -4.44879389 | 0.07544366  | 5.21160793 |
| 8  | 3.25430632  | -0.28815633 | 0.07370805  | 1 | -4.29029417 | -1.65645635 | 4.85270786 |
| 6  | -1.48999393 | -4.18545628 | 0.28010803  | 1 | -2.90519381 | -0.74205637 | 5.45240784 |
| 1  | -1.70309389 | -3.19405627 | -0.12319195 | 6 | -2.32289386 | -1.45725632 | 2.96610808 |
| 1  | -1.38789392 | -4.10765648 | 1.36510813  | 1 | -1.92139387 | -1.29815638 | 1.96590805 |
| 6  | 4.11670589  | 0.63154364  | 0.48500803  | 1 | -1.48229384 | -1.49295640 | 3.66960812 |
| 6  | 4.77520609  | 0.49944368  | 1.75560808  | 1 | -2.82059383 | -2.43385625 | 2.98610806 |
| 6  | 5.51210594  | 1.58334363  | 2.24400806  | 6 | -2.61939383 | 1.01404369  | 3.44380808 |

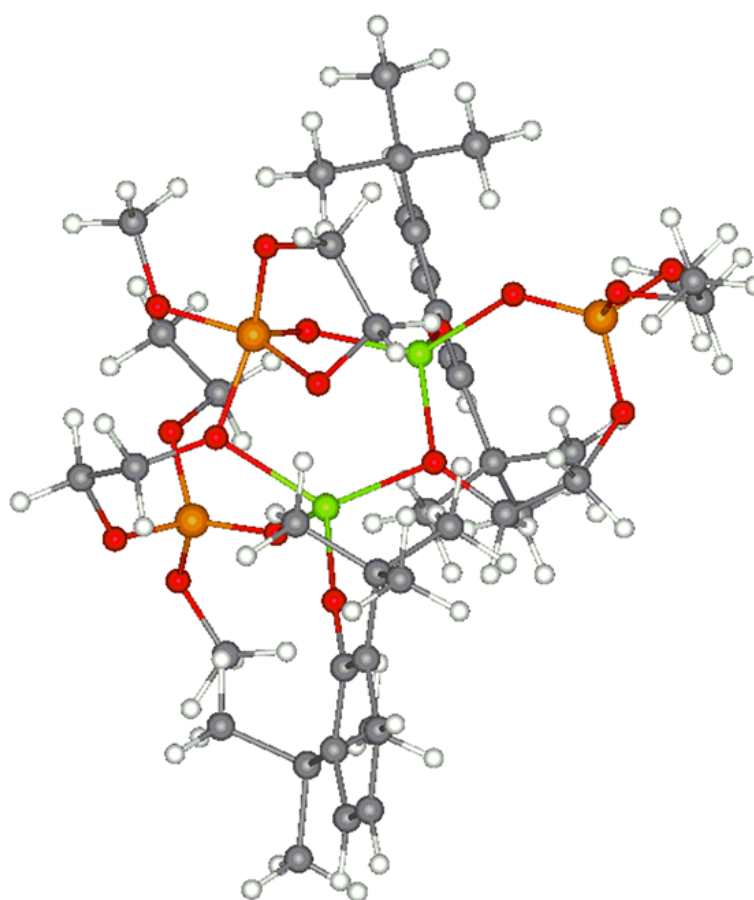
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|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1  | 5.97870588  | 1.52044368  | 3.22150803  | 1  | -3.32199383 | 1.77894366  | 3.79390812  |
| 6  | 5.69220591  | 2.75024366  | 1.50870812  | 1  | -1.78009391 | 0.98184359  | 4.14920807  |
| 6  | 5.19790602  | 2.80134368  | 0.20950803  | 1  | -2.23939371 | 1.32334363  | 2.46930814  |
| 1  | 5.42510605  | 3.67804384  | -0.38879195 | 6  | -2.54909372 | -5.19435644 | -0.09619195 |
| 6  | 4.44690609  | 1.75914359  | -0.34409195 | 1  | 1.82560611  | 1.00024366  | 2.22440815  |
| 6  | 4.74720621  | -0.81585634 | 2.56130815  | 1  | -7.90509415 | -0.53045630 | 2.38780808  |
| 6  | 4.05730581  | 1.81644368  | -1.83459187 | 1  | 6.26140594  | 3.58104372  | 1.91880798  |
| 6  | 5.14960623  | -1.99195635 | 1.64800811  | 8  | 1.15200615  | -2.68295622 | 0.77490807  |
| 1  | 4.46600580  | -2.09245634 | 0.80400807  | 15 | 1.14820611  | -4.10565615 | 0.30310804  |
| 1  | 5.15410614  | -2.93015623 | 2.21760798  | 8  | 2.22820616  | -4.48275614 | -0.79229194 |
| 1  | 6.16000605  | -1.83895636 | 1.25300813  | 8  | 1.46000612  | -1.90315640 | -1.98539197 |
| 6  | 3.36580634  | -1.08025634 | 3.18630815  | 6  | 2.08890629  | -4.24005604 | -2.21739197 |
| 1  | 2.59520626  | -1.24275637 | 2.43140817  | 6  | 2.37760615  | -2.80085635 | -2.59229183 |
| 1  | 3.06040621  | -0.24265634 | 3.82320809  | 1  | 1.08710611  | -4.53735638 | -2.52599192 |
| 1  | 3.40340614  | -1.97285640 | 3.82470798  | 1  | 2.82840633  | -4.89785624 | -2.68029189 |
| 6  | 5.75710583  | -0.80065632 | 3.72430801  | 1  | 3.37850618  | -2.51815629 | -2.25419188 |
| 1  | 5.49550581  | -0.07215634 | 4.49930763  | 1  | 2.34890628  | -2.70815635 | -3.68319201 |
| 1  | 6.77550602  | -0.58935630 | 3.38220811  | 8  | 1.44660616  | -5.12305641 | 1.48390806  |
| 1  | 5.76770592  | -1.78645635 | 4.20330763  | 6  | 2.51030612  | -4.88175631 | 2.42690802  |
| 6  | 4.75590611  | 2.97154379  | -2.57589197 | 1  | 3.47670627  | -5.04995632 | 1.94720817  |
| 1  | 5.84600592  | 2.91464376  | -2.49059200 | 1  | 2.45020628  | -3.86465621 | 2.81500816  |
| 1  | 4.43500614  | 3.95674372  | -2.21999192 | 1  | 2.36420631  | -5.60165644 | 3.23150802  |
| 1  | 4.50470591  | 2.91814375  | -3.64149189 | 1  | -3.51389384 | -4.86475611 | 0.29940805  |
| 6  | 2.54660630  | 2.03224373  | -2.02109194 | 1  | -2.63729382 | -5.28545618 | -1.18149197 |
| 1  | 1.95260608  | 1.26964366  | -1.51669192 | 1  | -2.31809378 | -6.17815638 | 0.32010806  |
| 1  | 2.28560615  | 2.00854373  | -3.08529186 | 8  | -0.25279382 | 3.52174377  | 1.41030812  |
| 1  | 2.24040627  | 3.00804377  | -1.62929189 | 1  | 1.55600607  | 3.32004380  | 2.32260799  |
| 6  | 4.50380611  | 0.51824367  | -2.53539181 | 1  | 1.58280611  | 2.87834382  | 0.60170805  |
| 1  | 5.59270620  | 0.41134366  | -2.47649193 | 8  | -0.31529382 | -0.64395630 | -1.35179198 |
| 1  | 4.21880579  | 0.53684366  | -3.59449196 | 15 | 0.00400617  | -1.26295638 | -2.74669194 |
| 1  | 4.04800606  | -0.35355633 | -2.06799197 | 8  | 1.00190616  | -0.60265636 | -3.87689185 |
| 12 | -1.34779394 | 0.58464360  | -0.16479194 | 8  | -1.34779394 | -0.54285634 | -3.49139190 |
| 8  | 0.32910618  | 0.52984369  | 0.88390809  | 6  | 0.37570617  | 0.26914367  | -4.82059193 |
| 8  | -3.05849385 | 0.14984366  | 0.49050805  | 6  | -1.09759390 | -0.11675633 | -4.81369209 |
| 6  | 0.82750618  | 1.33794367  | 1.91580796  | 1  | 0.85970616  | 0.12104367  | -5.78829193 |
| 6  | 1.01860607  | 2.79154372  | 1.53250813  | 1  | 0.52390617  | 1.30074358  | -4.48859215 |
| 1  | 0.18260616  | 1.28974366  | 2.80410814  | 1  | -1.75019383 | 0.72934365  | -5.04209232 |
| 6  | -4.28379393 | -0.04445634 | 0.96710813  | 1  | -1.30029392 | -0.92145634 | -5.53539228 |
| 6  | -5.41919422 | -0.01905634 | 0.08960805  | 8  | -0.44859383 | -2.80195618 | -3.03609204 |
| 6  | -6.69559383 | -0.19055635 | 0.63460809  | 6  | -1.67339385 | -3.19285631 | -3.66909194 |
| 1  | -7.56529379 | -0.16525635 | -0.01289195 | 1  | -2.53599381 | -2.71665621 | -3.20469189 |

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|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -6.90019417 | -0.40085635 | 1.99300814  | 1  | -1.65659392 | -2.96135616 | -4.73759222 |
| 6 | -5.79689407 | -0.45355633 | 2.83610797  | 1  | -1.73049390 | -4.27605629 | -3.54489183 |
| 1 | -5.97129393 | -0.63165629 | 3.89170814  | 15 | -0.97419381 | 3.76484370  | 0.02110805  |
| 6 | -4.49019384 | -0.28595632 | 2.36690807  | 8  | -1.31309390 | 2.51694369  | -0.73069191 |
| 6 | -5.26969385 | 0.16234367  | -1.43209195 | 8  | -2.21059370 | 4.67464352  | 0.40920803  |
| 6 | -3.32069373 | -0.35395634 | 3.36670804  | 8  | -0.08589384 | 4.70844364  | -0.88459194 |
| 6 | -4.65029383 | 1.53164363  | -1.76949191 | 6  | -3.29239368 | 4.15964365  | 1.22420812  |
| 1 | -3.67079377 | 1.67024362  | -1.31299198 | 6  | 0.33180618  | 6.02644396  | -0.42699197 |
| 1 | -4.53469419 | 1.64444363  | -2.85459185 | 1  | -4.06289387 | 4.92904377  | 1.20990813  |
| 1 | -5.30419397 | 2.33874369  | -1.41909194 | 1  | -3.68319368 | 3.23274374  | 0.80200809  |
| 6 | -4.41399384 | -0.98105633 | -2.00919199 | 1  | -2.93919373 | 3.99794388  | 2.24360800  |
| 1 | -3.42879367 | -1.01885629 | -1.54379189 | 6  | 1.10660613  | 6.68064356  | -1.54759192 |
| 1 | -4.91169405 | -1.94325638 | -1.84039187 | 1  | -0.56189382 | 6.59954357  | -0.16659194 |
| 1 | -4.27389383 | -0.84985638 | -3.08849192 | 1  | 0.94780618  | 5.90344381  | 0.46860805  |
| 6 | -6.62049389 | 0.10794365  | -2.16959190 | 1  | 1.43570614  | 7.67394352  | -1.22849190 |
| 1 | -7.13599396 | -0.84775639 | -2.02689195 | 1  | 1.98880613  | 6.09194374  | -1.80929196 |
| 1 | -7.29629421 | 0.91344368  | -1.86249197 | 1  | 0.48260617  | 6.79194355  | -2.43779182 |
| 1 | -6.44559383 | 0.22554365  | -3.24519181 |    |             |             |             |

## DTS-78



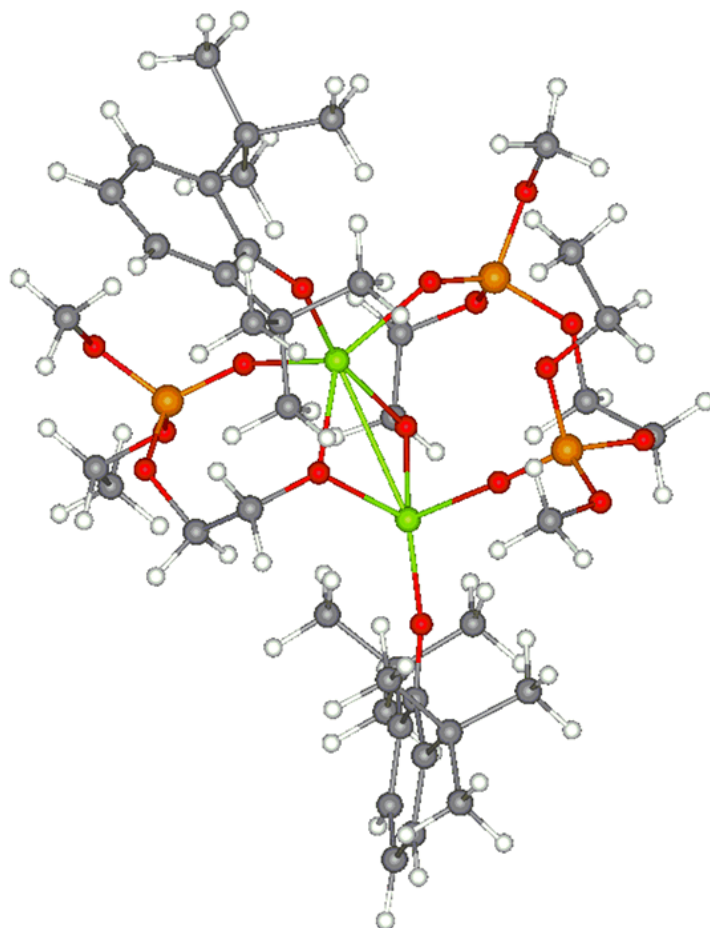
Zero-point vibrational energy

2985272.5 (Joules/Mol)

|                                              |                             |
|----------------------------------------------|-----------------------------|
|                                              | 713.49726 (Kcal/Mol)        |
| Zero-point correction=                       | 1.137030 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.210878                    |
| Thermal correction to Enthalpy=              | 1.211822                    |
| Thermal correction to Gibbs Free Energy=     | 1.025295                    |
| Sum of electronic and zero-point Energies=   | -4232.442930                |
| Sum of electronic and thermal Energies=      | -4232.369082                |
| Sum of electronic and thermal Enthalpies=    | -4232.368138                |
| Sum of electronic and thermal Free Energies= | -4232.554665                |

| cartesian |             |             |             |    |             |             |             |  |  |  |  |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|--|--|
| 12        | 1.64996374  | -0.42086893 | -0.40770584 | 6  | -3.51003647 | -1.99146891 | 4.37699413  |  |  |  |  |
| 8         | -0.86923635 | -3.51226878 | -1.57580578 | 1  | -4.41643620 | -1.58826888 | 4.84079409  |  |  |  |  |
| 8         | 3.45936370  | -0.25196892 | 0.14969414  | 1  | -3.65123630 | -3.06676888 | 4.22439384  |  |  |  |  |
| 6         | -2.20643640 | -3.32756877 | -1.01800585 | 1  | -2.69273639 | -1.87276888 | 5.09749413  |  |  |  |  |
| 1         | -2.39263630 | -2.25546885 | -0.95570588 | 6  | -1.84573627 | -1.90036893 | 2.55799413  |  |  |  |  |
| 1         | -2.23293638 | -3.75526881 | -0.01300585 | 1  | -1.48483622 | -1.43126893 | 1.64299417  |  |  |  |  |
| 6         | 4.69826365  | -0.10866892 | 0.61729419  | 1  | -1.05183625 | -1.82626891 | 3.31179404  |  |  |  |  |
| 6         | 5.24686384  | -1.05666888 | 1.54579413  | 1  | -2.01033640 | -2.96436882 | 2.35349417  |  |  |  |  |
| 6         | 6.54016352  | -0.85616893 | 2.03839397  | 6  | -2.88803649 | 0.21253109  | 3.46509409  |  |  |  |  |
| 1         | 6.96096373  | -1.56116891 | 2.74669409  | 1  | -3.79633641 | 0.65603107  | 3.88899422  |  |  |  |  |
| 6         | 7.32416344  | 0.22253110  | 1.65139413  | 1  | -2.09743643 | 0.27813107  | 4.22329426  |  |  |  |  |
| 6         | 6.80376339  | 1.12693107  | 0.73519409  | 1  | -2.59023643 | 0.80473107  | 2.59939408  |  |  |  |  |
| 1         | 7.42916346  | 1.95953107  | 0.43229416  | 6  | -3.18913627 | -4.02446890 | -1.92850578 |  |  |  |  |
| 6         | 5.51776361  | 0.99563110  | 0.20219415  | 1  | 1.69996369  | 0.92613107  | 2.11409402  |  |  |  |  |
| 6         | 4.46756363  | -2.30206871 | 2.00289416  | 1  | -7.35533619 | -2.75636888 | 1.64909422  |  |  |  |  |
| 6         | 5.02656364  | 2.04843116  | -0.80640590 | 1  | 8.32676315  | 0.35223109  | 2.05159402  |  |  |  |  |
| 6         | 4.15136385  | -3.18426871 | 0.78149414  | 8  | 0.74766368  | -2.24816871 | 0.08419415  |  |  |  |  |
| 1         | 3.54876351  | -2.65156889 | 0.04659414  | 15 | 0.43206367  | -3.49746871 | -0.68590581 |  |  |  |  |
| 1         | 3.61196351  | -4.08996868 | 1.08199418  | 8  | 1.55246377  | -3.95396876 | -1.71460581 |  |  |  |  |
| 1         | 5.08076382  | -3.49836874 | 0.29389414  | 8  | 1.39516377  | -1.12156892 | -2.37240601 |  |  |  |  |
| 6         | 3.18396354  | -1.89266896 | 2.74909401  | 6  | 1.64266372  | -3.43236876 | -3.06270599 |  |  |  |  |
| 1         | 2.49176359  | -1.35256898 | 2.10369396  | 6  | 2.22766352  | -2.03806877 | -3.08740592 |  |  |  |  |
| 1         | 3.42946362  | -1.24896896 | 3.60119414  | 1  | 0.65396369  | -3.44586873 | -3.52190590 |  |  |  |  |
| 1         | 2.66606355  | -2.77656889 | 3.14079404  | 1  | 2.30606365  | -4.12356901 | -3.58770585 |  |  |  |  |
| 6         | 5.27116346  | -3.18026876 | 2.97959399  | 1  | 3.20726371  | -2.02416873 | -2.59950590 |  |  |  |  |
| 1         | 5.52156353  | -2.65256882 | 3.90619421  | 1  | 2.34876370  | -1.72326887 | -4.12690592 |  |  |  |  |
| 1         | 6.19836378  | -3.55676889 | 2.53529406  | 8  | 0.24776369  | -4.75106859 | 0.26859415  |  |  |  |  |
| 1         | 4.66746378  | -4.05216885 | 3.25679398  | 6  | 0.72766370  | -4.81076860 | 1.62459421  |  |  |  |  |
| 6         | 6.08206367  | 3.12903118  | -1.10420585 | 1  | 1.67836368  | -5.34636879 | 1.63929415  |  |  |  |  |
| 1         | 6.99556351  | 2.70973110  | -1.53820586 | 1  | 0.84746367  | -3.80926871 | 2.03699398  |  |  |  |  |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1  | 6.35616350  | 3.70413113  | -0.21310586 | 1  | -0.02063631 | -5.36536884 | 2.19149399  |
| 1  | 5.67256355  | 3.83683109  | -1.83450580 | 1  | -4.20093632 | -3.86786890 | -1.54440582 |
| 6  | 3.80476356  | 2.78483129  | -0.22780585 | 1  | -3.13603640 | -3.61736870 | -2.94120598 |
| 1  | 2.97046351  | 2.10033131  | -0.07180586 | 1  | -2.99073648 | -5.09906864 | -1.96940589 |
| 1  | 3.48016357  | 3.58943129  | -0.90000582 | 8  | -0.69603634 | 3.29883122  | 2.03369403  |
| 1  | 4.06246376  | 3.23903108  | 0.73599410  | 1  | 1.12786376  | 3.04513121  | 2.88199401  |
| 6  | 4.69296360  | 1.38143110  | -2.15410590 | 1  | 1.18406379  | 3.18503118  | 1.10989416  |
| 1  | 5.59206343  | 0.91523105  | -2.57230592 | 8  | -0.86923635 | -0.06126891 | -1.99710584 |
| 1  | 4.33476353  | 2.12503123  | -2.87770605 | 15 | 0.24586369  | 0.02513109  | -3.04700589 |
| 1  | 3.92606354  | 0.61583108  | -2.04790592 | 8  | 1.37206376  | 1.11293113  | -2.32240605 |
| 12 | -1.46673632 | 0.68713105  | -0.28350586 | 8  | -0.13843630 | 1.22593105  | -4.14660597 |
| 8  | 0.32806367  | 0.71313107  | 0.58139420  | 6  | 0.98106366  | 2.46853113  | -2.48220587 |
| 8  | -3.07583642 | 0.01953109  | 0.43979415  | 6  | 0.31866369  | 2.53523111  | -3.85920596 |
| 6  | 0.67106366  | 1.21583104  | 1.85049427  | 1  | 1.87416375  | 3.09083128  | -2.42440605 |
| 6  | 0.65256369  | 2.73083115  | 1.94999421  | 1  | 0.28496367  | 2.75323129  | -1.68870580 |
| 1  | 0.01636369  | 0.80593109  | 2.63249397  | 1  | -0.53003633 | 3.22413111  | -3.86680603 |
| 6  | -4.18443632 | -0.63276893 | 0.76799417  | 1  | 1.02856374  | 2.82813120  | -4.64040613 |
| 6  | -5.32103634 | -0.63466895 | -0.11020586 | 8  | -0.01353631 | -1.11016893 | -4.20630598 |
| 6  | -6.43023634 | -1.41356897 | 0.23769414  | 6  | -0.97523630 | -0.95416892 | -5.25510597 |
| 1  | -7.29253626 | -1.44516897 | -0.41920587 | 1  | -1.92523623 | -0.57906890 | -4.86780596 |
| 6  | -6.48083639 | -2.15516877 | 1.41219413  | 1  | -0.60433632 | -0.27916893 | -6.02850580 |
| 6  | -5.40873623 | -2.08826876 | 2.29419398  | 1  | -1.12173629 | -1.95356894 | -5.67170572 |
| 1  | -5.47923660 | -2.64156890 | 3.22449398  | 15 | -1.50723624 | 3.77013111  | 0.75309420  |
| 6  | -4.26443624 | -1.33336890 | 2.01879406  | 8  | -1.72873628 | 2.70253110  | -0.26810586 |
| 6  | -5.37303638 | 0.20543109  | -1.40370584 | 8  | -2.80853629 | 4.42193127  | 1.36879420  |
| 6  | -3.14343643 | -1.25586891 | 3.07469416  | 8  | -0.75713634 | 4.99183130  | 0.08159414  |
| 6  | -5.11603642 | 1.69283104  | -1.09170592 | 6  | -3.76113629 | 3.64013124  | 2.13319397  |
| 1  | -4.13493633 | 1.85123110  | -0.64430583 | 6  | -0.51643634 | 6.22913122  | 0.81219411  |
| 1  | -5.16933632 | 2.28963113  | -2.01070595 | 1  | -4.61623621 | 4.29533100  | 2.29189396  |
| 1  | -5.87803650 | 2.07383108  | -0.40160584 | 1  | -4.06573629 | 2.75533128  | 1.57319415  |
| 6  | -4.35503626 | -0.30196893 | -2.44170594 | 1  | -3.31693649 | 3.35753131  | 3.08849406  |
| 1  | -3.32953644 | -0.28656894 | -2.07360578 | 6  | 0.33546367  | 7.12393141  | -0.05810586 |
| 1  | -4.59193659 | -1.33056891 | -2.73500586 | 1  | -1.48523629 | 6.68293142  | 1.03489423  |
| 1  | -4.39233637 | 0.31903109  | -3.34590602 | 1  | -0.01433631 | 5.98923111  | 1.75429416  |
| 6  | -6.75303650 | 0.14243110  | -2.08490586 | 1  | 0.51956367  | 8.06773090  | 0.46349415  |
| 1  | -7.00683641 | -0.86726892 | -2.42490602 | 1  | 1.29916370  | 6.65743113  | -0.27670586 |
| 1  | -7.55603647 | 0.49783105  | -1.43030584 | 1  | -0.17033631 | 7.34413099  | -1.00130582 |
| 1  | -6.74373627 | 0.78643107  | -2.97140598 |    |             |             |             |



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2981995.1 (Joules/Mol)      |
|                                              | 712.71393 (Kcal/Mol)        |
| Zero-point correction=                       | 1.135782 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.211045                    |
| Thermal correction to Enthalpy=              | 1.211990                    |
| Thermal correction to Gibbs Free Energy=     | 1.020143                    |
| Sum of electronic and zero-point Energies=   | -4232.438967                |
| Sum of electronic and thermal Energies=      | -4232.363704                |
| Sum of electronic and thermal Enthalpies=    | -4232.362760                |
| Sum of electronic and thermal Free Energies= | -4232.554607                |

| cartesian |             |             |             |   |            |             |             |
|-----------|-------------|-------------|-------------|---|------------|-------------|-------------|
| 12        | -1.74398005 | -0.23436901 | 0.14263910  | 6 | 3.79741979 | -1.71646893 | -4.57186079 |
| 8         | 0.50751990  | -3.93466902 | 0.25553912  | 1 | 3.64251995 | -0.92576897 | -5.31416082 |
| 8         | -3.58428001 | 0.09163100  | -0.06926090 | 1 | 4.86251974 | -1.97066903 | -4.55786085 |
| 6         | 1.07331991  | -5.22046900 | 0.64103913  | 1 | 3.25051999 | -2.59816909 | -4.92606068 |
| 1         | 0.49471989  | -6.02076864 | 0.16763911  | 6 | 3.42082000 | -2.57206917 | -2.28116083 |
| 1         | 0.97091991  | -5.31436872 | 1.72533917  | 1 | 3.03792000 | -2.37876916 | -1.27776086 |
| 6         | -4.80008030 | 0.50373101  | -0.41906092 | 1 | 2.86301994 | -3.41286898 | -2.71476078 |
| 6         | -5.45637989 | -0.05426900 | -1.56496084 | 1 | 4.47241974 | -2.86956906 | -2.20146084 |
| 6         | -6.69748020 | 0.46343097  | -1.94796085 | 6 | 1.78381991 | -0.99446899 | -3.33586097 |

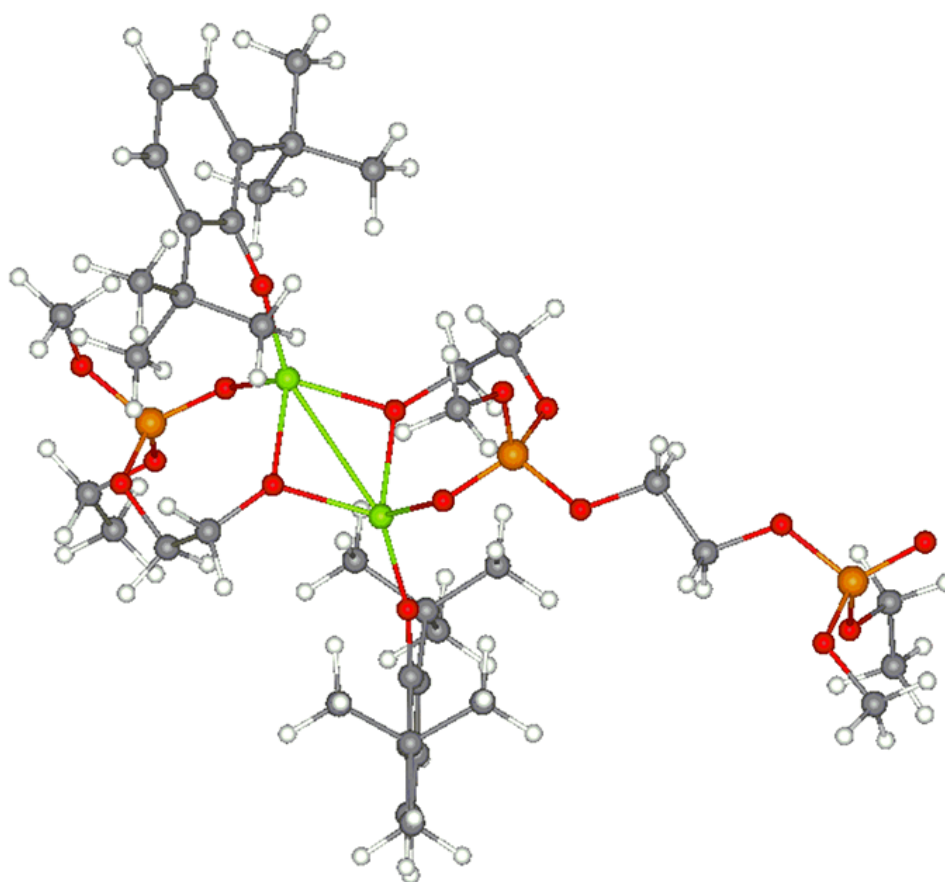
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 1  | -7.19867992 | 0.06883100  | -2.82526088 | 1  | 1.65171993  | -0.12846899 | -3.99406099 |
| 6  | -7.33028030 | 1.47463107  | -1.23496091 | 1  | 1.25271988  | -1.83916903 | -3.79596090 |
| 6  | -6.72478008 | 1.96173108  | -0.08286089 | 1  | 1.31601989  | -0.78286898 | -2.37466097 |
| 1  | -7.24738026 | 2.72483087  | 0.48393911  | 6  | 2.52061987  | -5.25806904 | 0.21043912  |
| 6  | -5.48218012 | 1.49653101  | 0.35843909  | 1  | -1.10928011 | 0.96943104  | -2.77426076 |
| 6  | -4.85768032 | -1.23396897 | -2.35266089 | 1  | 6.71352005  | 1.86323106  | -3.40106082 |
| 6  | -4.89058018 | 2.04983091  | 1.66703916  | 1  | -8.29297924 | 1.86153102  | -1.55996084 |
| 6  | -4.67377996 | -2.43716908 | -1.40736091 | 8  | -1.36638010 | -2.24946904 | 0.17703912  |
| 1  | -4.00318003 | -2.19986916 | -0.58056092 | 15 | -1.05538011 | -3.69246912 | 0.36453912  |
| 1  | -4.26957989 | -3.29956913 | -1.95126081 | 8  | -1.54918015 | -4.36286879 | 1.70863914  |
| 1  | -5.63988018 | -2.73546910 | -0.98556089 | 8  | 0.22121991  | -2.69386911 | 3.31063914  |
| 6  | -3.52158022 | -0.84386897 | -3.01056075 | 6  | -1.91578007 | -3.73766899 | 2.95813918  |
| 1  | -2.76808000 | -0.57106900 | -2.27096081 | 6  | -1.19868016 | -2.45346904 | 3.29623914  |
| 1  | -3.65878010 | 0.01273100  | -3.67946076 | 1  | -1.70888007 | -4.50356865 | 3.70763922  |
| 1  | -3.12588000 | -1.67346895 | -3.61016083 | 1  | -2.99158001 | -3.54166913 | 2.93713903  |
| 6  | -5.77688026 | -1.70876896 | -3.49266076 | 1  | -1.42128015 | -1.65106893 | 2.59203911  |
| 1  | -5.93738031 | -0.93496895 | -4.25116110 | 1  | -1.52308011 | -2.14796901 | 4.29703903  |
| 1  | -6.75377989 | -2.04026914 | -3.12596083 | 8  | -1.74718010 | -4.67196894 | -0.67766094 |
| 1  | -5.31158018 | -2.56396914 | -3.99626064 | 6  | -1.46468008 | -4.49666882 | -2.08436084 |
| 6  | -5.84248018 | 3.02623081  | 2.38173914  | 1  | -2.08398008 | -5.22586870 | -2.60416079 |
| 1  | -6.79938030 | 2.55853081  | 2.63603926  | 1  | -1.73028016 | -3.48756909 | -2.40296078 |
| 1  | -6.04478025 | 3.92343092  | 1.78733909  | 1  | -0.40818012 | -4.68946886 | -2.28646088 |
| 1  | -5.38108015 | 3.35693097  | 3.31943917  | 1  | 2.96771979  | -6.20086908 | 0.54103911  |
| 6  | -3.59758019 | 2.83373094  | 1.37873912  | 1  | 2.61401987  | -5.19236898 | -0.87506092 |
| 1  | -2.84528017 | 2.20083094  | 0.90613914  | 1  | 3.08081985  | -4.43096876 | 0.65043914  |
| 1  | -3.17078018 | 3.23903084  | 2.30403924  | 8  | 0.44781989  | 3.57363081  | -1.35486090 |
| 1  | -3.80598021 | 3.67243099  | 0.70473909  | 1  | -1.08428013 | 3.25953102  | -2.62326097 |
| 6  | -4.62567997 | 0.89833105  | 2.65783906  | 1  | -1.46328008 | 2.81713080  | -0.94676089 |
| 1  | -5.56597996 | 0.39763099  | 2.91413903  | 8  | 1.82661986  | -1.07126892 | 2.01263905  |
| 1  | -4.18578005 | 1.28323102  | 3.58653903  | 15 | 1.27681994  | -1.47826898 | 3.33813906  |
| 1  | -3.95378017 | 0.15143099  | 2.23163915  | 8  | -0.58138013 | 0.18803102  | 1.68413913  |
| 12 | 1.22661984  | 0.24933100  | 0.43493912  | 8  | 0.59781986  | -0.35916901 | 4.22373915  |
| 8  | -0.27248010 | 0.45603099  | -0.96066082 | 6  | -0.72768009 | 1.08033097  | 2.75203919  |
| 8  | 2.91731977  | -0.17576900 | -0.46106091 | 6  | 0.44321990  | 0.99873102  | 3.71363902  |
| 6  | -0.34318012 | 1.31553102  | -2.06296086 | 1  | -1.65258014 | 0.87243104  | 3.31203914  |
| 6  | -0.70328009 | 2.75743079  | -1.73086083 | 1  | -0.78018010 | 2.12883091  | 2.42093921  |
| 1  | 0.60431987  | 1.33443105  | -2.61636090 | 1  | 1.37791991  | 1.31013107  | 3.24153924  |
| 6  | 3.97881985  | 0.17223099  | -1.16256082 | 1  | 0.27401990  | 1.61273098  | 4.60073900  |
| 6  | 5.09902000  | 0.84593105  | -0.55266094 | 8  | 2.39291978  | -2.03996897 | 4.32153893  |
| 6  | 6.03942013  | 1.46123099  | -1.38806081 | 6  | 3.30561996  | -3.06096911 | 3.87913918  |
| 1  | 6.85491991  | 2.02953100  | -0.95156085 | 1  | 2.77811980  | -4.01266909 | 3.77063918  |

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|   |            |             |             |    |             |             |             |
|---|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 5.98562002 | 1.35313106  | -2.77456093 | 1  | 3.77831984  | -2.77086902 | 2.93943906  |
| 6 | 5.05381966 | 0.47983101  | -3.33106089 | 1  | 4.05951977  | -3.14836907 | 4.66073895  |
| 1 | 5.10551977 | 0.28913099  | -4.39846087 | 15 | 1.13791990  | 3.60923100  | 0.07283911  |
| 6 | 4.09062004 | -0.17356899 | -2.55746078 | 8  | 1.35181987  | 2.28793097  | 0.72383916  |
| 6 | 5.35831976 | 0.79953104  | 0.96883917  | 8  | 2.42662001  | 4.48293114  | -0.20686090 |
| 6 | 3.27371979 | -1.32646894 | -3.17726088 | 8  | 0.28091988  | 4.52733135  | 1.04403913  |
| 6 | 4.39391994 | 1.68163097  | 1.77693915  | 6  | 3.36781979  | 4.12383127  | -1.25346088 |
| 1 | 3.36031985 | 1.36983097  | 1.64633918  | 6  | -0.04598010 | 5.89973116  | 0.69373912  |
| 1 | 4.63461971 | 1.62783098  | 2.84693909  | 1  | 4.18892002  | 4.83283138  | -1.16136086 |
| 1 | 4.46702003 | 2.73133087  | 1.47203910  | 1  | 3.73941994  | 3.10813093  | -1.11046088 |
| 6 | 5.24071980 | -0.66276896 | 1.44393909  | 1  | 2.88571978  | 4.22733116  | -2.22696090 |
| 1 | 4.24631977 | -1.05846894 | 1.23153913  | 6  | -0.79588014 | 6.51033115  | 1.85573912  |
| 1 | 5.98521996 | -1.28796899 | 0.93783915  | 1  | 0.88471991  | 6.43573093  | 0.48963910  |
| 1 | 5.42401981 | -0.72356898 | 2.52503920  | 1  | -0.65458012 | 5.89013100  | -0.21556088 |
| 6 | 6.78251982 | 1.26733100  | 1.32313919  | 1  | -1.05478013 | 7.54623127  | 1.61743915  |
| 1 | 7.54882002 | 0.70473105  | 0.77983916  | 1  | -1.71908009 | 5.96173096  | 2.05753899  |
| 1 | 6.93571997 | 2.33433080  | 1.12743914  | 1  | -0.18088010 | 6.50743103  | 2.75913906  |
| 1 | 6.95321989 | 1.11213100  | 2.39473915  |    |             |             |             |

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## DI-5m



|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point vibrational energy                | 2979905.6 (Joules/Mol)      |
|                                              | 712.21453 (Kcal/Mol)        |
| Zero-point correction=                       | 1.134986 (Hartree/Particle) |
| Thermal correction to Energy=                | 1.211475                    |
| Thermal correction to Enthalpy=              | 1.212419                    |
| Thermal correction to Gibbs Free Energy=     | 1.010057                    |
| Sum of electronic and zero-point Energies=   | -4232.462628                |
| Sum of electronic and thermal Energies=      | -4232.386140                |
| Sum of electronic and thermal Enthalpies=    | -4232.385196                |
| Sum of electronic and thermal Free Energies= | -4232.587557                |

| cartesian |             |             |             |   |            |             |             |  |  |
|-----------|-------------|-------------|-------------|---|------------|-------------|-------------|--|--|
| 12        | -0.22144972 | 0.61003995  | -0.47804517 | 6 | 4.33225060 | -3.94045997 | -3.80264521 |  |  |
| 8         | -8.55114937 | -0.99805999 | 1.18885481  | 1 | 5.39775038 | -3.82346010 | -4.02634478 |  |  |
| 8         | -1.21794975 | 2.18973994  | -0.39924514 | 1 | 4.11545038 | -5.00975990 | -3.70924520 |  |  |
| 6         | -8.63914967 | -0.84736001 | 2.63055468  | 1 | 3.77755022 | -3.56796002 | -4.67144489 |  |  |
| 1         | -7.67004967 | -1.11386001 | 3.06555486  | 6 | 2.37795019 | -3.33586001 | -2.42644525 |  |  |
| 1         | -9.39224911 | -1.54226005 | 3.01095486  | 1 | 1.97695017 | -2.80426002 | -1.56284523 |  |  |
| 6         | -1.68954980 | 3.43023992  | -0.44734517 | 1 | 1.87545013 | -2.96725988 | -3.32974529 |  |  |

|    |             |             |             |    |              |             |             |
|----|-------------|-------------|-------------|----|--------------|-------------|-------------|
| 6  | -2.41844988 | 3.88163996  | -1.59604526 | 1  | 2.13715029   | -4.39866018 | -2.31194520 |
| 6  | -2.83744979 | 5.21473980  | -1.64104521 | 6  | 4.24825048   | -1.67656004 | -2.82944512 |
| 1  | -3.37654972 | 5.58163977  | -2.50814509 | 1  | 5.32375050   | -1.56446004 | -3.00614524 |
| 6  | -2.59554982 | 6.10173988  | -0.59764516 | 1  | 3.72135019   | -1.31516004 | -3.72114515 |
| 6  | -1.94484973 | 5.64024019  | 0.54115486  | 1  | 3.97555041   | -1.03666008 | -1.98884523 |
| 1  | -1.79394972 | 6.33633995  | 1.35945475  | 6  | -8.99704933  | 0.59113991  | 2.93105483  |
| 6  | -1.49344981 | 4.32193995  | 0.65715486  | 1  | 1.36685026   | 1.85944009  | -2.83924532 |
| 6  | -2.78454971 | 2.92903996  | -2.75044513 | 1  | 6.99005032   | -5.91525984 | -0.34594515 |
| 6  | -0.82274967 | 3.85743999  | 1.96375477  | 1  | -2.92954969  | 7.13454008  | -0.66244513 |
| 6  | -3.63584971 | 1.76243997  | -2.21054530 | 8  | -9.32724953  | -3.48476005 | 1.24715483  |
| 1  | -3.11284971 | 1.20863998  | -1.43144524 | 15 | -8.51564980  | -2.47406006 | 0.54985487  |
| 1  | -3.88804984 | 1.06394005  | -3.01844525 | 8  | -6.96744967  | -2.88195992 | 0.44925484  |
| 1  | -4.57234955 | 2.14474010  | -1.78914523 | 8  | -3.69334984  | -1.79535997 | -0.58894515 |
| 6  | -1.52254975 | 2.39274001  | -3.45154524 | 6  | -6.01814938  | -2.04416013 | -0.22534515 |
| 1  | -0.88444972 | 1.84593999  | -2.75644517 | 6  | -4.65514946  | -2.63005996 | 0.09225484  |
| 1  | -0.93544972 | 3.21623993  | -3.87384510 | 1  | -6.08394957  | -1.01416004 | 0.13645485  |
| 1  | -1.79224980 | 1.71334004  | -4.26924515 | 1  | -6.20744944  | -2.05726004 | -1.30164516 |
| 6  | -3.62354970 | 3.61953998  | -3.84054518 | 1  | -4.46664953  | -2.61016011 | 1.16775477  |
| 1  | -3.08604980 | 4.44233990  | -4.32444477 | 1  | -4.57814932  | -3.65806007 | -0.27164516 |
| 1  | -4.56924963 | 4.00884008  | -3.44944525 | 8  | -8.84974957  | -2.15646005 | -0.98204517 |
| 1  | -3.86934972 | 2.88894010  | -4.61954498 | 6  | -10.19794941 | -1.79916000 | -1.33994520 |
| 6  | -0.79844970 | 4.95974016  | 3.03795481  | 1  | -10.89174938 | -2.58656001 | -1.03694522 |
| 1  | -1.80384982 | 5.30463982  | 3.30105472  | 1  | -10.47334957 | -0.84925997 | -0.87454516 |
| 1  | -0.20684972 | 5.82883978  | 2.72985482  | 1  | -10.20524979 | -1.69345999 | -2.42424512 |
| 1  | -0.33904970 | 4.56264019  | 3.95035481  | 1  | -9.05714989  | 0.73464000  | 4.01415491  |
| 6  | 0.64465028  | 3.46194005  | 1.71595478  | 1  | -8.24314976  | 1.27603996  | 2.53445482  |
| 1  | 0.73025030  | 2.64984012  | 0.99355483  | 1  | -9.96594906  | 0.84943998  | 2.49565482  |
| 1  | 1.12565029  | 3.13463998  | 2.64505482  | 8  | 4.28005028   | 2.24354005  | -1.20204520 |
| 1  | 1.20775020  | 4.31943989  | 1.33065474  | 1  | 3.13705015   | 3.32764006  | -2.48104525 |
| 6  | -1.60824978 | 2.67603993  | 2.56985474  | 1  | 2.39405012   | 3.11824012  | -0.87844515 |
| 1  | -2.62024975 | 2.99404001  | 2.84425473  | 8  | -1.41714978  | -0.89506006 | -1.14194524 |
| 1  | -1.11184978 | 2.31044006  | 3.47775483  | 15 | -2.13094974  | -1.97106004 | -0.39154515 |
| 1  | -1.70024979 | 1.85044003  | 1.86245477  | 8  | 0.61655033   | -0.45626003 | 0.99015486  |
| 12 | 2.44315028  | -0.49896002 | 0.22665484  | 8  | -1.96314979  | -2.01356006 | 1.17415476  |
| 8  | 1.61775029  | 0.59343994  | -1.22774518 | 6  | 0.06905030   | -1.02516007 | 2.14655471  |
| 8  | 3.41155028  | -2.11145997 | 0.13485485  | 6  | -0.70374972  | -2.29895997 | 1.86505485  |
| 6  | 2.16265035  | 1.42724001  | -2.21514511 | 1  | -0.59864974  | -0.31516004 | 2.65475488  |
| 6  | 2.94475031  | 2.61353993  | -1.67664516 | 1  | 0.85415035   | -1.29296005 | 2.86885476  |
| 1  | 2.81835032  | 0.86023998  | -2.89054513 | 1  | -0.11684972  | -2.99916005 | 1.26585484  |
| 6  | 4.28315067  | -3.10825992 | 0.01845484  | 1  | -1.00914979  | -2.78636003 | 2.79325485  |
| 6  | 4.89815044  | -3.67765999 | 1.18335474  | 8  | -1.72034979  | -3.43635988 | -0.85284513 |

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|   |            |             |             |    |             |             |             |
|---|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 5.86655045 | -4.67165995 | 1.01155484  | 6  | -1.46744978 | -3.71975994 | -2.24914527 |
| 1 | 6.35485029 | -5.10275984 | 1.87895477  | 1  | -2.40834975 | -3.71846008 | -2.80464530 |
| 6 | 6.23025036 | -5.14415979 | -0.24434516 | 1  | -0.77814972 | -2.98446012 | -2.66504526 |
| 6 | 5.58535051 | -4.63556004 | -1.36554515 | 1  | -1.01924968 | -4.71116018 | -2.27484512 |
| 1 | 5.85485029 | -5.03885984 | -2.33574510 | 15 | 4.59555054  | 1.93063998  | 0.32345486  |
| 6 | 4.60915041 | -3.63845992 | -1.27364516 | 8  | 3.68675017  | 0.91674006  | 0.93665487  |
| 6 | 4.49575043 | -3.25286007 | 2.60825467  | 8  | 6.13055038  | 1.54903996  | 0.29875484  |
| 6 | 3.90335011 | -3.15095997 | -2.55264521 | 8  | 4.54955053  | 3.27083993  | 1.15585482  |
| 6 | 4.84765053 | -1.77646005 | 2.86785483  | 6  | 6.57945061  | 0.31383997  | -0.31464514 |
| 1 | 4.37455034 | -1.10376000 | 2.15365481  | 6  | 5.41615057  | 4.39813995  | 0.84005487  |
| 1 | 4.53575039 | -1.47586000 | 3.87605476  | 1  | 7.63615036  | 0.22963998  | -0.06654516 |
| 1 | 5.93165064 | -1.62795997 | 2.80005479  | 1  | 6.03175068  | -0.53736007 | 0.09285484  |
| 6 | 2.98655033 | -3.49695992 | 2.80835485  | 1  | 6.44995070  | 0.37393996  | -1.39634526 |
| 1 | 2.40185022 | -2.97995996 | 2.04635477  | 6  | 5.04735041  | 5.53694010  | 1.76235473  |
| 1 | 2.76125026 | -4.56686020 | 2.73565483  | 1  | 6.45195055  | 4.07984018  | 0.98285484  |
| 1 | 2.66685033 | -3.15165997 | 3.79985476  | 1  | 5.27105045  | 4.66784000  | -0.21044515 |
| 6 | 5.21685028 | -4.06845999 | 3.69635487  | 1  | 5.68925047  | 6.39703989  | 1.54995477  |
| 1 | 5.01425028 | -5.14156008 | 3.61625481  | 1  | 4.00685024  | 5.83684015  | 1.61835480  |
| 1 | 6.30185032 | -3.91966009 | 3.67815471  | 1  | 5.18705034  | 5.25053978  | 2.80745482  |
| 1 | 4.86365032 | -3.74185991 | 4.68115520  |    |             |             |             |

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## S2. Polymerization and polymer spectra

### S2.1. Polymerization experiments

Homopolymerization at 5 °C (Table 1, runs 1-4).

Solution of [(BHT)Mg( $\mu$ -OBn)(THF)]<sub>2</sub> (**Mg1**, 75 mg, 177  $\mu$ mol Mg) in CH<sub>2</sub>Cl<sub>2</sub> (1 mL) was added to the cooled (5 °C) and stirred solution of the monomer (17.7 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (the total volume of the solution is 16.5 mL). The resulting mixture of 1M monomer concentration was stirred for 10 min. Then, 1 mmol of AcOH in CH<sub>2</sub>Cl<sub>2</sub> (5 mL) was added, and the probe of the reaction mixture was analyzed by <sup>1</sup>H NMR spectroscopy. The product was separated by precipitation and filtration after the addition of Et<sub>2</sub>O (90 mL) and was dried *in vacuo*.

NMR spectra of poly( $\epsilon$ CL) and poly(MeOEP) are provided in Figures S2 and S3, respectively. NMR spectra of *rac*-LA and *L*-LA polymers are presented in the manuscript.

Homopolymerization of MeOEP at low temperatures (Table 1, runs 5 and 6).

The experiments were repeated using an external bath thermostatted at given temperature (–20 or –50 °C). The treatment of the mixture and separation of the polymer were performed as described above. NMR spectra are presented in Figures S4 and S5.

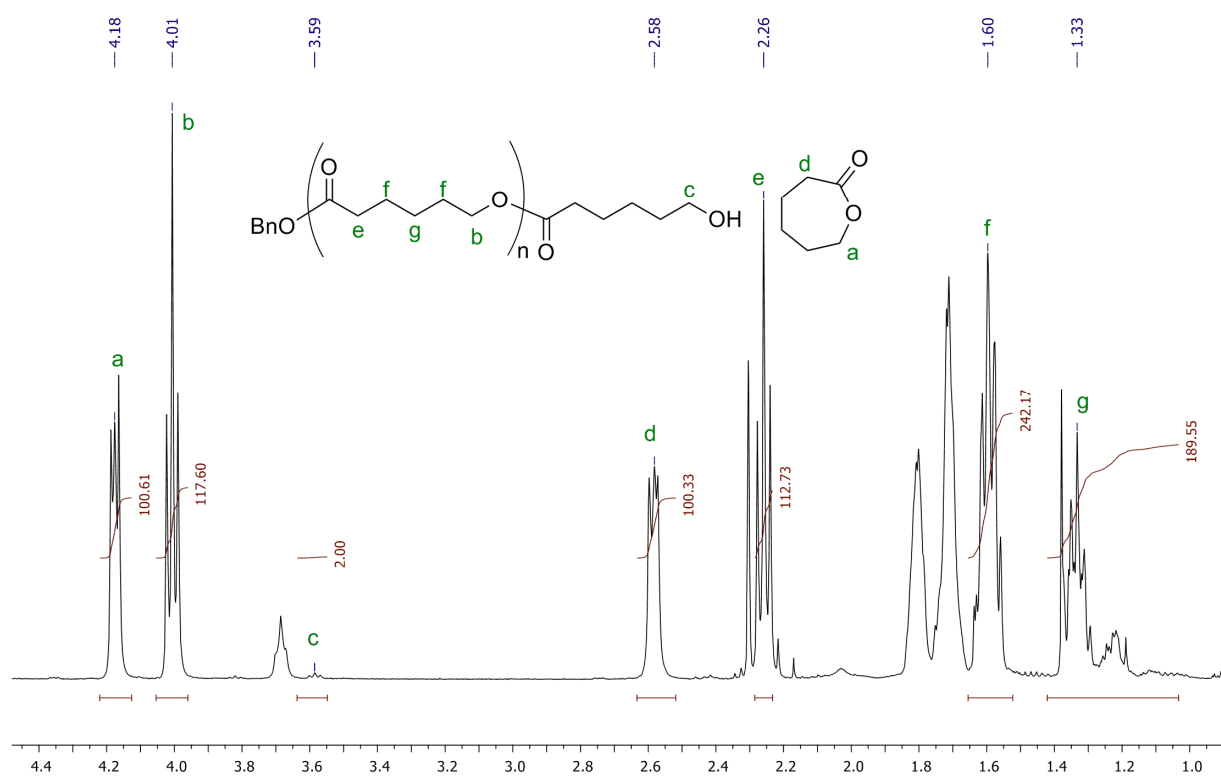
Prepolymerization of MeOEP with subsequent lactide polymerization (Table 1, runs 7 and 8).

MeOEP (0.239 g, 1.76 mmol) was dissolved in CH<sub>2</sub>Cl<sub>2</sub> (0.6 mL). The mixture was cooled to 0 °C, and the solution of the **Mg1** catalyst (75 mg, 177  $\mu$ mol Mg) in CH<sub>2</sub>Cl<sub>2</sub> (1 mL) was injected. After 3 min of stirring, the lactide solution prepared from 2.309 g (16.02 mmol) of *rac*-LA or *L*-LA in CH<sub>2</sub>Cl<sub>2</sub> (the total volume 14.2 mL) was injected into the reaction mixture. After 10 min of stirring, the polymerization was terminated by the addition of 1 mmol of AcOH in CH<sub>2</sub>Cl<sub>2</sub> (5 mL). The reaction mixture was analyzed by <sup>1</sup>H NMR spectroscopy, and the product was separated by precipitation and filtration after the addition of Et<sub>2</sub>O (90 mL) and was dried *in vacuo*.

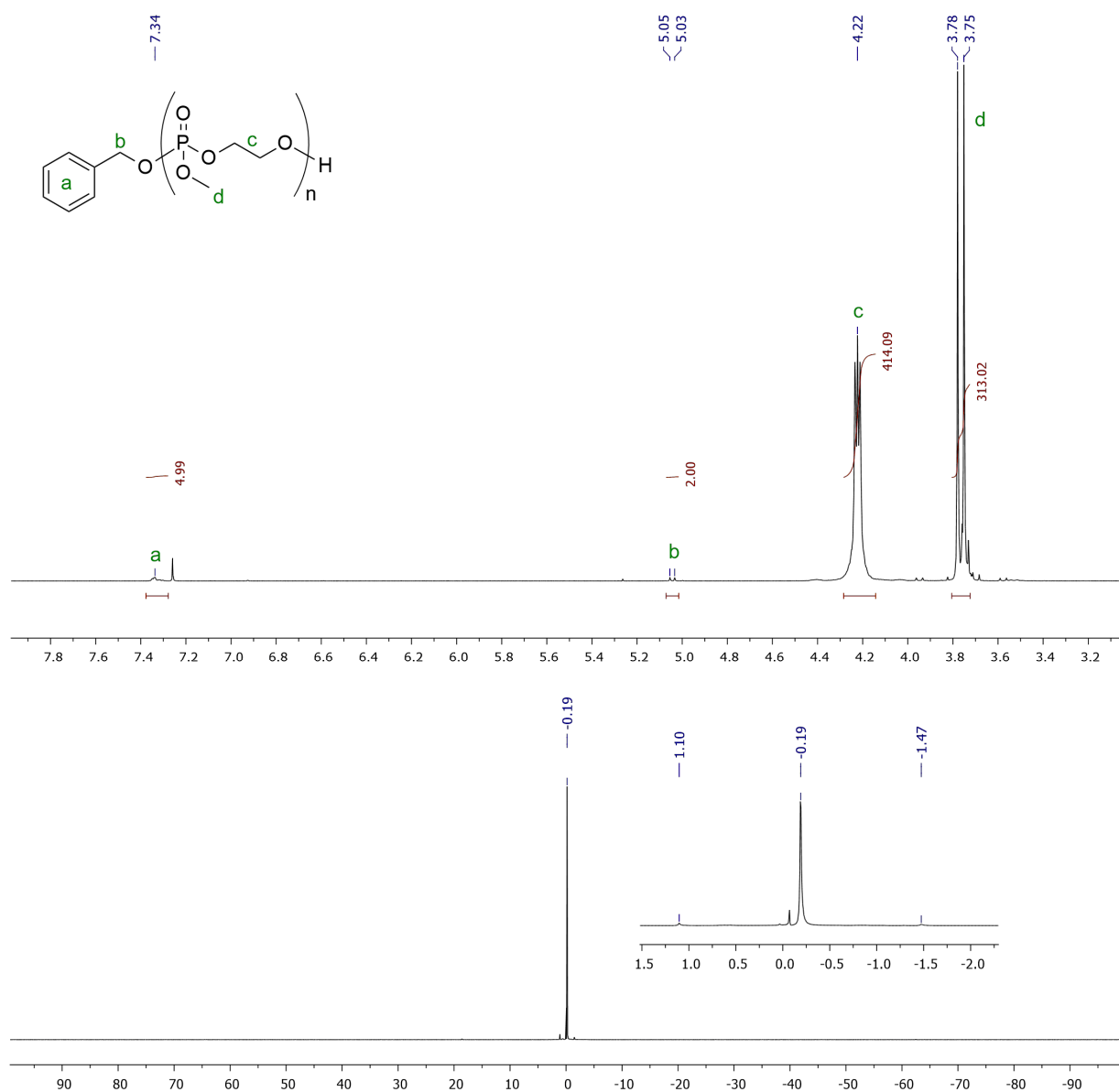
<sup>1</sup>H NMR spectra of copolymers are presented in the manuscript. <sup>31</sup>P NMR spectra are provided in Figures S6 and S7, respectively.

## S2.2. NMR spectra of polymers

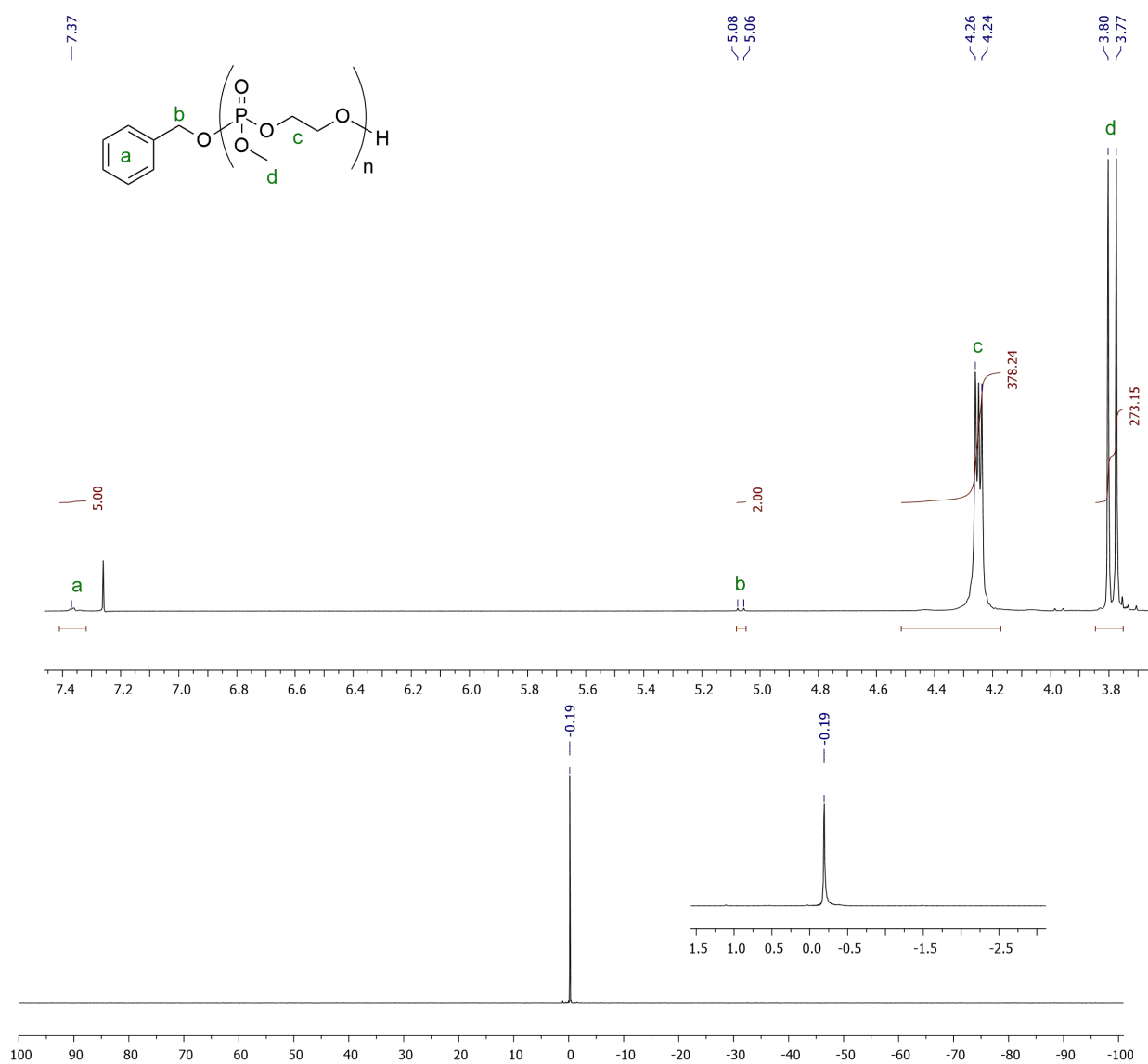
$^1\text{H}$  NMR spectra of the reaction mixtures and polymer samples were recorded in  $\text{CDCl}_3$  at 20 °C.  $M_n$  values of the polymers were determined by end-group analysis, by comparative integration of the  $\text{CH}_2\text{OH}$  end group for poly( $\epsilon\text{CL}$ ) or by initiator signals (benzyl group) for poly(MeOEP) and PLA.



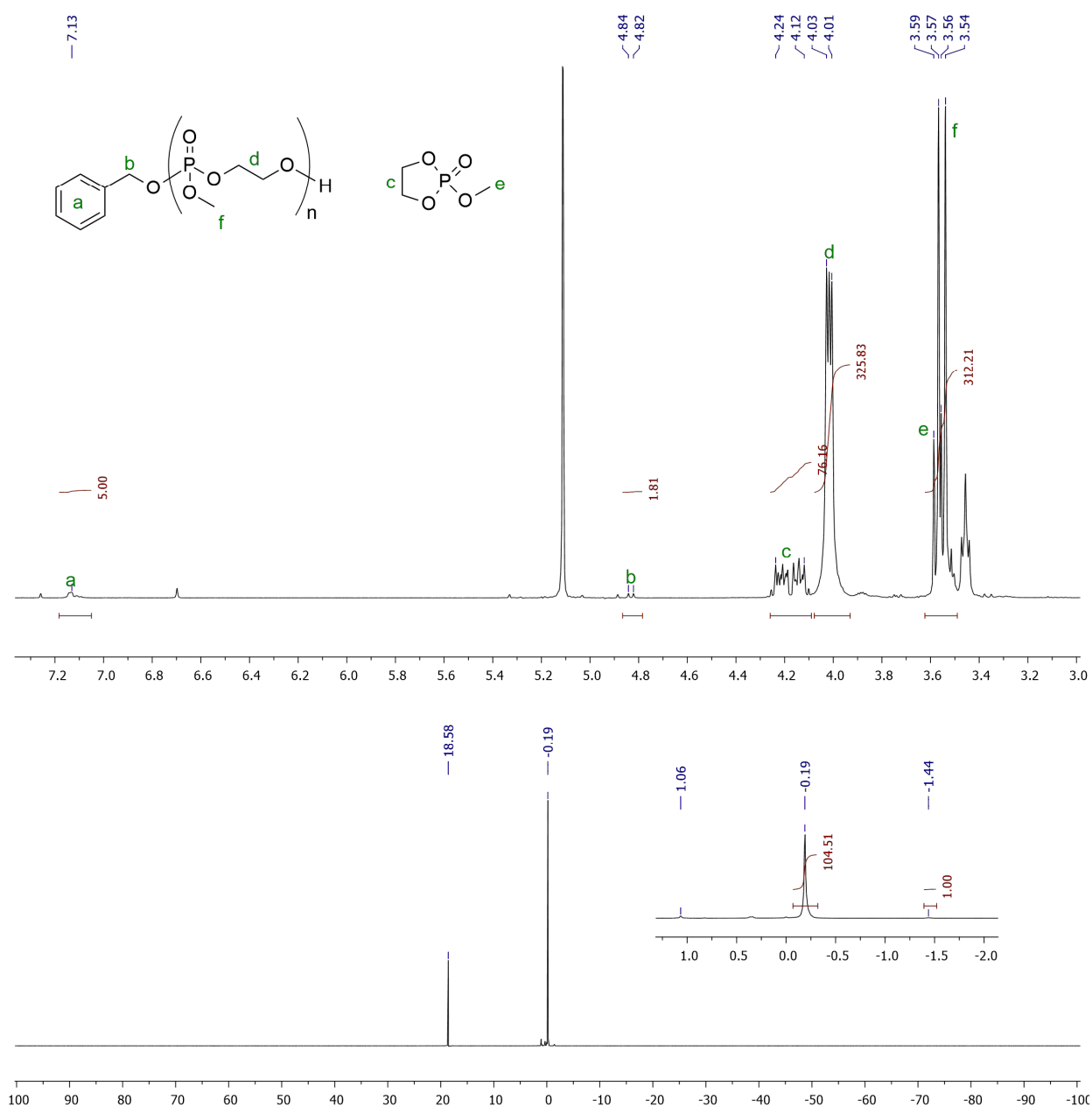
**Figure S2.**  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 20 °C) of poly( $\epsilon\text{CL}$ ) (Table 3, run 1)



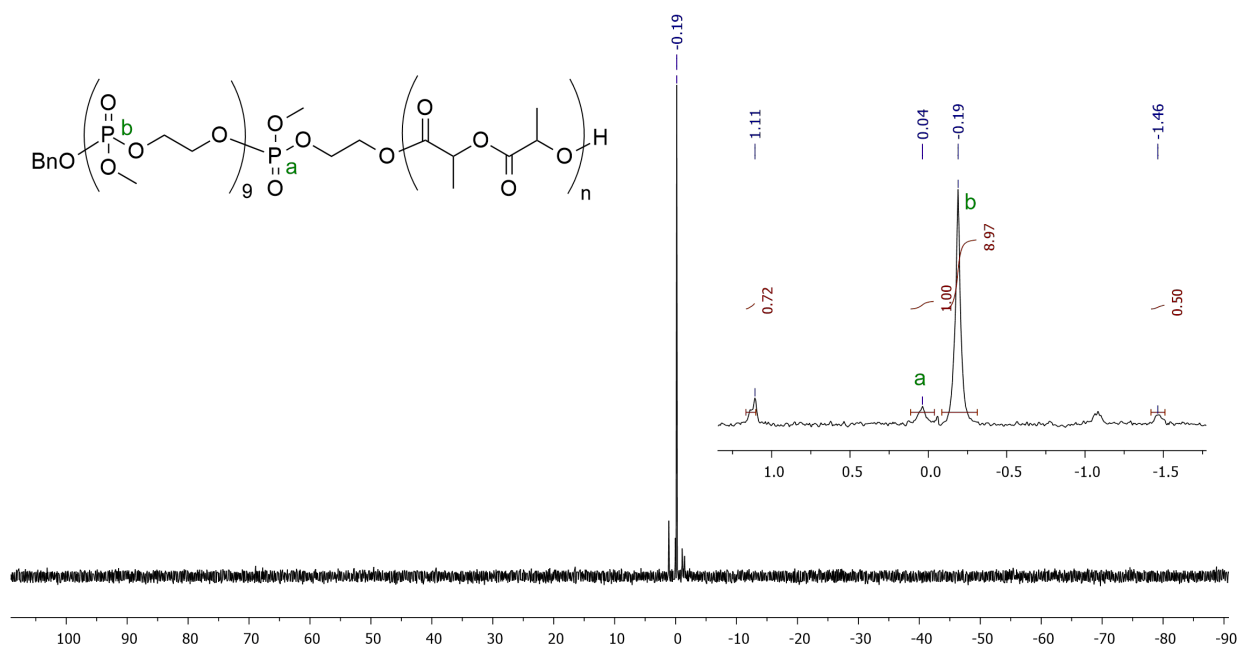
**Figure S3.**  $^1\text{H}$  and  $^{31}\text{P}$  NMR spectra ( $\text{CDCl}_3$ , 20  $^\circ\text{C}$ ) of poly(MeOEP) obtained at 5  $^\circ\text{C}$  (Table 3, run 4)



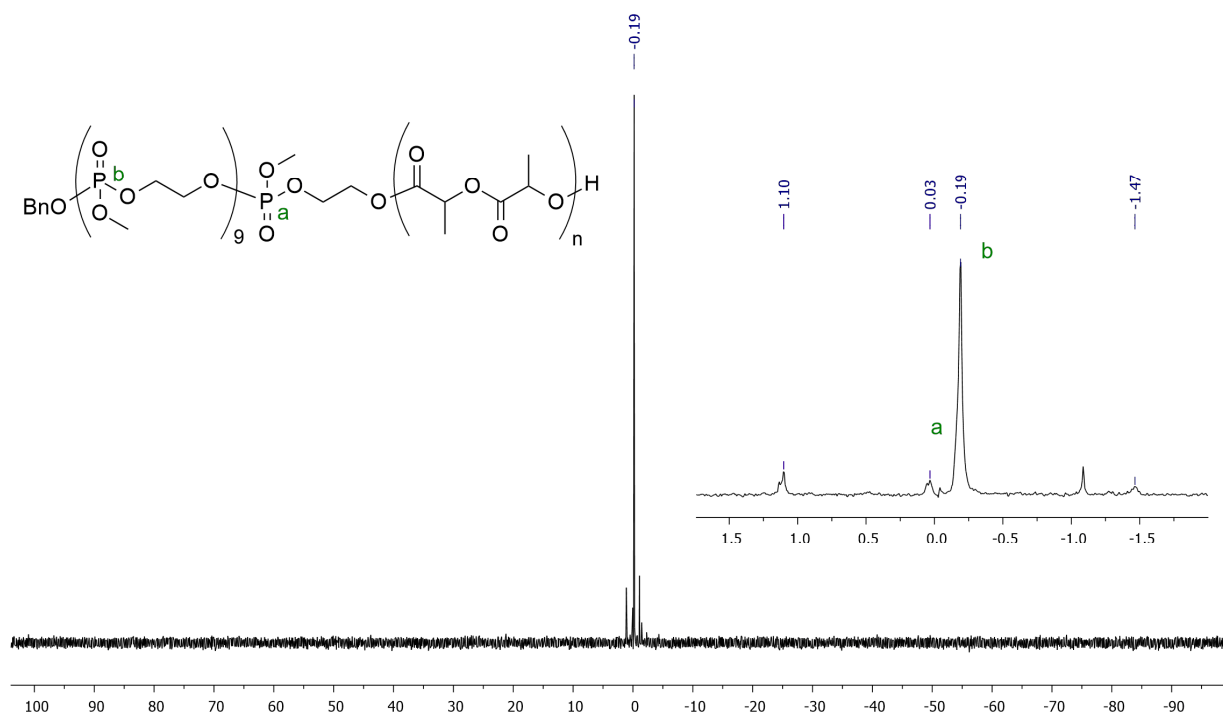
**Figure S4.**  $^1\text{H}$  and  $^{31}\text{P}$  NMR spectra ( $\text{CDCl}_3$ , 20 °C) of poly(MeOEP) obtained at  $-20$  °C (Table 3, run 5)



**Figure S5.** <sup>1</sup>H and <sup>31</sup>P NMR spectra (CDCl<sub>3</sub>, 20 °C) of the reaction mixture of MeOEP polymerization at -50 °C (Table 3, run 6)



**Figure S6.**  $^{31}\text{P}$  NMR spectrum (CDCl<sub>3</sub>, 20 °C) of the reaction mixture obtained by *rac*-LA polymerization after MeOEP pre-polymerization (Table 3, run 7)



**Figure S7.**  $^{31}\text{P}$  NMR spectrum (CDCl<sub>3</sub>, 20 °C) of the reaction mixture obtained by *rac*-LA polymerization after MeOEP pre-polymerization (Table 3, run 8)

## References

1. Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Petersson, G.A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A.; Bloino, J.; Janesko, B.G.; Gomperts, R.; Mennucci, B.; Hratchian, H.P.; Ortiz, J.V.; Izmaylov, A.F.; Sonnenberg, J.L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T. ; Ranasinghe, D.; Zakrzewski, V.G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J.A., Jr.; Peralta, J.E.; Ogliaro, F.; Bearpark, M.; Heyd, J.J.; Brothers, E.; Kudin, K.N.; Staroverov, V.N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J.C.; Iyengar, S.S.; Tomasi, J.; Cossi, M.; Millam, J.M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J.W.; Martin, R.L.; Morokuma, K.; Farkas, O.; Foresman J.B.; Fox, D.J. *Gaussian 09, Revision A.01*, Gaussian, Inc., Wallingford CT, **2016**.
2. Steitz, T.A.; Lipscomb, W.N. Molecular structure of methyl ethylene phosphate. *J. Am. Chem. Soc.* **1965**, *87*, 2488–2489, DOI: 10.1021/ja01089a031.
3. Nifant'ev, I.E.; Shlyakhtin, A.V.; Bagrov, V.V.; Minyaev, M.E.; Churakov, A.V.; Karchevsky, S.G.; Birin, K.P.; Ivchenko, P.V. Mono-BHT heteroleptic magnesium complexes: synthesis, molecular structure and catalytic behavior in the ring-opening polymerization of cyclic esters. *Dalton Trans.* **2017**, *46*, 12132–12146, DOI: 10.1039/c7dt02469j.