Supporting information

Mechanistic Insights on Acrylate Insertion Polymerization

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I. Materials and general considerations

Unless noted otherwise, all manipulations of air sensitive compounds were carried out under an inert atmosphere using standard glovebox or Schlenk techniques. Toluene, pentane and Et₂O were distilled from sodium; dmsO and methylene chloride from CaH₂ under argon. Ethylene (3.5 grade) supplied by Praxair and methyl acrylate supplied by Aldrich were used as received. [(tmeda)PdMe₂]¹, [2-(2-methoxyphenyl)phosphino]benzenesulfonic acid², and the corresponding **1-tmeda**,³ **1-dmsO**,³ **1-pyr**³ and [{(**1-Cl**)-μ-Na}₂]⁴ were prepared by known procedures. NMR spectra were recorded on a Varian Unity INOVA 400, a Bruker Avance DRX 600 spectrometer or a Bruker Avance III spectrometer, equipped with a cryoprobe head. ¹H and ¹³C NMR chemical shifts were referenced to the solvent signal. Multiplicities are given as follows (or combinations thereof): s: singlet, d: doublet, t: triplet, vt: virtual triplet, m: multiplet. The identity and purity of metal complexes was established by ¹H, ¹³C and ³¹P NMR, and elemental analysis. NMR assignments were confirmed by ¹H, ¹H gCOSY, ¹H, ¹³C gHSQC and ¹H, ¹³C gHMBC experiments. High-temperature NMR measurements of polyethylenes were performed in 1,1,2,2-tetrachloroethane-*d*₂ at 130 °C. For ethylene homopolymers and ethylene-methyl acrylate copolymers, gel permeation chromatography (GPC) was carried out in 1,2,4-trichlorobenzene at 160 °C on a Polymer Laboratories 220 instrument equipped with Olexis columns with differential refractive index, viscosity, and light scattering (15° and 90°) detectors. Data reported were determined directly against PE standard (for samples with $M_n < 10^4$ g mol⁻¹) and via universal calibration (for samples with 10^4 g mol⁻¹ < M_n < 10⁵ g mol⁻¹). These methods were in good agreement with one another. FAB mass spectra were obtained with a double-focusing Finnigan MAT 8200 mass spectrometer equipped with a Ion Tech (Teddington, U.K) FAB Ion Source. ESI mass spectra

were recorded on a Bruker Esquire 3000+ instrument. For improved ionisation $[\text{HNEt}_3][\text{B}(\text{C}_6\text{F}_5)_4]$ was added to the sample solutions.

II. Complex syntheses

$[(P^{\wedge}O)PdMe]_n$ ($P^{\wedge}O = \kappa^2\text{-}P,O\text{-}2\text{-}(2\text{-}MeOC_6H_4)_2PC_6H_4SO_3$) (**1_n**) was prepared by modification of a reported procedure.⁵ 100 mg (0.20 mmol) of **1-pyr** and 150 mg (30 mmol) of tris(pentafluorophenyl)borane were dissolved in 4 mL of dichloromethane at room temperature. This solution was layered with pentane, and stored overnight at room temperature. The crystals formed were washed twice with dichloromethane and once with pentane. 75 mg (86% yield) of **1_n** were obtained as a yellowish solid.

1H NMR (600 MHz, CD_2Cl_2 /acetone- d_6) δ 7.93 (ddd, $J = 1.1$, $J = 4.7$, $J = 7.8$, 2H, H-6), 7.61 (br. s, 2H, H-12), 7.46 (ddd, $J = 1.3$, $J = 2.7$, $J = 8.6$, 2H, H-10), 7.36 (vt, 1H, H-5), 7.25 (m, 1H, H-3), 7.22 (m, 1H, H-4), 6.96 (t, $J = 7.5$, 2H, H-11), 6.91 (dd, $J = 4.8$, $J = 8.2$, 2H, H-9), 3.56 (s, 6H, OCH_3), 0.02 (d, $J = 1.1$, 3H, Pd- CH_3). ^{13}C NMR (151 MHz, CD_2Cl_2 /acetone- d_6) δ 160.86 (s, C8), 149.11 (d, $^2J_{PC} = 14.6$, C1), 138.35 (br. s, C12), 135.00 (d, $^2J_{PC} = 2.8$, C3), 133.93 (s, C10), 130.58 (d, $^4J_{PC} = 2.2$, C5), 128.61 (d, $^3J_{PC} = 7.8$, C4), 127.75 (d, $^3J_{PC} = 8.8$, C6), 127.74 (d, $^1J_{PC} = 55.8$, C2), 120.88 (d, $^3J_{PC} = 12.6$, C11), 116.40 (d, $^1J_{PC} = 61.3$, C7), 111.87 (d, $^3J_{PC} = 4.5$, C9), 55.49 (s, OCH_3), -0.07 (d, $J = 1.7$, Pd- CH_3). ^{31}P NMR (161.8 MHz, CD_2Cl_2 /acetone- d_6): δ 24. Anal. Calcd. (%) for $\{C_{21}H_{21}O_5PdPS\}_n$: C, 48.37; H, 4.16; S, 6.13; Found: C, 48.19; H, 4.08; S, 5.89.

$[(P^{\wedge}O)Pd\{CH(COOMe)CH_2CH(C(OMe)O)CH_2CH_3\}]$ (**3-meso** and **3-rac**). 75 mg of **1_n** and 100 mg of BHT were dispersed in 5 mL of a 4 mol L⁻¹ methyl acrylate solution in dichloromethane. Sonication (by means of a heated ultrasound bath) was applied to the mixture for 3 hours at 60°C. Unreacted monomer and solvent were removed in vacuo. The non-volatiles were redissolved in dichloromethane, and centrifuged for 15 min at 4500 rpm in order to separate unreacted **1_n** from the reaction mixture. The supernatant was transferred to a Schlenk tube, and concentrated under vacuum. Addition of methanol resulted in the precipitation of polymethylacrylate (presumably formed by free-radical polymerization), which was separated via filtration over celite. Methanol was removed under vacuum, yielding a white product. This solid was washed twice with diethyl ether, (to remove BHT) and 30 mg (0.04 mmol, 30%) of **3-meso** and **3-rac** were isolated by filtration in the form of a white powder. Alternatively **3-meso**, **3-rac** could be prepared starting from $[\{(1\text{-Cl})\text{-}\mu\text{-Na}\}_2]$: To a suspension of 223 mg (0.36 mmol, 1.0 eq) $[\{(1\text{-Cl})\text{-}\mu\text{-Na}\}_2]$ and 62 mg (0.32 mmol, 0.9 eq) AgBF₄ in 12 mL dichloromethane were added 0.6 mL (6.62 mmol, 18 eq) methyl acrylate. The reaction mixture was stirred in the dark at 60 °C for 90 min in a sealed tube. The solvent was evaporated and 30 mL of toluene were added to the residue. The suspension was filtrated and ¾ of the solvent was removed in vacuum. The resulting precipitate was filtrated washed with Et₂O and dried in vacuum. The product was obtained as a slightly yellow powder (157 mg, 0.23 mmol, 72 %). Crystals suitable for X-ray diffraction analysis were obtained from saturated benzene/pentane solutions at 4 °C.

^1H NMR (600 MHz, CD_2Cl_2 ; resonances of minor diastereomer given in (brackets)) δ 8.48 (8.38) (m, 1H, 12-H or 18-H), 8.01 (8.01) (m, 2H, 6-H), 7.59 (7.59) (m, 4H, 10-H and 16-H), 7.46 (7.36) (m, 1H, 12-H or 18-H), 7.46 (7.46) (m, 1H, 5-H), 7.42 7.42 (m, 1H, 3-H), 7.31 (7.31) (m, 1H, 4-H), 7.16 and 7.06 (7.16 and 7.06) (m each, 1H each, 11-H and 17-H, 7.02 and 6.91 (7.02 and 6.91) (m each, 1H each, 9-H and 15-H), 3.95 (3.97) (s, 3H, 25-H), 3.67 (3.66) (s, 3H, ArOCH_3), 3.52 (3.50) (s, 3H, ArOCH_3), 3.44 (3.28) (s, 3H, 27-H), 3.16 (2.98) (m, 1H, 21-H), 2.07 (1.94) (m, 1H, 19-H), 1.81 and 1.39 (1.26 and 1.25) (m each, 1H each, 20-H), 1.24 and 0.92 (2.06 and 1.76) (m each, 1H each, 22-H), 0.93 (0.93) (m, 3H, 23-H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 185.68 (185.40) (s, C24), 179.63 (177.92) (s, C26), 161.29 (161.22) (s, C8 or C14), 160.58 (160.50) (d, $J = 2.9$, C8 or C14), 148.45 (148.59) (d, $J = 14.8$, C1), 142.08 (br. s, C12 or C18), 136.65 (br. s, C12 or C18), 134.94 (134.80) (s, C10 or C16), 134.86 (134.74) (d, $J = 2.7$, C3), 134.29 (134.14) (s, C10 or C16), 131.01 (130.91) (d, $J = 2.5$, C5), 128.66 (128.58) (d, $J = 8.3$, C4), 127.80 (127.98) (d, $J = 8.9$, C6), 127.03 (127.45) (d, $J = 56.5$, C2), 121.26 and 120.87 (121.17 and 120.83) (d each, $J = 11.1$ and 15.0 , C11 and C17), 115.86 and 114.49 (115.30 and 114.11) (d each, $J = 62.5$ and 61.5 , C7 and C13), 111.81 and 111.57 (111.77 and 111.68) (d each, $J = 5.0$ and 4.4 , C9 and C15), 55.90 (55.23) (s, C25), 55.78 (55.78) (s, ArOCH_3), 55.38 (55.38) (s, ArOCH_3), 52.06 (44.71) (s, C21), 51.39 (51.05) (s, C27), 32.44 (27.64) (s, C22), 27.19 (28.08) (s, C19), 24.30 (29.50) (s, C20), 12.43 (12.00) (s, C23). ^{31}P NMR (161.8 MHz, CD_2Cl_2). 22.99 (24.24). Anal. Calcd. (%) for

$\{C_{29}H_{33}O_9PdPS\}_n$: C, 50.11; H, 4.79; Found: C, 49.91; H, 4.80. MS(ESI): $m/z = 796.3$
[M+HNEt₃]⁺.

Thermolysis of **3-meso** and **3-rac** in methylene chloride-*d*₂ in a J. Young tube at 90 °C for 48 hours (in the absence of additional MA) yields 4-carbmethoxy-methylhexanoate by β-hydride elimination as the sole product.

Key NMR resonances of 4-carbmethoxy-methylhexanoate: ¹H NMR (400 MHz, CD₂Cl₂) δ 6.89 (m, 1H, H-4), 7.61 (d, *J* = 15.8 Hz, 1H, H-5), 3.10 (dt, *J* = 7.4, *J* = 8.3, 1H, 3-H) 1.82 and 1.63 (m, 2H, 2-H), 0.91 (t, *J* = 7.6, 3H, 1-H). ¹³C NMR (101 MHz, CD₂Cl₂) δ 123.57 (C4), 114.36 (C5), 50.48 (C3), 25.76 (C2), 11.87 (C1).

III. Homopolymerization of ethylene

Polymerizations were carried out in a 250 mL stainless steel mechanically stirred (750 rpm) pressure reactor equipped with a heating/cooling jacket supplied by a thermostat controlled by a thermocouple dipping into the polymerization mixture. A valve controlled by a pressure transducer allowed for applying and keeping up a constant ethylene pressure. The required flow of ethylene, corresponding to ethylene consumed by polymerization, was monitored by a mass flow meter and recorded digitally. Prior to a polymerization experiment, the reactor was heated under vacuum to the desired reaction temperature for 30 – 60 min and then back-filled with argon.

Standard procedure: A stock solution of the catalyst precursor ($1 \mu\text{mol mL}^{-1}$) in methylene chloride was prepared in the drybox, and kept in the refrigerator of the drybox (-30°C). These solutions were never stored longer than 12 hours. The reactor was vented, and in a slight argon stream, the solvent was transferred via cannula and the precursor solution was inserted by a syringe to the reactor. The reactor was closed and a constant ethylene pressure was applied. After the desired reaction time the reactor was rapidly vented and cooled to room temperature. The reaction mixture was stirred with an excess volume of methanol. The polymer was isolated by filtration, washed several times with methanol, and dried in vacuo at 50°C .

Polymerization with **1_n**

1_n is a single component precursor to very active ethylene polymerization catalysts (Table S1). With **1-dmsO** a polymerization activity of 10^5 TO h^{-1} which is independent of ethylene concentration is observed at an ethylene pressure of 5 bar. This contrasts to **1-pyr** or **1-lut**, in which a restricted dissociation of pyridine or lutidine, respectively, limits

polymerization rates under these conditions. The behaviour of **1_n** parallels polymerization with **1-dmsO**. In detail, at 5 bar the average activity observed with **1_n** in a 30 min polymerization experiment is somewhat lower (80 °C, 5 bar ethylene, 30 minutes polymerization run, **1-dmsO**: 1.0×10^5 TO h⁻¹; **1_n**: 6.6×10^4 TO h⁻¹). This appears to be due to a slow dissolution of the catalyst precursor **1_n** under reaction conditions, i.e. in the presence of ethylene monomer. Indeed, monitoring the ethylene uptake over time indicated a substantial increase of the consumption in the early stages of the reaction (first 5 min) with **1_n**. Also, addition of one equivalent of dmsO, which resulted in dissolution of **1_n** at the concentrations of NMR experiments to form **1-dmsO**, promoted the polymerization (Table S1).

Table S1. Ethylene polymerization with **1_n**

Entry	Pd [μmol]	p [bar]	TOF [mol (C ₂ H ₄) mol (Pd) ⁻¹ h ⁻¹]	polymer yield [g]	M _n ^a [10 ³ g mol ⁻¹]	branches ^b [/1000C]
S1-1	3.8	2	3.5×10^4	1.88	9.3	9
S1-2	4.4	5	6.6×10^4	4.09	11.7	4
S1-3	5.2	10	1.0×10^5	7.28	14.6	2
S1-4 ^c	4.0	5	8.1×10^4	4.52	11.9	4

Reaction conditions: 100 mL of toluene; 80 °C, 30 min polymerization time. ^a determined by ¹H NMR. ^b determined by ¹³C NMR, methyl branches observed exclusively. ^c addition of 1 equivalent of dmsO to the reaction mixture.

IV. Copolymerization of ethylene and methyl acrylate

An identical procedure as for ethylene homopolymerization was applied for copolymerization with methyl acrylate (MA). The solution of toluene and MA (with a total volume of 50 mL) was cannula transferred into the reactor under an argon counter stream. The catalyst precursor was dissolved in dichloromethane (1 mL) and inserted by a syringe to the reactor. In order to prevent any radical homopolymerization of methyl acrylate, the radical inhibitor 3,5-di-*t*-butyl-4-hydroxy-toluene (BHT) was added to the reaction mixture.

In order to prevent loss of any oligomeric material, toluene and comonomer were removed under vacuum, and the residue was dried in vacuo at 50 °C for several days. Polymer samples with more than 25 mol-% of incorporated MA were dissolved in diethyl ether and filtrated over celite, in order to remove residual ligand and also palladium black, formed in some experiments.

In ethylene-MA copolymerizations, **1_n**, **1-dmso** and **1-lut** afford polymers with virtually identical comonomer incorporation and molecular weights (Table S2). This confirms that the actual active species are identical. Again, the low solubility of **1_n** appears to slightly lower the observed average polymerization rate in a one hour experiment by comparison to **1-dmso**.

Table S2. Ethylene-methyl acrylate copolymerization

Entry	Catalyst precursor	Polymer yield [g]	TOF C ₂ H ₄	TOF MA	X _{MA} ^a	M _n ^a [10 ³ g mol ⁻¹]
S2-1	1-dmso	0.74	493	268	35%	3.1
S2-2	1_n	0.51	304	175	36%	3.3
S2-3	1-lut	0.40	245	135	33%	3.0

Reaction conditions: total volume toluene + MA: 50 mL; [MA] = 2.5 mol L⁻¹; 5 bar ethylene pressure; 95 °C; 20 μmol Pd(II); 1 h reaction time. ^a Determined by ¹H NMR at 130°C.

V. Homoligomerization of acrylate

Oligomerizations were performed in 8 mL screw-cap vials charged with a total volume of 5 mL of neat acrylate or acrylate solution in toluene, catalyst precursor, and BHT. The mixtures were stirred at 90°C. After the desired reaction time, unreacted monomers and solvent were removed in vacuo. The resulting liquid was dissolved in acetone and filtrated over silica, yielding a transparent viscous liquid (which still contains the initial BHT).

The oligomers were characterized by NMR and GPC. GPC is also useful to detect any high molecular weight polymer formed by free radical polymerization (cf. supporting information of [3]).

In acrylate insertion oligomerization, productivities observed in 12 h experiments with **1_n** are lower vs. **1-dmsO**, which again appears to be due to a slow dissolution of **1_n** (Table S3). At a higher reaction time of 24 h, with **1_n** the overall productivity is similar to **1-dmsO**. Under the reaction conditions (90 °C), catalyst decomposition appears to occur to a significant extent at the prolonged reaction times (≥ 12 h) studied. With **1_n**, fresh catalyst is provided gradually due to the slow dissolution of this catalyst precursor.

Table S3. Methyl acrylate oligomerization

Entry	Precursor	Reaction time [h ⁻¹]	TON [mol (A) mol (Pd) ⁻¹]	Oligomer yield [mg]	DP _n ^a (NMR)
S3-1	1-dmsO	12	98	170	8
S3-2	1-dmsO	16	98	169	9
S3-3	1_n	12	54	94	8
S3-4 ^b	1_n	24	113	222	9
S3-5	1-lut	16	42	72	9

Reaction conditions: 90 °C, 20 μ mol of Pd(II); ratio BHT / Pd = 35; 5 mL of neat monomers (entry 1, 4 and 5 [MA] = 6 mol L⁻¹ in toluene); ^a Determined by ¹H NMR; ^b Traces of poly(methyl acrylate) detected, presumably formed by free radical polymerization.

VI. NMR spectra of 3-meso,3-rac at 25°C

Figure S1. ^{31}P NMR spectrum of **3-meso,3-rac** in CD_2Cl_2 .

Figure S2. ^1H NMR spectrum of **3-meso,3-rac** in CD_2Cl_2 (aromatic region).

Figure S3. ^1H NMR spectrum of **3-meso,3-rac** in CD_2Cl_2 (aliphatic region, s = toluene).

Figure S4. ^{13}C NMR spectrum of **3-meso,3-rac** in CD_2Cl_2 (carbonyl region).

Figure S5. ^{13}C NMR spectrum of **3-meso,3-rac** in CD_2Cl_2 (aromatic region).

Figure S6. ^{13}C NMR spectrum of **3-meso,3-rac** in CD_2Cl_2 (aliphatic region).

Figure S7: $^1\text{H}\{^{13}\text{C}\}$ phase sensitive gHSQC (red: CH and CH_3 ; blue CH_2) spectrum of the aromatic region.

Figure S8: $^1\text{H}\{^{13}\text{C}\}$ phase sensitive gHSQC (red: CH and CH_3 ; blue CH_2) spectrum of the aliphatic region.

Figure S9: $^1\text{H}\{^{13}\text{C}\}$ gHMBC spectrum of the aromatic region.

Figure S10: $^1\text{H}\{^{13}\text{C}\}$ gHMBC spectrum of the aliphatic region.

Figure S11: $^1\text{H}\{^{13}\text{C}\}$ gHMBC spectrum of the carbonyl region.

Figure S12: ^1H - ^1H -gCOSY spectrum of the aliphatic region.

Figure S13: ^1H ^1H -gCOSY spectrum of the aromatic region.

VII. Single crystal X-ray diffraction of **3-meso,3-rac**

The crystal structure analysis was carried out at 100 K using a STOE IPDS-II diffractometer (graphite monochromated Mo-K α radiation, $\lambda = 0.71073$ Å). The structures were solved and refined using the SHELXS-97^{6a}, SHELXL-97^{6b} and PLATON⁷ software packages. The drawn ellipsoids represent 50% probability.

Crystals suitable for X-ray diffraction analysis were obtained from saturated benzene/pentane solutions after cooling to 4 °C within weeks. Two different crystals were subjected to X-ray diffraction analysis. The quality of the modelled solutions were very similar for both crystals.

The structure is disordered with respect to the stereocenter at C3 (**3-meso**), C39 (**3-rac**), respectively, of the palladium complex; i.e. both diastereomers crystallize in the unit cell in identical positions. The disorder was treated after identifying split positions in the electron density map, i.e. C3, C8, and C9 for **3-meso** and, C39, C40 C41 for **3-rac**, while C1, C2, C4, and O1 of the palladacycle were refined on their averaged positions for both diastereomers. This treatment results in artificially altered bond lengths and distances in vicinity to C3 and C39, e.g. C3-C8 1.62(3) Å and C8-C9 1.38(3) Å. Refinement converged to an occupancy of 64:36 (1.8:1) which is close to ratio determined by ¹H NMR analysis (1.6:1) of the crystallization experiment. Further refinement proceeded to convergence with a unit cell containing disordered **3-meso**, **3-rac** and three molecules of benzene. However, one molecule of benzene (C33-C38) exhibits unusual anisotropic displacement parameters, which is likely due to unresolved disorder. At this point residual electron density was detected at the position 0.0, 0.0, 0.0, which was identified as ca. 2 molecules of pentane per unit cell by NMR analysis of the diffracted crystal. However, pentane could not be modelled satisfactory due to

unreasonable bonding distances and angles. Further improvement was achieved using the SQUEEZE routine implemented in PLATON⁷ by which 128 e⁻ were removed from a 553 Å³ solvent accessible void. Results of the SQUEEZE routine are appended at the end of the cif-file. The calculated density and F000 were based on the pentane free structure, while absorption correction was applied assuming two molecules of pentane in the unit cell.

Table S4. Crystallographic Data of Complex **3-meso,3-rac**

CCDC deposit no	759055
Crystal description	colourless prism
Formula	C ₃₈ H ₄₂ O ₉ PPdS (C ₂₉ H ₃₃ O ₉ PPdS, 1.5 C ₆ H ₆); pentane squeezed out by Platon ^[7]
Crystal Size [mm ³]	0.45 × 0.317 × 0.1
Crystal System	triclinic
Space group	<i>P</i> ₋₁ (2)
<i>a</i> [Å]	11.2956(11)
<i>b</i> [Å]	11.9428(10)
<i>c</i> [Å]	17.5109(16)
α [°]	77.449(7)
β [°]	76.951(7)
γ [°]	77.429(7)
<i>V</i> [Å ³]	2210.7(3)
<i>Z</i>	2
<i>M_r</i> [g·mol ⁻¹]	812.15 (squeezed pentane not considered)
ρ_{calc} [g·cm ⁻³]	1.220 (squeezed pentane not considered)
μ (Mo-K α) [mm ⁻¹]	0.548
<i>F</i> (000) [e]	838 (squeezed pentane not considered)
<i>T</i> [K]	100
Wavelength [Å]	0.71073 (Mo-K α)
Diffractometer	STOE IPDS 2T
Scan	ω -scan
$\theta_{\text{min-max}}$ [°]	1.78-25.77
($\sin\theta/\lambda$) _{max} [Å ⁻¹]	0.59
Data total / unique	27509/ 8369
<i>R</i> _{int}	0.0760
<i>R</i> _{sigma}	0.0576
Data obs (<i>F</i> ² ≥ 4σ(<i>F</i> ²))	5638
<i>hkl</i> -range	-13/13, -14/14, -21/21
Absorption correction	numerical Integration ^[8] ; (two molecules of Pentane per unit cell considered)
Structure Solution	SHELXS-97 ^[6a]
Structure Refinement	SHELXL-97 ^[6b]
H atoms	mixed
Number Parameters	488
<i>R</i> (<i>F</i>) obs. / all	0.0488/ 0.0656
w <i>R</i> (<i>F</i> ²) all	0.1393
<i>w</i> (<i>a</i> , <i>b</i>) ^[a]	0.0748, 0.7133
Go <i>F</i> (<i>F</i> ²)	1.057
d <i>U</i> _{max}	0.000
$\Delta\rho_{\text{fin}}$ (min./max.) [e·Å ⁻³]	0.74/-1.05
remarks	Disordered pentane at 0.0, 0.0, 0.0 was removed by the PLATON SQUEEZE ^[7] routine; further disorder was modelled anisotropically

[a] weighting scheme: $w = 1/[\sigma^2(\text{Fo}^2) + (a \cdot \text{P})^2 + b \cdot \text{P}]$, $\text{P} = [\max(\text{Fo}^2, 0) + 2 \text{Fc}^2]/3$.

Figure S14. Molecular structure and numbering of **3-meso** (64 %) at 50% probability ellipsoids. All hydrogen atoms and co-crystallized solvent molecules are omitted for clarity.

Figure S15. Molecular structure and numbering of **3-rac** (36 %) at 50% probability ellipsoids. All hydrogen atoms and co-crystallized solvent molecules are omitted for clarity.

VIII. Determination of K_1 at variable temperatures

The equilibrium constant K_1 was determined via the ^{13}C shift of the Δ -carbonyl signal for two different dmso concentrations (Table S4). In the temperature interval from 5 °C to 35 °C the equilibrium (**3-meso,3-rac** + dmso $\rightleftharpoons$ **3-meso-dmso,3-rac-dmso**) is fast on NMR timescale and only one signal (δ , average of **3-meso,3-rac** and **3-meso-dmso, 3-rac-dmso**) is observed. Thus, the resonances for the dmso-opened chelate, **3-meso-dmso, 3-rac-dmso** (δ_{opened}) are not directly accessible. It was assumed that the Δ -carbonyl signal has a similar shift as in **3-meso-pyr, 3-rac-pyr**, which only exists in its open form (Figure S16-4). The mole fractions were calculated according to (SI1), and K_1 was determined according to (SI2) from the known concentrations of **3-meso,3-rac** and dmso. To avoid errors by temperature dependence of the shifts the spectra for **3-meso,3-rac** (δ_{closed}) and **3-meso-pyr,3-rac-pyr** (δ_{opened}) were also recorded for every temperature investigated. With increasing temperature the Δ -carbonyl signals of **3-meso** and **3-rac** are variably shifted (Figure S17). In some spectra two different carbonyl resonances for the two diastereoisomers were detected (25 °C, 35 °C); a weighted average of the two chemical shifts was used.

$$\delta = \alpha\delta_{\text{closed}} + \beta\delta_{\text{opened}} \quad (\text{SI1})$$

$$K_1 = \frac{\beta}{\alpha[\text{dmso}]_0 - \alpha\beta[\text{3-meso,3-rac}]_0} \quad (\text{SI2})$$

Figure S16. ^{13}C NMR spectra (carbonyl region, 150 MHz, CD_2Cl_2 , 5 °C) of **3-meso,3-rac** (1) at two different dmsol concentrations (2 & 3) and in presence of 1 equiv. pyridine (4).

Figure S17: ^{13}C NMR spectra (carbonyl region, 150 MHz, CD_2Cl_2 , 5 °C to 35 °C) of **3-meso,3-rac** ([dmsol] = 0.73 mol/L) at variable temperature.

Table S4. Determination of $K_1(T)$ at variable temperatures for two different dmso concentrations

Temp [K]	278		288		298		308	
$\delta_{\text{chelate}}^a$ [ppm]	185.39		185.39		185.40		185.42	
δ_{open}^b [ppm]	175.87		175.95		176.02		176.09	
3-meso,3-rac conc. [10^{-2} mol L $^{-1}$]	4.18	4.34	4.09	3.92	3.86	3.60	3.58	3.16
dmso conc. [mol L $^{-1}$]	0.23	0.73	0.23	0.73	0.23	0.73	0.23	0.73
δ_{measured} [ppm]	181.95	179.22	182.07	179.38	182.20	179.53	182.28	179.62
chelate open [%]	36.13	64.81	35.17	63.67	34.12	62.58	33.65	62.17
K_1 [L mol $^{-1}$]	2.57	2.61	2.46	2.47	2.34	2.35	2.28	2.30
$\text{Ln}(K_1)$	0.946	0.959	0.900	0.904	0.848	0.854	0.822	0.833
$\text{Ln}(K_1)_{\text{average}}$	0.952		0.902		0.851		0.828	
$1/T$ [10^3 K]	3.60		3.47		3.36		3.25	

^a Chemical shift of the carbonyl atom Δ , determined by ^{13}C NMR of **3-meso** and **3-rac** in CD_2Cl_2 (0.46 mol L $^{-1}$); ^b Chemical shift of the carbonyl atom Δ , determined by ^{13}C NMR of **3-meso-pyr**, **3-rac-pyr** in CD_2Cl_2 (0.39 mol L $^{-1}$).

Plotting the natural logarithm of the averaged equilibrium constants for the two dmso concentrations against the temperature (Van't Hoff plot) gave the values of the reaction enthalpy $\Delta H^\circ = -3.0(6)$ kJ mol $^{-1}$ and entropy $\Delta S^\circ = -3(2)$ J mol $^{-1}$ K $^{-1}$ (Figure S19).

Figure S18: Van't Hoff plot of $K_1(T)$ with two different dmsol ratios (ca. 5 and ca. 15 equiv.), determined from the ^{13}C NMR resonance of the Δ -carbonyl moiety at $T = 278$ to 308 K, CD_2Cl_2 .

Figure S19. Van't Hoff plot of the equilibrium between **3-meso,3-rac** and **3-meso-dmsol**, **3-rac-dmsol**, determined by variable temperature ^{13}C NMR spectroscopy at $T = 278$ to 308 K, CD_2Cl_2 .

The chelate opening of **3-meso,3-rac** with dmsO was also investigated at -80 °C. At this temperature the chemical equilibrium is slow on the NMR timescale, so that the individual resonances of **3-meso,3-rac** and **3-meso-dmsO,3-rac-dmsO** are observed in the ^{13}C -NMR spectra (Figure S20). The spectra show a higher complexity resulting from different conformers (also seen in ^{31}P -NMR) and hence no quantitative determination of K_1 was possible. However, the results are in reasonable qualitative agreement with $K_1(193\text{ K}) \approx 5(4)$ extrapolated from the thermodynamic data obtained at 278 to 308 K.

Comparison of the chemical shifts for the Δ -carbonyl signal (δ_Δ) for **3-meso-dmsO,3-rac-dmsO**, and **3-meso-pyr,3-rac-pyr** at -80 °C confirm the validity of the assumption that the resonance δ_Δ for the opened chelate is essentially independent of the nature of L.

Figure S20. ^{13}C NMR spectra of the carbonyl region of **3-meso,3-rac** at four different dmsO concentrations at -80 °C ($[\mathbf{3-meso,3-rac}]_0 \sim 0.05\text{ mol L}^{-1}$; 150 MHz, CD_2Cl_2).

IX. Binding strength of ethylene versus dmso

The ratio of the measured activity TOF to the maximum activity $TOF_{\max}$ is identical to the ratio of Pd atoms coordinated with ethylene ($Pd_{C_2H_4}$) to all Pd atoms in the polymerization mixture.

$$\frac{TOF}{TOF_{\max}} = \frac{[Pd_{C_2H_4}]}{[Pd]_0} \quad (SI3)$$

$$[Pd_{C_2H_4}] = \frac{TOF}{TOF_{\max}} \cdot [Pd]_0 \quad (SI4)$$

The equilibrium binding constant K_3 ($\mathbf{1-dmso} \rightleftharpoons \mathbf{1-C_2H_4} + \text{dmso}$) is defined according to (SI5) :

$$K_3 = \frac{[Pd_{C_2H_4}][dmso]}{[Pd_{dmso}][C_2H_4]} \quad (SI5)$$

Substitution of (SI3) and the mass conservation (SI6) into equation (SI5) results in (SI7).

$$[Pd]_0 = [Pd_{dmso}]_0 = [Pd_{dmso}] + [Pd_{C_2H_4}] \quad (SI6)$$

$$\Rightarrow K_3 = \frac{[Pd]_0 \cdot \frac{TOF}{TOF_{\max}}}{[Pd]_0 \cdot \left(1 - \frac{TOF}{TOF_{\max}}\right)} \cdot \frac{[dmso]}{[C_2H_4]} \quad (SI7)$$

$$\Leftrightarrow K_3 = \frac{TOF}{TOF_{\max} - TOF} \cdot \frac{[dmso]}{[C_2H_4]} \quad (SI8)$$

$$\Leftrightarrow \frac{TOF_{\max}}{TOF} = \frac{[dmso]}{[C_2H_4]} \cdot \frac{1}{K_3} + 1 \quad (SI9)$$

Consequently K_3 can be determined by a plot of the $\text{TOF}_{\text{max}}/\text{TOF}$ ratio versus the $[\text{dmsO}]/[\text{C}_2\text{H}_4]$ ratio. This includes the assumption that the relative binding of ethylene vs. dmsO is similar in **3-meso,3-rac** and the non-substituted alkyls $[(\text{P}^{\wedge}\text{O})\text{PdR}]$ occurring in ethylene homopolymerization. The rate of ethylene homopolymerization in the absence of essential inhibition by coordination of dmsO (TOF_{max}) was derived from ethylene polymerizations with **1-dmsO** as a catalyst precursor without additional dmsO at ethylene pressures higher than 5 bar (*vide infra*). The observed independence of polymerization rate from ethylene concentration in this pressure regime shows that indeed no significant inhibition by the dmsO introduced with the catalyst precursor occurred. With increasing amount of added dmsO (36 to 117 equivalents with respect to **1-dmsO**), the TOF values decreased (Table S5, Figure S21).

Table S5. Ethylene polymerization with **1-dmsO** in presence of dmsO.

Entry	[dmsO] [mol L ⁻¹]	TOF [mol (C ₂ H ₄) mol (Pd) ⁻¹ h ⁻¹]	polymer yield [g]	M _n ^a [10 ³ g mol ⁻¹]	M _w /M _n ^a
S5-1	0.04×10^{-3}	9.41×10^4 (= TOF_{max})	4.62	16.2	1.9
S5-2	1.27×10^{-3}	3.45×10^4	1.69	7.8	2.2
S5-3	2.06×10^{-3}	2.20×10^4	1.08	5.6	1.7
S5-4	4.11×10^{-3}	1.44×10^4	0.71	n.d.	n.d.

Reaction conditions: 100 mL of toluene; 80 °C; 30 min polymerization time; 3.5 μmol Pd; 10 bar ethylene pressure. ^a determined by GPC.

Figure S21: Activity in ethylene polymerisation at different concentrations of added dmso (catalyst precursor: **1-dmso**; $[\mathbf{1-dmso}]_0 = 3.5 \times 10^{-5} \text{ mol L}^{-1}$; 80 °C; 10 bar ethylene).

The solubility of ethylene was determined experimentally. A 70 mL steel autoclave was filled with 40 mL of toluene, heated to 80 °C, and pressurised with ethylene under stirring until equilibration was attained. The amount of ethylene taken up was determined by the weight gain of the reactor. The solubility was calculated by correcting this value for the amount of ethylene in the gas phase. For this purpose, in a similar experiment the amount of ethylene in the gas phase was determined with the reactor filled with 40 mL of solid glass pearls. The solubilities determined agree with values determined by Lee et al. for the solubility of ethylene in toluene at 50 °C and 100 °C,⁹

From a plot of $\text{TOF}_{\text{max}}/\text{TOF}$ versus $[\text{dmso}]/[\text{ethylene}]$, $K_3 = 1.1(2) \times 10^{-3}$ was determined according to equation SI9 (Figure S22).

Figure S22. Plot of $\text{TOF}_{\text{max}}/\text{TOF}$ in ethylene polymerizations with variable amounts of added dmso vs. the ratio of dmso to ethylene concentration in the polymerization mixture (●). Note that dmso liberated by dissociation of the catalyst precursor, **1-dmso**, is not considered, which results in a negligible error given that added dmso is in excess (≥ 30 equiv.). The $\text{TOF}_{\text{max}}/\text{TOF}$ for a polymerization without added dmso is also shown (■).

X. Mass spectrometry of higher insertion products

Insertion of methyl acrylate

Beyond the ESI-MS studies (cf. manuscript and vide supra) in a preliminary experiment a solution of **3-meso,3-rac** in a 4 mol L⁻¹ MA solution in benzene was kept for 12 hours at 60 °C. After removing the volatiles in vacuo, the remaining yellow powder was analyzed by FAB mass spectrometry and three different chelates were detected in their protonated form (M+1, Figure S23). The starting material ($m/z = 695.6$), the product of two consecutive insertion MA into a palladium hydride ($m/z = 681.6$) originating from β -hydride elimination and the product of insertion of one MA unit into **3-meso,3-rac** ($m/z = 781.8$).

Figure S23. FAB-mass spectrum of oligomerization solution.

As the detected intensities of the relevant species are low with fast atom bombardment (FAB) ionization, further mass spectrometry experiments were carried out with the milder electrospray ionization (ESI) technique.

For the MA insertion 23 mg (33 μmol , 1 eq) **3-meso,3-rac**, 12 mg (96 μmol , 3 eq) *p*-methoxyphenol and 82 mg (953 μmol , 29 eq) methyl acrylate were dissolved in 2 ml benzene and heated for 6 h at 60 °C in the dark. The solvent was evaporated and the residue suspended in Et₂O and filtrated. The yellow filtrate was layered with pentane yielding a white precipitate which was isolated as a dry powder. For mass spectrometry a few drops of a solution of [HNEt₃][B(C₆F₅)₄] in MeOH ($\sim 0.006 \text{ mol L}^{-1}$) were added to a solution of the aforementioned precipitate in MeOH. This solution was injected into the ESI-mass spectrometer.

Note that experiments under the same conditions with known substances led to the expected results: **1-dmso** ($m/z = 624$ [M-dmso+HNEt₃]⁺), **1_n** ($m/z = 624$ [M+HNEt₃]⁺), **3-meso,3-rac** ($m/z = 796$ [M+HNEt₃]⁺).

Figure S24. ESI-mass spectrum of insertion of MA into **3-meso,3-rac** (full).

Figure S25. Recorded isotope pattern for $[(\text{PO})\text{Pd}(\text{C}_4\text{H}_6\text{O}_2)_2\text{Me}]$ ($\text{C}_{35}\text{H}_{49}\text{NO}_9\text{PPdS}$).

Figure S26. Simulated isotope pattern for $[(\text{PO})\text{Pd}(\text{C}_4\text{H}_6\text{O}_2)_2\text{Me}]$ ($\text{C}_{35}\text{H}_{49}\text{NO}_9\text{PPdS}$).

Figure S27. ESI-mass spectrum of insertion of MA into **3-meso,3-rac** ($m/z = 500-620$).

Figure S28. ESI-mass spectrum of insertion of MA into **3-meso,3-rac** ($m/z = 690-1280$).

Insertion of butyl acrylate

In a similar experiment as described above for MA, a solution of **3-meso,3-rac**, *p*-methoxyphenol and butyl acrylate in benzene was heated for 24 h at 60 °C (Scheme S1). After workup ESI-mass spectra of the yellow solid were recorded.

Scheme S1. Insertion of butyl acrylate (BA) into complexes **3-meso,3-rac** (M represents major mass of the isotope pattern, detected by ESI-MS as the HNEt₃-adducts (M+102.13).

The signals for products of multiple insertion of butyl acrylate into **3-meso,3-rac** (m/z = 924, 1052, 1180, 1308, 1436) are rather weak in comparison to the signals for consecutive insertion of butyl acrylate into (P^{Ar}O)PdH (m/z = 866, 944, 1122, 1250, 1378), but can clearly be assigned (Figure S29). The prevalent observation of insertion products into the hydride can be related to the propensity of the catalyst for β -hydride elimination.

Figure S29. Multiple insertions of butyl acrylate into **3-meso,3-rac**.

Figure S30. ESI-mass spectrum of insertion of BA into **3-meso,3-rac** (full).

Figure S31. ESI-mass spectrum of insertion of BA into **3-meso,3-rac** (m/z = 980-1450).

XI. DFT calculations

Computational Details:

The Amsterdam Density Functional (ADF) program¹⁰ was used. The electronic configuration of the molecular systems was described by a triple- ζ STO basis set on Pd (ADF basis set TZV).^{10a} Double- ζ STO basis sets, augmented by one polarization function, were used for main group atoms (ADF basis sets DZVP).^{10a} The inner shells on Pd (including 3d), P and S (including 2p) C and O (1s), were treated within the frozen core approximation. Energies and geometries were evaluated using the local exchange-correlation potential by Vosko et al.,¹¹ augmented in a self-consistent manner with Becke's¹² exchange gradient correction and Perdew's¹³ correlation gradient correction (BP86 functional). The transition states were approached through a linear transit procedure starting from the coordination intermediates. The forming C-C bond was assumed as reaction coordinate during the linear transit scans. Full transition state searches were started from the maxima along the linear transit paths. All geometries were localized in the gas phase at 0 K.

Molecular models, cartesian coordinates and total energies (a.u.):

1

E = -11.10574744 a.u.

Pd	0.00000	0.00000	0.00000
P	2.25186	0.00000	0.00000
C	3.10754	0.21885	1.60846
C	3.07913	-1.44587	-0.77222
C	2.82483	1.43493	-1.01576
C	2.91451	-0.70461	2.66095
O	2.14909	-1.79059	2.36968
C	1.86023	-2.71104	3.42763
H	1.20839	-3.47033	2.98388
H	2.78099	-3.18647	3.79791

H	1.33662	-2.20465	4.25188
C	3.51318	-0.48664	3.90318
H	3.36768	-1.19267	4.71744
C	4.29810	0.64750	4.10694
H	4.75360	0.80836	5.08458
C	4.49066	1.56781	3.08224
H	5.09039	2.46253	3.24333
C	3.89002	1.35265	1.84402
H	4.01939	2.08897	1.05219
C	2.61335	-1.91640	-2.02350
O	1.61879	-1.19110	-2.59392
C	1.12139	-1.60781	-3.87181
H	0.34641	-0.88015	-4.13097
H	0.68534	-2.61555	-3.81154
H	1.92100	-1.58237	-4.62659
C	3.18539	-3.05293	-2.60046
H	2.83135	-3.42361	-3.56000
C	4.22464	-3.71547	-1.94747
H	4.66444	-4.59908	-2.41155
C	4.70153	-3.25513	-0.72363
H	5.52036	-3.76713	-0.21916
C	4.12351	-2.12600	-0.14319
H	4.49983	-1.75855	0.81175
C	3.95841	1.26531	-1.82225
H	4.47962	0.30807	-1.82886
C	4.43632	2.30659	-2.61443
H	5.32245	2.15022	-3.22984
C	3.78289	3.53443	-2.61320
H	4.15002	4.35513	-3.23078
C	2.65119	3.71714	-1.82195
H	2.11731	4.66757	-1.80442
C	2.16259	2.68181	-1.02476
S	0.69542	3.05214	0.00000

O	0.32496	4.42832	-0.31985
O	1.12019	2.73932	1.37004
O	-0.33362	2.05949	-0.52977
C	-0.10535	-2.01390	0.35996
H	0.79785	-2.62203	0.23939
H	-0.86255	-2.29288	-0.39718
H	-0.50103	-2.10157	1.38404

lMA-cis

E= -13.69111340 a.u.

Pd	0.00000	0.00000	0.00000
P	2.37872	0.00000	0.00000
C	3.06473	1.41306	-0.97540
C	2.43157	2.67146	-0.97730
S	0.93409	3.01069	0.00000
O	-0.09024	2.08800	-0.65758
O	1.26378	2.57675	1.36519
O	0.61546	4.41577	-0.23536
C	3.08348	0.02699	1.69409
C	3.11849	-1.47821	-0.80012
C	2.93704	3.70540	-1.76674
C	4.05579	3.49860	-2.56828
C	4.67523	2.25103	-2.58658
C	4.18230	1.21759	-1.79583
C	0.08212	-2.04447	0.39259
H	2.42505	4.66729	-1.73743
H	4.43971	4.31324	-3.18373
H	5.54736	2.07795	-3.21782
H	4.67545	0.24609	-1.81134
H	0.76455	-2.29426	1.21676
C	-2.29398	-0.01473	0.11555
H	-2.53070	-0.98692	-0.32522
C	-2.86323	1.18340	-0.56396

C	-1.78378	0.10253	1.38829
H	-1.73781	1.09353	1.84779
H	-1.64438	-0.76754	2.02919
H	0.44566	-2.50127	-0.53992
C	4.00376	-2.34204	-0.15409
C	4.48156	-3.48977	-0.78920
C	4.06463	-3.78174	-2.08411
C	3.16168	-2.94788	-2.74560
C	2.68055	-1.80497	-2.10470
H	4.32825	-2.11564	0.86118
H	5.17743	-4.14835	-0.27020
H	4.43594	-4.67186	-2.59326
H	2.83698	-3.19732	-3.75367
O	1.77944	-0.94182	-2.64523
C	4.44957	0.26436	1.96240
C	4.90237	0.31390	3.28427
C	4.00936	0.12269	4.33639
C	2.66030	-0.11013	4.08722
C	2.20860	-0.14360	2.77098
O	5.26307	0.40566	0.88317
H	5.95161	0.50258	3.49966
H	4.37984	0.16596	5.36110
H	1.95788	-0.24092	4.90940
H	1.14912	-0.27644	2.56026
C	6.59429	0.88742	1.10692
H	7.01504	1.05458	0.11004
H	6.57210	1.83538	1.66315
H	7.19896	0.14134	1.64375
C	1.31573	-1.18832	-3.97858
H	0.62190	-0.37147	-4.19744
H	2.15394	-1.16689	-4.69027
H	0.79027	-2.15274	-4.03672
O	-3.05030	0.93387	-1.88852

O	-3.15436	2.22489	-0.01131
C	-3.57717	2.07243	-2.61581
H	-3.67197	1.73456	-3.65157
H	-4.55227	2.36175	-2.20476
H	-2.88120	2.91560	-2.53263
H	-0.93066	-2.40259	0.62481

1MA-isom

E= -13.67727321 a.u.

Pd	-1.274840	0.061542	0.500571
P	0.830411	-1.721757	0.390923
C	2.299808	-0.910653	-0.415657
C	2.433480	0.488671	-0.496241
S	1.183189	1.615384	0.176184
O	-0.023766	1.398113	-0.730515
O	0.870692	1.091600	1.532279
O	1.738082	2.958773	0.069756
C	1.567773	-2.283153	1.990461
C	0.731864	-3.274051	-0.604888
C	3.544585	1.062973	-1.115758
C	4.537586	0.254908	-1.662880
C	4.417294	-1.130224	-1.594738
C	3.306010	-1.703174	-0.981436
C	-2.706437	0.297606	-0.965649
H	3.613022	2.149956	-1.153251
H	5.405580	0.709402	-2.141889
H	5.191898	-1.771927	-2.015626
H	3.223351	-2.789519	-0.933931
H	-2.935618	1.370313	-0.976489
H	-2.145493	-0.018730	-1.851620
C	-2.636420	-1.077768	1.719262
H	-2.031257	-1.565834	2.484916

H	-3.242369	-1.719259	1.076556
C	-2.954180	0.277787	1.875881
H	-3.796676	0.738046	1.354738
C	-2.423484	1.025771	3.048338
H	-3.592311	-0.322010	-0.785966
C	1.083787	-4.540761	-0.139767
C	0.925394	-5.674149	-0.940995
C	0.406083	-5.540068	-2.224802
C	0.050398	-4.283274	-2.718647
C	0.212019	-3.154459	-1.914032
H	1.506766	-4.642763	0.859965
H	1.214236	-6.653906	-0.561316
H	0.277352	-6.416376	-2.861051
H	-0.348681	-4.193882	-3.726905
O	-0.086468	-1.883721	-2.305183
C	2.815389	-1.832282	2.430115
C	3.307693	-2.171063	3.690916
C	2.545949	-2.973039	4.532545
C	1.291341	-3.429210	4.126410
C	0.796712	-3.075625	2.870460
H	3.414173	-1.195442	1.780036
H	4.282213	-1.801362	4.008200
H	2.917318	-3.246553	5.520657
H	0.702088	-4.045461	4.801526
O	-0.424499	-3.468335	2.397351
C	-0.480490	-1.670293	-3.664887
H	-0.574276	-0.585049	-3.772938
H	0.289986	-2.042779	-4.356293
H	-1.445833	-2.155111	-3.875104
C	-1.220447	-4.314004	3.235148
H	-2.129614	-4.522411	2.662270
H	-0.696906	-5.258178	3.450373
H	-1.479471	-3.804997	4.175904

O	-1.777536	0.534573	3.956385
O	-2.758844	2.339607	2.963634
C	-2.196522	3.153116	4.023925
H	-2.541158	4.169980	3.817848
H	-2.555467	2.801845	4.998821
H	-1.102189	3.091663	3.991496

1MA-trans

E= -13.68447195 a.u.

Pd	0.00000	0.00000	0.00000
P	2.51266	0.00000	0.00000
C	3.18648	1.63943	-0.56592
C	2.42745	2.82315	-0.46482
S	0.67348	2.81588	0.00000
O	0.05495	2.00517	-1.12194
O	0.56474	2.02510	1.26848
O	0.25293	4.21011	0.05751
C	3.20330	-0.21488	1.69739
C	3.34183	-1.20400	-1.10596
C	2.97076	4.04785	-0.85402
C	4.25918	4.10967	-1.37718
C	4.99882	2.94065	-1.53057
C	4.46663	1.71921	-1.12530
C	-2.06084	0.32811	0.08855
H	2.35501	4.94130	-0.75425
H	4.67486	5.07100	-1.68121
H	5.99764	2.97581	-1.96661
H	5.04829	0.80831	-1.25073
H	-2.21541	1.14530	-0.62486
H	-2.66104	-0.55743	-0.15216
C	-0.38130	-1.92780	-0.84468
H	0.52496	-2.29375	-1.33567

H	-1.27723	-1.83619	-1.46160
C	-0.48940	-2.06809	0.54988
H	-1.46567	-2.03277	1.03959
C	0.56178	-2.79050	1.31174
H	-2.20555	0.65412	1.12810
C	4.57754	-0.22122	2.03231
C	4.97362	-0.33031	3.36895
C	4.01782	-0.40484	4.38050
C	2.66256	-0.36986	4.07305
C	2.27052	-0.27335	2.73982
O	5.45947	-0.12777	1.00184
H	6.02890	-0.34160	3.63132
H	4.34760	-0.47663	5.41759
H	1.91031	-0.39934	4.86051
H	1.21066	-0.21331	2.49847
C	4.12508	-2.27070	-0.66638
C	4.62661	-3.21020	-1.56729
C	4.34229	-3.08527	-2.92438
C	3.53962	-2.04229	-3.38940
C	3.02568	-1.11389	-2.48215
H	4.33212	-2.37941	0.39629
H	5.23299	-4.03972	-1.20476
H	4.73536	-3.81121	-3.63713
H	3.30954	-1.96619	-4.45034
O	2.19247	-0.09157	-2.81154
C	1.85390	0.10705	-4.18778
H	1.19711	0.98235	-4.19578
H	2.75537	0.30870	-4.78511
H	1.32058	-0.76751	-4.58970
C	6.84848	0.00717	1.32115
H	7.35979	0.12413	0.36008
H	7.01854	0.89706	1.94472
H	7.22644	-0.89261	1.82930

O	0.17361	-2.95319	2.60900
O	1.60829	-3.21731	0.85762
C	1.11750	-3.70535	3.41124
H	0.66138	-3.77268	4.40320
H	1.26609	-4.70208	2.97698
H	2.07865	-3.17865	3.45429

1MA-inser

E= -13.67046549 a.u.

Pd	0.00000	0.00000	0.00000
P	2.37377	0.00000	0.00000
C	3.08774	1.43951	-0.92804
C	2.47543	2.70726	-0.89898
S	0.92867	3.00877	0.00000
O	-0.02741	2.04493	-0.71381
O	1.17716	2.60090	1.38814
O	0.56215	4.39608	-0.27135
C	3.02277	3.76949	-1.61944
C	4.16853	3.58259	-2.38681
C	4.76515	2.32557	-2.44474
C	4.22788	1.26496	-1.72110
H	2.51832	4.73452	-1.57333
H	4.58626	4.41816	-2.94990
H	5.65238	2.16468	-3.05799
H	4.70414	0.28651	-1.77040
C	3.09074	0.04614	1.69311
C	3.14867	-1.44575	-0.82601
H	-2.25175	-1.94295	0.00887
C	-1.56421	-1.49716	0.72979
C	-0.22434	-1.99637	0.68583
H	-1.98361	-1.26656	1.71070
C	0.05837	-3.03004	-0.34603
C	-2.20934	0.44407	0.00273

H	-2.16224	0.67450	-1.06887
H	0.32526	-2.12223	1.62316
H	-3.16122	-0.02720	0.24988
H	-2.03322	1.32477	0.63083
C	4.46305	0.25488	1.95958
C	4.91433	0.34214	3.28004
C	4.01347	0.22456	4.33615
C	2.65789	0.02933	4.09114
C	2.20954	-0.04557	2.77530
O	5.28517	0.33707	0.88099
H	5.96862	0.50669	3.49077
H	4.38272	0.29894	5.35951
H	1.94872	-0.03762	4.91515
H	1.14469	-0.13583	2.56890
C	4.05603	-2.30397	-0.20478
C	4.57948	-3.40737	-0.88072
C	4.18540	-3.65965	-2.19162
C	3.25170	-2.83874	-2.82464
C	2.72612	-1.73702	-2.14473
H	4.36099	-2.10902	0.82268
H	5.29670	-4.05964	-0.38268
H	4.59811	-4.51148	-2.73425
H	2.93921	-3.05862	-3.84374
O	1.81734	-0.87484	-2.66398
C	1.19435	-1.21304	-3.91111
H	0.47405	-0.41099	-4.09782
H	1.93576	-1.23865	-4.72326
H	0.67066	-2.17529	-3.82159
C	6.62847	0.78797	1.09216
H	7.05760	0.90330	0.09138
H	6.63283	1.75727	1.61092
H	7.21005	0.04619	1.65976
O	-0.48701	-3.11824	-1.43590

O	0.96478	-3.92630	0.12630
C	1.19568	-5.05723	-0.74765
H	1.98879	-5.63561	-0.26502
H	0.27533	-5.64947	-0.83916
H	1.51050	-4.71344	-1.73886

2KP

E = -13.71546880 a.u.

Pd	0.00000	0.00000	0.00000
P	2.30597	0.00000	0.00000
C	2.94310	1.44173	-0.97388
C	2.29790	2.69474	-0.95077
S	0.77670	2.99532	0.00000
O	-0.19702	2.02971	-0.68454
O	1.07946	2.58674	1.37792
O	0.40125	4.38309	-0.25425
C	2.79203	3.75019	-1.71786
C	3.91165	3.57209	-2.52518
C	4.53786	2.32956	-2.57674
C	4.05657	1.27501	-1.80648
H	2.26601	4.70389	-1.67496
H	4.28530	4.40373	-3.12392
H	5.40435	2.17506	-3.22047
H	4.55601	0.30774	-1.84962
C	3.05090	0.07042	1.67544
C	3.05898	-1.45184	-0.82667
H	-1.90913	-0.28750	0.12571
C	-1.91744	-1.33385	0.62727
C	-0.52592	-1.88576	0.72117
H	-2.50371	-1.90639	-0.11086
C	-0.19752	-2.99103	-0.21063
C	-2.64326	-1.15258	1.96048
H	-2.03815	-0.56073	2.66167

H	-0.14387	-2.05730	1.73523
H	-2.83814	-2.13584	2.41472
H	-3.60404	-0.63758	1.82125
C	4.41929	0.33510	1.90838
C	4.89551	0.44485	3.21828
C	4.02457	0.28823	4.29431
C	2.67463	0.02744	4.08073
C	2.19952	-0.06641	2.77586
O	5.21202	0.44333	0.81003
H	5.94603	0.65525	3.40556
H	4.41324	0.38185	5.30891
H	1.98910	-0.07687	4.92072
H	1.13732	-0.21405	2.59035
C	3.99523	-2.28624	-0.21353
C	4.50319	-3.40373	-0.87664
C	4.06191	-3.69734	-2.16424
C	3.10013	-2.90141	-2.78617
C	2.59223	-1.78194	-2.12174
H	4.33411	-2.05976	0.79687
H	5.24328	-4.03627	-0.38683
H	4.45923	-4.56294	-2.69637
H	2.75044	-3.15526	-3.78501
O	1.66161	-0.94156	-2.63519
C	0.98602	-1.32895	-3.84150
H	0.25766	-0.53423	-4.02826
H	1.69262	-1.38632	-4.68237
H	0.46809	-2.28649	-3.69023
C	6.53857	0.95591	0.98859
H	6.94041	1.08332	-0.02194
H	6.51014	1.92797	1.50142
H	7.16459	0.24493	1.54819
O	-0.69555	-3.16625	-1.31581
O	0.72434	-3.82622	0.34381

C	1.05848	-4.97484	-0.46991
H	1.81339	-5.52211	0.10247
H	0.16423	-5.59097	-0.63365
H	1.46220	-4.65257	-1.43631

2

E= -13,72149122 a.u.

C	4.10550	1.22622	-1.76727
C	2.97770	1.41836	-0.96053
C	2.35563	2.68263	-0.94851
C	2.88472	3.72586	-1.70886
C	4.01710	3.52384	-2.49307
C	4.62265	2.27017	-2.52870
P	2.28485	0.00000	0.00000
C	2.96820	-1.48607	-0.83577
C	3.79804	-2.41277	-0.20076
C	4.20121	-3.58151	-0.84820
C	3.76751	-3.83145	-2.14681
C	2.92921	-2.92883	-2.80247
C	2.52238	-1.76219	-2.15142
O	1.69683	-0.83099	-2.69162
C	1.22464	-1.02698	-4.03044
S	0.83636	3.01522	0.00000
O	0.47694	4.40160	-0.28756
Pd	0.00000	0.00000	0.00000
O	-2.18156	-0.59704	0.21515
C	-1.62769	-1.47183	0.93280
O	-2.08370	-1.79664	2.15628
C	-3.21877	-1.00811	2.61220
O	-0.15563	2.04773	-0.65036
C	-0.35532	-2.04529	0.50298
H	-0.41072	-2.41801	-0.53168
C	3.03130	0.02655	1.67520

C	4.41983	0.14903	1.90667
C	4.90564	0.21656	3.21569
C	4.02128	0.16872	4.29171
C	2.65032	0.06408	4.07849
C	2.16757	0.00567	2.77432
H	1.09505	-0.02424	2.58749
O	1.15120	2.63943	1.38454
O	5.21625	0.16927	0.80576
H	5.97259	0.31253	3.40323
H	4.41742	0.22579	5.30617
H	1.95682	0.05173	4.91826
H	4.13451	-2.21981	0.81756
H	4.85278	-4.28927	-0.33640
H	4.07848	-4.73954	-2.66474
H	2.59522	-3.14176	-3.81591
H	2.37896	4.69086	-1.67586
H	4.42053	4.34692	-3.08423
H	5.50076	2.10003	-3.15240
H	4.58346	0.24772	-1.79825
H	0.58880	-0.16152	-4.23916
H	2.06611	-1.05229	-4.73824
H	0.63532	-1.95248	-4.10460
C	0.44463	-2.91774	1.43579
H	-3.43806	-1.38382	3.61547
H	-2.94967	0.05432	2.63766
H	-4.07264	-1.15511	1.94097
C	-0.12829	-4.34086	1.52802
H	1.47996	-2.98075	1.06660
H	0.48113	-2.46909	2.44072
H	0.48473	-4.95875	2.20161
H	-1.15821	-4.32576	1.91338
H	-0.13639	-4.82285	0.53818
C	6.60621	0.46387	0.98987

H	7.03092	0.51086	-0.01809
H	6.73251	1.43430	1.49109
H	7.10559	-0.33111	1.56386

2

2MA-meso-cis

2MA-meso-isom

2MA-meso-trans

3MA-meso-inser

3-meso-KP

3-meso

2

E = -13.72118138 a.u.

C	4.08036	1.20113	-1.80794
C	2.94277	1.39767	-1.01558
C	2.31548	2.65976	-1.02301
C	2.83294	3.68795	-1.81087
C	3.96628	3.47777	-2.59281
C	4.59054	2.23360	-2.59140
P	2.28975	0.00000	0.00000
C	3.05806	-1.47855	-0.77697
C	3.97391	-2.29280	-0.10843
C	4.50008	-3.43432	-0.71553
C	4.10858	-3.76450	-2.00932

C	3.19745	-2.96652	-2.70283
C	2.66747	-1.82764	-2.09204
O	1.78067	-0.98407	-2.67910
C	1.37435	-1.25316	-4.02627
S	0.85316	3.03112	0.00000
O	0.49768	4.41613	-0.29802
Pd	0.00000	0.00000	0.00000
O	-2.18386	-0.65992	0.45438
C	-1.45043	-1.49576	1.04276
O	-1.60286	-1.80956	2.34793
C	-2.60431	-1.01532	3.04476
O	-0.19398	2.06704	-0.55360
C	-0.30415	-2.06989	0.34084
C	-0.58324	-2.77641	-0.96957
C	-1.16742	-4.18111	-0.73580
H	-1.34136	-4.69176	-1.69546
C	3.19875	0.17796	1.59230
C	4.15261	1.18853	1.74331
C	4.83801	1.36580	2.94301
C	4.56369	0.52769	4.01750
C	3.60615	-0.47827	3.90098
C	2.91623	-0.65316	2.69851
O	1.97307	-1.61931	2.50921
C	1.55449	-2.37188	3.65615
O	1.26565	2.68358	1.36570
H	4.35432	1.86275	0.91252
H	5.57229	2.16528	3.03300
H	5.09104	0.65301	4.96365
H	3.40060	-1.12123	4.75328
H	4.29515	-2.02144	0.89731
H	5.21846	-4.05337	-0.17885
H	4.51622	-4.65092	-2.49680
H	2.90849	-3.23632	-3.71662

H	2.32365	4.65174	-1.79262
H	4.36053	4.29036	-3.20445
H	5.47927	2.05998	-3.19856
H	4.57961	0.23161	-1.80832
H	0.71610	-2.98705	3.31512
H	2.37017	-3.01360	4.02209
H	1.21048	-1.69917	4.45490
H	0.68456	-0.44463	-4.28627
H	2.24095	-1.23752	-4.70355
H	0.85713	-2.22197	-4.09274
H	0.43433	-2.56541	0.97780
H	-1.28583	-2.18042	-1.57348
H	0.35707	-2.86992	-1.53259
H	-0.47783	-4.79931	-0.14040
H	-2.12698	-4.12400	-0.19892
H	-2.60506	-1.39556	4.07018
H	-2.32469	0.04430	3.01815
H	-3.58595	-1.14933	2.57590

2MA-meso-cis

E = -16.29353001 a.u.

Pd	0.00000	0.00000	0.00000
P	2.39674	0.00000	0.00000
C	3.12516	1.44203	-0.90731
C	2.50287	2.70527	-0.90413
S	0.96215	3.03494	0.00000
O	-0.01567	2.06618	-0.66817
O	1.24310	2.65709	1.39200
O	0.61570	4.42159	-0.29481
C	3.06175	-0.00347	1.71157
C	3.16984	-1.45480	-0.81480
C	3.05499	3.76102	-1.63169

C	4.21535	3.57376	-2.37579
C	4.82866	2.32312	-2.39774
C	4.28665	1.26875	-1.67012
C	0.02075	-2.12446	0.26195
H	2.54345	4.72303	-1.60431
H	4.63530	4.40478	-2.94405
H	5.73408	2.16425	-2.98451
H	4.77732	0.29640	-1.68849
H	1.03823	-2.39210	0.58071
C	-0.93976	-2.54511	1.31560
C	-2.29345	0.15407	-0.22754
H	-2.58067	-0.83180	-0.59465
H	-2.40317	1.02758	-0.87502
C	-2.04208	0.33382	1.10611
C	-1.98275	1.69280	1.72580
H	-2.11129	-0.50305	1.80214
C	-0.31433	-2.71072	-1.10336
H	0.21456	-2.15243	-1.89113
H	-1.39423	-2.60602	-1.28774
C	0.07074	-4.19617	-1.19459
H	1.15610	-4.32627	-1.05609
H	-0.20367	-4.60982	-2.17774
H	-0.45245	-4.78120	-0.42205
C	3.94624	-2.38504	-0.12067
C	4.45771	-3.51510	-0.76052
C	4.19363	-3.71703	-2.11171
C	3.40822	-2.81152	-2.82605
C	2.88488	-1.69027	-2.18000
H	4.15679	-2.22295	0.93696
H	5.06402	-4.22783	-0.20200
H	4.59415	-4.59201	-2.62497
H	3.20110	-2.99139	-3.87914
O	2.08510	-0.76394	-2.77360

C	4.42107	0.24011	2.01612
C	4.83819	0.29561	3.34888
C	3.91881	0.09613	4.37674
C	2.58125	-0.15741	4.09111
C	2.16071	-0.19264	2.76407
O	5.26474	0.38278	0.96089
H	5.87983	0.49358	3.59143
H	4.26170	0.14490	5.41099
H	1.86071	-0.30690	4.89380
H	1.10951	-0.35848	2.53479
C	6.58499	0.87804	1.21813
H	7.03145	1.04473	0.23220
H	6.53955	1.82863	1.76860
H	7.18223	0.14008	1.77403
C	1.84097	-0.87445	-4.18175
H	1.22350	-0.00759	-4.43581
H	2.78656	-0.83735	-4.74264
H	1.29778	-1.80243	-4.41458
O	-0.36157	-2.53445	2.55796
O	-2.10734	-2.86841	1.13558
C	-1.23275	-2.96795	3.62669
H	-0.60614	-2.97588	4.52364
H	-2.07279	-2.27237	3.74857
H	-1.62640	-3.97016	3.41552
O	-1.44303	1.60137	2.96774
O	-2.39110	2.71392	1.21081
C	-1.25333	2.88251	3.62528
H	-0.94376	2.63798	4.64549
H	-0.46721	3.43581	3.09731
H	-2.19135	3.45036	3.61789

2MA-meso-isom

E = -16.27800518 a.u.

Pd	0.00000	0.00000	0.00000
P	2.80599	0.00000	0.00000
C	3.42585	1.64662	0.62562
C	2.62367	2.80539	0.61328
S	0.92398	2.78319	0.00000
O	0.19471	1.91555	1.02563
O	0.98089	2.06425	-1.29696
O	0.45707	4.16382	0.00302
C	3.54044	-0.05503	-1.69294
C	3.92507	-1.13514	0.94395
C	3.10937	4.01858	1.10181
C	4.39832	4.09975	1.62075
C	5.19973	2.96283	1.65281
C	4.71531	1.75234	1.16219
C	-1.33443	-0.51205	1.57385
H	2.45607	4.88999	1.06561
H	4.77106	5.05115	2.00178
H	6.21077	3.01082	2.05818
H	5.35830	0.87312	1.19558
C	-2.71257	-0.06150	1.20930
H	-0.87178	0.17393	2.29906
C	-0.20642	-1.81725	-1.21060
H	0.59866	-1.76030	-1.94462
H	-0.23319	-2.69079	-0.55908
C	-1.34165	-1.03290	-1.40265
H	-2.28709	-1.24704	-0.89765
C	-1.40237	-0.11284	-2.57506
C	-1.24549	-1.96718	1.96100
C	5.05916	-1.73179	0.39205
C	5.87469	-2.57821	1.14493
C	5.55251	-2.83399	2.47379
C	4.42337	-2.25282	3.05264
C	3.60922	-1.40873	2.29328

H	5.32538	-1.51041	-0.64190
H	6.76091	-3.02331	0.69310
H	6.18278	-3.48757	3.07770
H	4.18916	-2.46066	4.09438
O	2.49768	-0.78479	2.77863
C	4.07283	1.07526	-2.31560
C	4.51322	1.03120	-3.63884
C	4.42188	-0.15719	-4.35463
C	3.89003	-1.30181	-3.75940
C	3.44214	-1.25014	-2.43993
H	4.13801	2.01102	-1.76100
H	4.91971	1.92882	-4.10345
H	4.75971	-0.20511	-5.39021
H	3.81708	-2.22240	-4.33416
O	2.90851	-2.31761	-1.77310
C	2.22471	-0.90766	4.17956
H	1.34909	-0.27781	4.36337
H	3.07447	-0.54070	4.77466
H	1.99818	-1.95066	4.44754
C	2.82827	-3.56887	-2.46345
H	2.40327	-4.27382	-1.74160
H	3.82788	-3.91330	-2.76917
H	2.17078	-3.49358	-3.34295
O	-0.61814	-0.11705	-3.50612
O	-2.45747	0.73581	-2.46070
C	-2.52039	1.73018	-3.51341
H	-3.39815	2.33979	-3.28161
H	-2.62685	1.23958	-4.48847
H	-1.60556	2.33477	-3.50193
O	-2.86306	1.27571	1.36873
O	-3.60787	-0.80407	0.82113
C	-4.14655	1.78657	0.93921
C	-1.93442	-2.22072	3.31533

H	-0.18781	-2.26602	2.02545
H	-1.74080	-2.58606	1.19770
H	-4.08759	2.86782	1.09132
H	-4.95252	1.34546	1.53912
H	-4.30574	1.54468	-0.11867
H	-1.84440	-3.28111	3.59628
H	-3.00391	-1.97051	3.25520
H	-1.47975	-1.61288	4.11308

2MA-meso-trans

E= -16.28466811 a.u.

Pd	1.080313	-0.154601	0.333417
P	-1.006805	-1.414024	-0.272694
C	-2.541415	-0.384537	-0.134722
C	-2.513666	0.980199	-0.476188
S	-0.982611	1.786053	-1.012479
O	-0.103505	1.657915	0.242423
O	-0.456760	0.961135	-2.109980
O	-1.319829	3.182620	-1.266688
C	-1.038356	-2.213595	-1.928391
C	-1.297612	-2.776505	0.927038
C	-3.661865	1.763300	-0.357355
C	-4.843041	1.202396	0.119962
C	-4.872172	-0.139465	0.493595
C	-3.730023	-0.925548	0.367192
C	2.644395	1.278863	0.791702
H	-3.600852	2.815107	-0.636376
H	-5.738300	1.818785	0.210190
H	-5.789646	-0.579949	0.885173
H	-3.759262	-1.973553	0.661845
H	1.964976	2.137872	0.706146

C	3.123289	1.123659	2.185803
C	2.119024	-1.752061	1.487360
H	1.296881	-2.157749	2.080565
H	2.990511	-1.351808	2.012456
C	2.240150	-2.080892	0.148491
C	3.556454	-1.981062	-0.547321
H	1.522414	-2.749794	-0.333458
C	3.734938	1.277295	-0.254382
H	3.293107	1.100150	-1.249256
H	4.455293	0.476692	-0.037104
C	4.475681	2.627339	-0.281671
H	5.268590	2.614188	-1.045628
H	3.784738	3.451539	-0.516283
H	4.944355	2.829673	0.693396
O	2.217634	1.631335	3.085608
C	2.640703	1.527760	4.461017
H	1.840738	1.991210	5.046542
H	2.777368	0.476313	4.745905
H	3.589615	2.058842	4.611444
O	4.180682	0.615920	2.535874
C	-2.149752	-2.917089	-2.449102
C	-2.097488	-3.451647	-3.739616
C	-0.952623	-3.290017	-4.517535
C	0.143902	-2.591078	-4.024485
C	0.087885	-2.049799	-2.742418
O	-3.224278	-3.050862	-1.627594
H	-2.948952	-3.991684	-4.147091
H	-0.930757	-3.711865	-5.523025
H	1.032212	-2.446457	-4.637358
H	0.928847	-1.467917	-2.372876
C	-1.302398	-4.129942	0.583834
C	-1.422397	-5.120300	1.560833
C	-1.544046	-4.755691	2.898404

C	-1.527332	-3.411024	3.273252
C	-1.388313	-2.424723	2.295603
H	-1.215114	-4.416975	-0.464204
H	-1.425782	-6.170883	1.271882
H	-1.647462	-5.520252	3.669193
H	-1.613951	-3.141034	4.323983
O	-1.310680	-1.092466	2.550500
C	-1.463241	-0.638282	3.900724
H	-1.382465	0.451361	3.845684
H	-2.449649	-0.923061	4.295648
H	-0.665470	-1.040994	4.541853
C	-4.429939	-3.588393	-2.184347
H	-5.179274	-3.510995	-1.389822
H	-4.750635	-2.998039	-3.054783
H	-4.299176	-4.644221	-2.464676
O	3.390256	-2.065041	-1.895886
O	4.636078	-1.880108	0.001373
C	4.631224	-2.023229	-2.643498
H	4.339435	-2.114114	-3.693271
H	5.148550	-1.074126	-2.460374
H	5.279509	-2.854502	-2.340395

2MA-meso-inser

E= -16.27189776 a.u.

Pd	0.00000	0.00000	0.00000
P	2.33896	0.00000	0.00000
C	3.05832	1.43171	-0.92714
C	2.45003	2.70218	-0.90059
S	0.90290	3.02403	0.00000
O	-0.06722	2.06235	-0.69761
O	1.15637	2.62852	1.39031

O	0.54955	4.41192	-0.28522
C	3.01250	3.76212	-1.61271
C	4.16826	3.57096	-2.36464
C	4.76044	2.31165	-2.41787
C	4.20776	1.25147	-1.70531
H	2.51450	4.73068	-1.57012
H	4.59945	4.40636	-2.91762
H	5.65750	2.15026	-3.01648
H	4.67431	0.26842	-1.75206
C	3.10397	0.01679	1.66914
C	3.00378	-1.47569	-0.86701
H	-1.88043	-2.01699	-0.87249
C	-1.55526	-1.76769	0.13973
C	-0.19452	-2.05919	0.46859
H	-2.29292	-1.91664	0.93124
C	0.10202	-2.38051	1.88984
C	-2.34149	0.27714	0.17411
H	-1.96025	1.13695	-0.39959
H	0.42482	-2.58279	-0.26785
C	-3.53902	-0.25837	-0.53747
C	-2.56870	0.59262	1.63681
H	-1.59922	0.73188	2.13950
H	-3.07140	-0.25559	2.12551
C	-3.40630	1.86826	1.80775
H	-3.55806	2.07859	2.87729
H	-4.39472	1.75391	1.33793
H	-2.89804	2.73460	1.35853
C	4.49942	0.07306	1.88933
C	4.99769	0.15377	3.19298
C	4.12042	0.19190	4.27528
C	2.74484	0.15349	4.07343
C	2.24936	0.07561	2.77452
O	5.29161	0.02445	0.78544

H	6.06966	0.19764	3.37093
H	4.52748	0.26318	5.28466
H	2.05489	0.20688	4.91464
H	1.17363	0.08726	2.60814
C	3.76143	-2.45993	-0.23124
C	4.15718	-3.61290	-0.91034
C	3.78782	-3.78841	-2.24075
C	3.01282	-2.83019	-2.89555
C	2.60826	-1.68295	-2.21003
H	4.04144	-2.32547	0.81243
H	4.75221	-4.36863	-0.39840
H	4.09512	-4.68330	-2.78320
H	2.72216	-2.98692	-3.93239
O	1.82270	-0.70898	-2.73872
C	1.44436	-0.80566	-4.11674
H	0.85296	0.09325	-4.31495
H	2.33407	-0.81773	-4.76348
H	0.83350	-1.70320	-4.29269
C	6.69300	0.26825	0.95542
H	7.11357	0.27504	-0.05544
H	6.86044	1.24394	1.43390
H	7.16459	-0.53288	1.54393
O	-3.40955	-0.14273	-1.89185
O	-4.51821	-0.74500	0.00360
C	-4.55722	-0.61564	-2.63630
H	-4.29490	-0.47630	-3.68908
H	-4.75055	-1.67250	-2.41392
H	-5.44518	-0.02645	-2.37531
O	-0.58158	-2.05656	2.84836
O	1.24224	-3.11835	1.98351
C	1.59351	-3.50703	3.33323
H	2.41843	-4.21712	3.22245
H	1.91380	-2.62695	3.90484

H	0.73359	-3.97386	3.82892
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3-meso-KP

E = -16.30193569 a.u.

Pd	0.00000	0.00000	0.00000
P	2.27700	0.00000	0.00000
C	3.04869	-1.51821	-0.67956
C	3.16396	0.29279	1.58108
C	2.88619	1.36420	-1.08612
C	2.67595	-1.94686	-1.97757
O	1.81012	-1.13471	-2.63533
C	1.41116	-1.49690	-3.96427
H	2.28244	-1.53277	-4.63462
H	0.72802	-0.70524	-4.28520
H	0.88796	-2.46390	-3.96518
C	3.18876	-3.13637	-2.49890
H	2.91487	-3.46478	-3.49929
C	4.05292	-3.91525	-1.72895
H	4.44674	-4.84193	-2.14785
C	4.40273	-3.52318	-0.44058
H	5.06763	-4.13880	0.16433
C	3.89491	-2.33207	0.07793
H	4.15851	-2.02965	1.09079
C	2.49451	0.38469	2.82112
O	1.16764	0.12076	2.84114
C	0.39013	0.64706	3.92937
H	0.51123	1.73842	3.97723
H	0.67034	0.17818	4.88465
H	-0.64434	0.38052	3.69292
C	3.22057	0.72734	3.96808
H	2.71186	0.82431	4.92453
C	4.59070	0.95516	3.89569
H	5.13454	1.21778	4.80386

C	5.26089	0.86529	2.67762
H	6.33015	1.06243	2.61257
C	4.53890	0.55072	1.53053
H	5.05294	0.52453	0.56984
C	3.96434	1.13667	-1.94964
H	4.42818	0.15070	-1.99083
C	4.45606	2.15601	-2.76195
H	5.30001	1.95792	-3.42300
C	3.86863	3.41659	-2.72622
H	4.24732	4.21936	-3.35994
C	2.78738	3.65516	-1.88105
H	2.30166	4.63020	-1.83994
C	2.28864	2.64206	-1.06320
S	0.86507	3.06016	0.00000
O	1.30699	2.76679	1.36823
O	0.50711	4.43540	-0.33647
O	-0.20708	2.08556	-0.48444
C	-1.53007	-2.26054	-0.49690
C	-2.52877	-1.06907	-0.37025
H	-2.08856	-0.16072	0.11630
C	-3.01728	-0.63489	-1.74506
C	-3.72551	-1.44539	0.53766
H	-3.28668	-1.85173	1.46145
H	-4.26403	-2.26756	0.03135
C	-4.67663	-0.29974	0.86865
H	-5.15685	0.11557	-0.02906
H	-5.46867	-0.65084	1.54704
H	-4.14210	0.52216	1.37071
O	-3.18999	-1.39041	-2.68640
O	-3.26782	0.69299	-1.77852
C	-3.77855	1.18356	-3.04389
H	-3.05605	0.97959	-3.84286
H	-3.90821	2.25935	-2.89992

H	-4.73147	0.69458	-3.28123
C	-0.19964	-2.06673	0.22313
H	-2.02924	-3.17452	-0.12359
H	-1.33773	-2.43204	-1.56496
C	-0.21185	-2.32309	1.68357
H	0.62331	-2.60597	-0.26222
O	-1.14124	-2.09269	2.45063
O	0.96844	-2.87788	2.08927
C	1.05888	-3.13678	3.50635
H	1.97692	-3.71775	3.63742
H	1.12265	-2.18967	4.05496
H	0.18274	-3.70051	3.85036

3-meso

E = -16.32160953 a.u.

Pd	0.00000	0.00000	0.00000
P	2.30544	0.00000	0.00000
C	3.15439	-0.16667	1.62750
C	3.13133	-1.20960	-1.12203
C	3.03685	1.58693	-0.65692
C	2.60801	-1.36163	-2.42747
O	1.51510	-0.61024	-2.71684
C	1.02874	-0.60406	-4.06446
H	0.66074	-1.59957	-4.35392
H	1.81592	-0.27245	-4.75747
H	0.20431	0.11543	-4.06806
C	3.22417	-2.22704	-3.33614
H	2.82690	-2.34484	-4.34197
C	4.36598	-2.93272	-2.95852
H	4.84008	-3.60100	-3.67841
C	4.90486	-2.77659	-1.68455
H	5.80974	-3.31101	-1.39641
C	4.28477	-1.91688	-0.77754

H	4.72302	-1.77428	0.20918
C	3.23738	-1.39777	2.31838
O	2.79643	-2.49867	1.65029
C	2.79216	-3.75069	2.34220
H	3.81162	-4.04400	2.63581
H	2.13569	-3.69985	3.22283
H	2.39878	-4.47868	1.62465
C	3.78096	-1.44621	3.60342
H	3.85716	-2.39358	4.13235
C	4.22275	-0.27671	4.22083
H	4.63975	-0.33090	5.22721
C	4.12793	0.94481	3.56337
H	4.45800	1.86471	4.04448
C	3.59521	0.99224	2.27620
H	3.50266	1.95449	1.77416
C	4.33658	1.53885	-1.18021
H	4.88005	0.59565	-1.20223
C	4.95286	2.67997	-1.68674
H	5.96569	2.61155	-2.08397
C	4.27226	3.89370	-1.68973
H	4.74435	4.79042	-2.09316
C	2.97933	3.96030	-1.18066
H	2.41563	4.89332	-1.17517
C	2.35881	2.82140	-0.66365
S	0.68181	3.01993	0.00000
O	0.79958	2.63833	1.41563
O	0.28024	4.38934	-0.31604
O	-0.10466	2.00648	-0.82054
C	-0.24879	-1.94924	0.74561
H	0.72294	-2.45178	0.75502
C	-1.21710	-2.66067	-0.19846
H	-0.86343	-2.50658	-1.23347
H	-1.13173	-3.74960	-0.01734

C	-2.71328	-2.31900	-0.11866
H	-3.15148	-2.81015	0.76569
C	-2.98440	-0.84865	0.08928
C	-3.48278	-2.81144	-1.36759
O	-2.19068	0.08592	-0.04821
C	-3.40467	-4.32474	-1.56245
O	-4.26447	-0.61701	0.40017
H	-4.02734	-4.63514	-2.41484
C	-4.59231	0.77790	0.66366
H	-4.40187	1.38313	-0.22940
H	-3.98065	1.14456	1.49527
H	-5.65434	0.77143	0.92267
H	-3.08474	-2.29477	-2.25982
H	-4.53714	-2.50931	-1.26477
H	-2.37783	-4.66336	-1.76156
H	-3.77002	-4.85345	-0.66758
C	-0.72565	-1.68709	2.12774
O	-1.89275	-1.52851	2.47799
O	0.31338	-1.60068	3.01155
C	-0.06288	-1.13408	4.32662
H	-0.71275	-1.86640	4.82332
H	0.88116	-1.01092	4.86685
H	-0.58909	-0.17484	4.24816

2

2E-cis

2E-isom

2E-trans

3E-inser

3E-KP

3E

2

E = -13.72118138 a.u.

C	4.08036	1.20113	-1.80794
C	2.94277	1.39767	-1.01558
C	2.31548	2.65976	-1.02301
C	2.83294	3.68795	-1.81087
C	3.96628	3.47777	-2.59281
C	4.59054	2.23360	-2.59140
P	2.28975	0.00000	0.00000
C	3.05806	-1.47855	-0.77697
C	3.97391	-2.29280	-0.10843
C	4.50008	-3.43432	-0.71553
C	4.10858	-3.76450	-2.00932
C	3.19745	-2.96652	-2.70283
C	2.66747	-1.82764	-2.09204

O	1.78067	-0.98407	-2.67910
C	1.37435	-1.25316	-4.02627
S	0.85316	3.03112	0.00000
O	0.49768	4.41613	-0.29802
Pd	0.00000	0.00000	0.00000
O	-2.18386	-0.65992	0.45438
C	-1.45043	-1.49576	1.04276
O	-1.60286	-1.80956	2.34793
C	-2.60431	-1.01532	3.04476
O	-0.19398	2.06704	-0.55360
C	-0.30415	-2.06989	0.34084
C	-0.58324	-2.77641	-0.96957
C	-1.16742	-4.18111	-0.73580
H	-1.34136	-4.69176	-1.69546
C	3.19875	0.17796	1.59230
C	4.15261	1.18853	1.74331
C	4.83801	1.36580	2.94301
C	4.56369	0.52769	4.01750
C	3.60615	-0.47827	3.90098
C	2.91623	-0.65316	2.69851
O	1.97307	-1.61931	2.50921
C	1.55449	-2.37188	3.65615
O	1.26565	2.68358	1.36570
H	4.35432	1.86275	0.91252
H	5.57229	2.16528	3.03300
H	5.09104	0.65301	4.96365
H	3.40060	-1.12123	4.75328
H	4.29515	-2.02144	0.89731
H	5.21846	-4.05337	-0.17885
H	4.51622	-4.65092	-2.49680
H	2.90849	-3.23632	-3.71662
H	2.32365	4.65174	-1.79262
H	4.36053	4.29036	-3.20445

H	5.47927	2.05998	-3.19856
H	4.57961	0.23161	-1.80832
H	0.71610	-2.98705	3.31512
H	2.37017	-3.01360	4.02209
H	1.21048	-1.69917	4.45490
H	0.68456	-0.44463	-4.28627
H	2.24095	-1.23752	-4.70355
H	0.85713	-2.22197	-4.09274
H	0.43433	-2.56541	0.97780
H	-1.28583	-2.18042	-1.57348
H	0.35707	-2.86992	-1.53259
H	-0.47783	-4.79931	-0.14040
H	-2.12698	-4.12400	-0.19892
H	-2.60506	-1.39556	4.07018
H	-2.32469	0.04430	3.01815
H	-3.58595	-1.14933	2.57590

2E-cis

E = -14,89154621 a.u.

Pd	0.00000	0.00000	0.00000
P	2.38728	0.00000	0.00000
C	3.08841	1.44248	-0.92819
C	2.45547	2.70057	-0.92065
S	0.92144	3.00796	0.00000
O	-0.06063	2.06522	-0.70519
O	1.19275	2.57902	1.37738
O	0.56856	4.40334	-0.24941
C	3.09062	-0.03337	1.69413
C	3.13037	-1.45307	-0.84527
C	2.98569	3.75835	-1.66127
C	4.13431	3.57663	-2.42515
C	4.75437	2.32946	-2.45681
C	4.23390	1.27339	-1.71555

C	0.01993	-2.07845	0.48863
H	2.46866	4.71729	-1.62697
H	4.53966	4.40933	-3.00145
H	5.64955	2.17480	-3.06015
H	4.73012	0.30384	-1.74074
H	1.03848	-2.29498	0.84237
C	-0.87097	-2.28739	1.66399
C	-2.27788	0.04391	-0.38998
H	-2.61513	-0.98318	-0.53687
H	-2.28948	0.71753	-1.25023
C	-2.06808	0.53512	0.86916
H	-1.89506	1.60047	1.03373
H	-2.21916	-0.08345	1.75547
C	-0.28704	-2.87478	-0.77465
H	0.29147	-2.45556	-1.61285
H	-1.35061	-2.77908	-1.03866
C	0.07288	-4.36051	-0.62454
H	1.15128	-4.48044	-0.43425
H	-0.17560	-4.91625	-1.54235
H	-0.48012	-4.81684	0.21124
C	3.95441	-2.37065	-0.19072
C	4.43262	-3.50500	-0.84906
C	4.08401	-3.72529	-2.17806
C	3.25484	-2.82892	-2.85426
C	2.76863	-1.70181	-2.18997
H	4.22818	-2.19474	0.85015
H	5.07742	-4.20770	-0.32185
H	4.45370	-4.60625	-2.70435
H	2.98615	-3.01974	-3.89154
O	1.93118	-0.78462	-2.74402
C	4.44800	0.24169	1.97722
C	4.89668	0.24812	3.30055
C	4.01333	-0.04226	4.33912

C	2.68015	-0.33449	4.07296
C	2.22514	-0.31356	2.75662
O	5.26119	0.45486	0.90852
H	5.93641	0.47251	3.52758
H	4.38224	-0.03750	5.36557
H	1.98448	-0.56554	4.87847
H	1.17677	-0.52953	2.55970
C	6.57325	0.97294	1.15838
H	6.99106	1.19861	0.17155
H	6.51684	1.89453	1.75532
H	7.20271	0.22607	1.66499
C	1.60764	-0.90940	-4.13407
H	0.97138	-0.04827	-4.35993
H	2.51875	-0.87142	-4.74926
H	1.05775	-1.84262	-4.32696
O	-2.11424	-2.74970	1.31305
O	-0.56892	-2.07261	2.83171
C	-2.99188	-2.99300	2.43706
H	-3.93113	-3.34667	2.00091
H	-2.55639	-3.75333	3.09830
H	-3.15058	-2.07326	3.01381

2E-isom

E = -14,87044981a.u.

Pd	0.00000	0.00000	0.00000
P	2.81097	0.00000	0.00000
C	3.42418	1.63987	0.64830
C	2.61990	2.79699	0.63927
S	0.92864	2.78162	0.00000
O	0.18081	1.91868	1.01617
O	1.00470	2.06454	-1.29726
O	0.47067	4.16493	-0.00397
C	3.57383	-0.04652	-1.68161

C	3.90368	-1.14428	0.96221
C	3.09600	4.00366	1.15315
C	4.37618	4.07908	1.69407
C	5.17951	2.94337	1.72199
C	4.70505	1.73943	1.20635
C	-1.38029	-0.52752	1.51625
H	2.44194	4.87461	1.11922
H	4.74132	5.02514	2.09527
H	6.18380	2.98749	2.14422
H	5.34814	0.86027	1.23907
C	-2.73887	-0.03368	1.14004
H	-0.92333	0.12485	2.27595
C	-0.16105	-1.79920	-1.25208
H	0.70445	-1.73893	-1.91276
H	-0.22230	-2.68942	-0.62333
C	-1.27965	-1.00475	-1.47533
H	-2.24570	-1.24516	-1.02605
H	-1.29046	-0.28661	-2.30030
C	-1.33295	-1.99526	1.86677
C	5.05598	-1.73581	0.44346
C	5.84224	-2.59429	1.21389
C	5.47156	-2.86725	2.52681
C	4.32401	-2.29088	3.07283
C	3.53981	-1.43403	2.29643
H	5.35883	-1.50205	-0.57769
H	6.74309	-3.03621	0.78868
H	6.07795	-3.53118	3.14391
H	4.05171	-2.51245	4.10250
O	2.41357	-0.81300	2.74934
C	4.08081	1.09789	-2.30028
C	4.53292	1.06743	-3.62017
C	4.48075	-0.12214	-4.33798
C	3.97480	-1.28172	-3.74726

C	3.51289	-1.24305	-2.43156
H	4.11762	2.03421	-1.74376
H	4.91963	1.97622	-4.08006
H	4.83036	-0.16049	-5.37002
H	3.93588	-2.20475	-4.32169
O	2.99331	-2.32360	-1.77448
C	2.08425	-0.95882	4.13588
H	1.20324	-0.32967	4.29467
H	2.91001	-0.60399	4.77082
H	1.84481	-2.00558	4.37645
C	2.98224	-3.58293	-2.45383
H	2.57158	-4.29900	-1.73471
H	4.00221	-3.88604	-2.73470
H	2.34218	-3.54561	-3.34872
O	-2.87682	1.29160	1.40176
O	-3.63401	-0.72721	0.66915
C	-4.15177	1.85091	1.01329
C	-2.05085	-2.26943	3.20091
H	-0.28358	-2.32033	1.94159
H	-1.82564	-2.58231	1.07671
H	-1.98927	-3.33823	3.45679
H	-3.11370	-1.99389	3.13087
H	-1.59730	-1.69233	4.02207
H	-4.08036	2.91565	1.25187
H	-4.96400	1.37262	1.57518
H	-4.31905	1.70127	-0.06051

2E-trans

E = -14.88638969 a.u.

Pd	0.00000	0.00000	0.00000
P	2.50058	0.00000	0.00000
C	3.15133	-1.51928	-0.81880
C	3.61464	0.17053	1.46428

C	3.13012	1.35019	-1.10390
C	2.63135	-1.85310	-2.09332
O	1.76254	-0.94869	-2.61584
C	1.20387	-1.20257	-3.91033
H	1.99651	-1.25488	-4.67121
H	0.54928	-0.34980	-4.11304
H	0.61625	-2.13195	-3.90558
C	3.00296	-3.04294	-2.72035
H	2.61377	-3.29486	-3.70491
C	3.87506	-3.92185	-2.07482
H	4.15495	-4.85196	-2.57080
C	4.37768	-3.62105	-0.81324
H	5.05141	-4.31143	-0.30646
C	4.01530	-2.42189	-0.19473
H	4.41112	-2.18543	0.79349
C	3.11293	0.14134	2.78194
O	1.78619	-0.10945	2.93843
C	1.18709	0.26145	4.18889
H	1.41906	1.30991	4.42340
H	1.51934	-0.40299	5.00049
H	0.10827	0.14883	4.04201
C	3.97919	0.35503	3.86085
H	3.59750	0.34388	4.87921
C	5.33405	0.58391	3.64062
H	5.99215	0.74825	4.49455
C	5.84326	0.61276	2.34499
H	6.90013	0.80598	2.16493
C	4.97780	0.41855	1.27213
H	5.37090	0.48245	0.25854
C	4.18725	1.13023	-1.99309
H	4.63336	0.13774	-2.07067
C	4.67989	2.16563	-2.78517
H	5.51143	1.97520	-3.46414

C	4.11497	3.43546	-2.70488
H	4.50328	4.25041	-3.31679
C	3.04170	3.66446	-1.84719
H	2.56552	4.64254	-1.77704
C	2.54675	2.62996	-1.05517
S	1.11291	2.96565	0.00000
O	1.49008	2.49175	1.33905
O	0.78002	4.37439	-0.18420
O	0.03481	2.06896	-0.62798
C	-0.12152	-2.22130	0.01207
C	-2.11101	0.31398	-0.26090
H	-2.01966	0.95454	-1.15052
C	-2.84102	-0.93488	-0.57212
C	-2.64192	1.05698	0.94920
H	-1.92312	1.83694	1.24045
H	-2.75877	0.35808	1.79203
C	-4.00078	1.71720	0.65130
H	-3.90728	2.44493	-0.16917
H	-4.74990	0.96259	0.36640
H	-4.37146	2.24977	1.54121
O	-3.42339	-1.65105	0.23352
O	-2.78278	-1.23700	-1.91378
C	-3.51477	-2.42641	-2.28259
H	-3.14598	-3.29997	-1.72958
H	-3.34970	-2.54670	-3.35784
H	-4.58370	-2.29959	-2.06682
C	-0.43540	-1.75927	1.27750
H	0.32996	-1.72198	2.05478
H	-0.90802	-2.50001	-0.69175
H	0.87905	-2.59527	-0.21532
H	-1.48111	-1.67594	1.58389

2E-inser

E= -14.86220609 a.u.

Pd	0.00000	0.00000	0.00000
P	2.32251	0.00000	0.00000
C	3.04105	1.43614	-0.91790
C	2.41431	2.69804	-0.90451
S	0.86624	3.01383	0.00000
O	-0.11518	2.07647	-0.70561
O	1.12844	2.58842	1.38283
O	0.53245	4.41372	-0.25001
C	2.96314	3.75749	-1.62821
C	4.11910	3.57312	-2.38130
C	4.72700	2.32085	-2.42399
C	4.19025	1.26188	-1.69784
H	2.45477	4.72093	-1.59087
H	4.53863	4.40855	-2.94323
H	5.62318	2.16416	-3.02512
H	4.66834	0.28380	-1.73644
C	3.06320	-0.02171	1.68152
C	3.00642	-1.47189	-0.86106
H	-1.95699	-2.19790	-0.47039
C	-1.50710	-1.80730	0.44544
C	-0.09978	-2.00298	0.59916
H	-2.14478	-1.87648	1.33015
H	0.42352	-2.58725	-0.16526
C	-2.35027	0.17146	0.24761
H	-2.03190	0.92374	-0.49314
H	0.29896	-2.12385	1.61170
C	-3.58917	-0.48146	-0.26348
C	-2.48358	0.73991	1.64706
H	-1.48733	1.00281	2.03691
H	-2.92180	-0.02354	2.30990
C	-3.36028	2.00015	1.66145
H	-3.44443	2.39232	2.68636

H	-4.37370	1.77610	1.29601
H	-2.91919	2.78656	1.03123
C	4.45223	0.06474	1.92841
C	4.92843	0.09016	3.24271
C	4.03561	0.03629	4.31116
C	2.66481	-0.03532	4.08517
C	2.19251	-0.05335	2.77561
O	5.26137	0.09478	0.83695
H	5.99566	0.15744	3.44051
H	4.42507	0.06127	5.32951
H	1.96380	-0.05391	4.91860
H	1.12117	-0.05885	2.58277
C	3.77018	-2.44911	-0.22126
C	4.16540	-3.60805	-0.89234
C	3.79105	-3.79464	-2.21966
C	3.01280	-2.84193	-2.87932
C	2.61045	-1.68882	-2.20259
H	4.05823	-2.30644	0.82012
H	4.76375	-4.35789	-0.37564
H	4.09785	-4.69325	-2.75618
H	2.71858	-3.00738	-3.91385
O	1.82702	-0.71740	-2.73722
C	1.41179	-0.84297	-4.10194
H	0.81331	0.05081	-4.30218
H	2.28344	-0.86668	-4.77252
H	0.79801	-1.74476	-4.24219
C	6.65284	0.36734	1.04215
H	7.08701	0.44167	0.03988
H	6.78567	1.31970	1.57526
H	7.13798	-0.45161	1.59398
O	-3.58801	-0.56233	-1.62673
O	-4.49466	-0.91144	0.43298
C	-4.76722	-1.19280	-2.18094

H	-4.60447	-1.20704	-3.26255
H	-4.87946	-2.21026	-1.78586
H	-5.66183	-0.60992	-1.92896

3E-KP

E= -14.89597529 a.u.

Pd	0.00000	0.00000	0.00000
P	2.27854	0.00000	0.00000
C	3.07351	-1.43019	-0.83917
C	3.18573	0.15928	1.58955
C	2.87126	1.44745	-0.99278
C	2.55719	-1.85335	-2.08737
O	1.53961	-1.10670	-2.58773
C	1.00586	-1.45485	-3.87061
H	1.78253	-1.38357	-4.64627
H	0.22052	-0.71808	-4.06413
H	0.57526	-2.46683	-3.85453
C	3.10226	-2.96670	-2.73179
H	2.70960	-3.29732	-3.69103
C	4.16637	-3.65458	-2.14864
H	4.58628	-4.51866	-2.66494
C	4.69429	-3.24083	-0.92907
H	5.53500	-3.76987	-0.48118
C	4.14289	-2.13431	-0.28232
H	4.56451	-1.80060	0.66584
C	3.07207	-0.83262	2.58965
O	2.31749	-1.92084	2.26840
C	2.19041	-2.95849	3.24662
H	1.71237	-2.57811	4.16157
H	3.17201	-3.39463	3.48711
H	1.55469	-3.72019	2.78405
C	3.73108	-0.67675	3.81073

H	3.65534	-1.43993	4.58184
C	4.48382	0.47244	4.05269
H	4.98575	0.58584	5.01412
C	4.58730	1.46559	3.08511
H	5.16140	2.37129	3.27641
C	3.93664	1.30525	1.86334
H	4.00426	2.09266	1.11430
C	4.01622	1.29228	-1.78549
H	4.54468	0.33907	-1.79362
C	4.49581	2.34254	-2.56524
H	5.39141	2.19774	-3.16954
C	3.83196	3.56526	-2.56753
H	4.19821	4.39114	-3.17869
C	2.69204	3.73591	-1.78667
H	2.14999	4.68171	-1.76628
C	2.20484	2.69107	-1.00160
S	0.72100	3.03217	0.00000
O	1.11411	2.66249	1.36709
O	0.36350	4.42246	-0.27004
O	-0.29577	2.06781	-0.59437
C	-1.58818	-2.21960	-0.14441
C	-2.58624	-1.06266	0.19462
H	-2.12273	-0.05703	0.04234
C	-3.72811	-1.11058	-0.81142
C	-3.10470	-1.14411	1.63142
H	-2.25445	-1.35024	2.30051
H	-3.78609	-2.01013	1.68603
C	-3.82000	0.12703	2.08470
O	-4.74748	-1.76007	-0.67136
O	-3.43732	-0.36882	-1.90874
C	-4.46138	-0.37966	-2.93562
H	-4.61951	-1.40100	-3.30265
H	-4.07861	0.27104	-3.72683

H	-5.40198	0.01145	-2.52975
C	-0.21895	-1.99351	0.47045
H	-2.04576	-3.16522	0.21304
H	-1.49716	-2.31057	-1.23960
H	-0.20909	-2.04662	1.56891
H	0.55887	-2.64426	0.04871
H	-4.18471	0.02545	3.11741
H	-3.14184	0.99437	2.05015
H	-4.68803	0.34415	1.44303

E-TP-3

E -14.91075862 a.u.

Pd	0.00000	0.00000	0.00000
P	2.28353	0.00000	0.00000
C	3.21742	0.11595	1.58556
C	3.03342	-1.45011	-0.85958
C	2.95880	1.41661	-0.98183
C	2.54260	-1.78917	-2.14389
O	1.59878	-0.95426	-2.64969
C	1.12089	-1.18701	-3.97810
H	0.61276	-2.16046	-4.04886
H	1.94676	-1.13726	-4.70337
H	0.40885	-0.37894	-4.17274
C	3.03621	-2.91043	-2.81403
H	2.66264	-3.17255	-3.80190
C	4.02247	-3.69701	-2.21712
H	4.40210	-4.56904	-2.75118
C	4.52361	-3.37001	-0.96105
H	5.30289	-3.97717	-0.50112
C	4.02514	-2.25006	-0.29168
H	4.42643	-1.98638	0.68697
C	3.03494	-0.84429	2.60514
O	2.21637	-1.89033	2.29951

C	1.94737	-2.85126	3.32375
H	2.86802	-3.37096	3.63063
H	1.47590	-2.37213	4.19495
H	1.25459	-3.57043	2.87447
C	3.69111	-0.70833	3.82997
H	3.55450	-1.44806	4.61545
C	4.52113	0.38956	4.05509
H	5.02144	0.48885	5.01896
C	4.70192	1.34956	3.06604
H	5.33737	2.21655	3.24224
C	4.04720	1.21007	1.84326
H	4.17197	1.97813	1.08152
C	4.11872	1.22188	-1.74287
H	4.61191	0.24970	-1.73907
C	4.65732	2.25621	-2.50454
H	5.56381	2.08142	-3.08459
C	4.03731	3.50244	-2.51858
H	4.45232	4.31693	-3.11405
C	2.88325	3.71171	-1.76762
H	2.37808	4.67786	-1.75502
C	2.33810	2.68208	-0.99912
S	0.86090	3.06569	0.00000
O	1.26841	2.72567	1.37085
O	0.53246	4.45893	-0.30192
O	-0.18530	2.11463	-0.55233
C	-0.09197	-2.03251	0.36606
H	0.87081	-2.51848	0.16256
C	-1.19001	-2.65725	-0.48239
H	-1.10787	-2.34028	-1.53848
H	-1.02615	-3.75036	-0.48691
C	-2.62675	-2.42898	0.00066
H	-2.67455	-2.71054	1.07458
C	-2.99626	-0.95845	-0.01438

C	-3.66220	-3.29665	-0.74732
O	-2.21033	-0.01348	-0.08396
C	-3.45555	-4.79853	-0.55420
O	-4.31506	-0.74311	0.09044
C	-4.70758	0.66049	0.14670
H	-4.38339	1.17344	-0.76526
H	-4.24731	1.13919	1.01800
H	-5.79741	0.64175	0.22968
H	-3.62252	-3.04683	-1.82293
H	-4.66834	-3.02379	-0.39765
H	-0.31186	-2.11477	1.44513
H	-4.27097	-5.36073	-1.03309
H	-2.51186	-5.15101	-0.99362
H	-3.45049	-5.06058	0.51606

2

2MA-rac-cis

2MA-rac-isom

2MA-rac-trans

3MA-rac-inser

3-rac-KP

3-rac

2

E = -13.72118138 a.u.

C	4.08036	1.20113	-1.80794
C	2.94277	1.39767	-1.01558
C	2.31548	2.65976	-1.02301
C	2.83294	3.68795	-1.81087
C	3.96628	3.47777	-2.59281
C	4.59054	2.23360	-2.59140
P	2.28975	0.00000	0.00000
C	3.05806	-1.47855	-0.77697
C	3.97391	-2.29280	-0.10843
C	4.50008	-3.43432	-0.71553
C	4.10858	-3.76450	-2.00932
C	3.19745	-2.96652	-2.70283
C	2.66747	-1.82764	-2.09204

O	1.78067	-0.98407	-2.67910
C	1.37435	-1.25316	-4.02627
S	0.85316	3.03112	0.00000
O	0.49768	4.41613	-0.29802
Pd	0.00000	0.00000	0.00000
O	-2.18386	-0.65992	0.45438
C	-1.45043	-1.49576	1.04276
O	-1.60286	-1.80956	2.34793
C	-2.60431	-1.01532	3.04476
O	-0.19398	2.06704	-0.55360
C	-0.30415	-2.06989	0.34084
C	-0.58324	-2.77641	-0.96957
C	-1.16742	-4.18111	-0.73580
H	-1.34136	-4.69176	-1.69546
C	3.19875	0.17796	1.59230
C	4.15261	1.18853	1.74331
C	4.83801	1.36580	2.94301
C	4.56369	0.52769	4.01750
C	3.60615	-0.47827	3.90098
C	2.91623	-0.65316	2.69851
O	1.97307	-1.61931	2.50921
C	1.55449	-2.37188	3.65615
O	1.26565	2.68358	1.36570
H	4.35432	1.86275	0.91252
H	5.57229	2.16528	3.03300
H	5.09104	0.65301	4.96365
H	3.40060	-1.12123	4.75328
H	4.29515	-2.02144	0.89731
H	5.21846	-4.05337	-0.17885
H	4.51622	-4.65092	-2.49680
H	2.90849	-3.23632	-3.71662
H	2.32365	4.65174	-1.79262
H	4.36053	4.29036	-3.20445

H	5.47927	2.05998	-3.19856
H	4.57961	0.23161	-1.80832
H	0.71610	-2.98705	3.31512
H	2.37017	-3.01360	4.02209
H	1.21048	-1.69917	4.45490
H	0.68456	-0.44463	-4.28627
H	2.24095	-1.23752	-4.70355
H	0.85713	-2.22197	-4.09274
H	0.43433	-2.56541	0.97780
H	-1.28583	-2.18042	-1.57348
H	0.35707	-2.86992	-1.53259
H	-0.47783	-4.79931	-0.14040
H	-2.12698	-4.12400	-0.19892
H	-2.60506	-1.39556	4.07018
H	-2.32469	0.04430	3.01815
H	-3.58595	-1.14933	2.57590

2Ma-rac-cis

E = -16.29280319 a.u.

Pd	0.00000	0.00000	0.00000
P	2.39849	0.00000	0.00000
C	3.10827	1.43061	-0.93618
C	2.47839	2.68998	-0.93495
S	0.95476	3.01503	0.00000
O	-0.03722	2.05866	-0.67051
O	1.24700	2.61333	1.38112
O	0.60446	4.40472	-0.27452
C	3.06692	0.01296	1.70946
C	3.17903	-1.46975	-0.78106
C	3.00672	3.73899	-1.68941
C	4.14961	3.54700	-2.45901
C	4.76884	2.29915	-2.48005
C	4.25087	1.25160	-1.72550

C	0.00473	-2.11658	0.32515
H	2.49236	4.69957	-1.66051
H	4.55204	4.37249	-3.04748
H	5.66028	2.13700	-3.08690
H	4.74707	0.28176	-1.74174
H	1.02627	-2.39098	0.62601
C	-0.93636	-2.51019	1.40791
C	-2.33786	0.06933	0.14847
H	-2.61795	-0.97868	0.01395
C	-2.88566	1.05036	-0.82883
C	-1.79113	0.50448	1.33002
H	-1.68088	1.57610	1.51272
H	-1.65170	-0.17402	2.17135
C	-0.36962	-2.71945	-1.02278
H	0.17035	-2.19370	-1.82518
H	-1.44596	-2.57557	-1.20183
C	-0.03706	-4.21861	-1.09416
H	1.04432	-4.38614	-0.96549
H	-0.33576	-4.63536	-2.06907
H	-0.57381	-4.77440	-0.30977
C	3.97890	-2.36250	-0.06467
C	4.49387	-3.51102	-0.66771
C	4.20236	-3.77410	-2.00248
C	3.39754	-2.90446	-2.73963
C	2.87800	-1.76011	-2.13220
H	4.20330	-2.15628	0.98238
H	5.12144	-4.19166	-0.09295
H	4.59908	-4.66790	-2.48539
H	3.17496	-3.12869	-3.78092
O	2.07085	-0.85954	-2.75439
C	4.41182	0.32068	2.01569
C	4.82515	0.38633	3.34944
C	3.91997	0.12397	4.37553

C	2.59905	-0.20323	4.08711
C	2.18147	-0.24485	2.75973
O	5.24843	0.50815	0.96260
H	5.85446	0.63884	3.59392
H	4.26003	0.18055	5.41023
H	1.88849	-0.40201	4.88808
H	1.14446	-0.47631	2.52714
C	6.53939	1.07247	1.22599
H	6.97806	1.26829	0.24199
H	6.44131	2.01601	1.78153
H	7.17321	0.36429	1.78022
C	1.80766	-1.03683	-4.15195
H	1.17886	-0.18798	-4.43630
H	2.74465	-1.01811	-4.72788
H	1.26952	-1.97915	-4.33321
O	-0.34450	-2.45726	2.64473
O	-2.10237	-2.85028	1.25785
C	-1.19887	-2.88911	3.72882
H	-0.59607	-2.77526	4.63465
H	-2.10551	-2.27344	3.78000
H	-1.49024	-3.93774	3.58609
O	-3.08799	0.44944	-2.03606
O	-3.15923	2.20820	-0.58584
C	-3.65039	1.33742	-3.03271
H	-3.73933	0.73366	-3.94031
H	-4.63301	1.69712	-2.70244
H	-2.98483	2.19508	-3.18700

2MA-rac-isom

E = -16.27428148

Pd	0.00000	0.00000	0.00000
P	2.55403	0.00000	0.00000
C	3.31142	1.70069	-0.03539

C	2.53997	2.87795	-0.12064
S	0.71817	2.94117	0.00000
O	0.20771	1.93637	-1.03744
O	0.41994	2.49553	1.37197
O	0.34504	4.30433	-0.37172
C	3.25539	-0.93435	1.41385
C	3.43221	-0.72838	-1.46778
C	3.17720	4.11646	-0.23784
C	4.56564	4.20397	-0.26157
C	5.33355	3.04668	-0.17361
C	4.70612	1.80898	-0.07272
C	-1.66068	-0.31570	-1.31557
H	2.55590	5.00832	-0.31221
H	5.04448	5.17929	-0.35516
H	6.42211	3.10112	-0.19726
H	5.31664	0.90787	-0.03028
C	-2.78146	0.68058	-1.19351
H	-1.01030	-0.13807	-2.18634
C	-0.24063	-1.67888	1.39155
H	0.61062	-1.65158	2.07741
H	-0.39221	-2.59640	0.82133
C	-1.30574	-0.80140	1.60016
H	-2.29331	-1.00866	1.18106
C	-1.26366	0.19152	2.71451
C	-2.06148	-1.74515	-1.23578
C	4.65895	-1.39544	-1.39424
C	5.31711	-1.84017	-2.54169
C	4.75087	-1.60703	-3.79137
C	3.54242	-0.92200	-3.90005
C	2.88762	-0.47507	-2.74848
H	5.12300	-1.56466	-0.42419
H	6.27245	-2.35684	-2.45391
H	5.25311	-1.95028	-4.69669

H	3.11573	-0.73153	-4.88263
O	1.73431	0.23637	-2.76508
C	3.51066	-2.30887	1.33692
C	3.81624	-3.05164	2.47712
C	3.84421	-2.42141	3.71894
C	3.54390	-1.06501	3.83185
C	3.23247	-0.32226	2.68880
H	3.45051	-2.81673	0.37480
H	4.01996	-4.11859	2.39038
H	4.08178	-2.99092	4.61798
H	3.53071	-0.59159	4.81117
O	2.85542	0.97365	2.69059
C	1.28515	0.78238	-4.01297
H	0.47242	1.46553	-3.74690
H	2.09559	1.34484	-4.49990
H	0.91693	-0.01293	-4.67794
C	2.58802	1.61564	3.94640
H	2.21031	2.60635	3.67627
H	1.81505	1.06076	4.49418
H	3.51254	1.70684	4.53566
C	-3.67067	0.64105	-2.45105
H	-3.39294	0.46139	-0.30592
H	-2.35076	1.68606	-1.08098
H	-4.46994	1.39369	-2.37800
H	-3.08064	0.85803	-3.35554
H	-4.13764	-0.34849	-2.56895
O	-1.16870	-2.55065	-1.89123
O	-3.04837	-2.17939	-0.65741
C	-1.49098	-3.95896	-1.84184
H	-0.65533	-4.46366	-2.33532
H	-1.59574	-4.29523	-0.80254
H	-2.43278	-4.15189	-2.37175
O	-2.35062	1.00092	2.65724

O	-0.40139	0.25054	3.57348
C	-2.36031	2.05524	3.65208
H	-3.28944	2.60577	3.47854
H	-2.34214	1.62422	4.66077
H	-1.48731	2.70140	3.50222

2MA-rac-trans

E = -16.28328954 a.u.

Pd	0.00000	0.00000	0.00000
P	2.53740	0.00000	0.00000
C	3.25092	1.42975	0.94305
C	2.61905	2.68634	0.91136
S	1.07393	2.93520	0.00000
O	0.11054	2.02659	0.77981
O	1.32301	2.40916	-1.35057
O	0.71812	4.34076	0.15996
C	3.36200	-0.02044	-1.64422
C	3.23476	-1.46973	0.86361
C	3.14343	3.76207	1.62813
C	4.28934	3.59455	2.39999
C	4.90257	2.34525	2.46729
C	4.38642	1.27311	1.74522
C	-2.12911	0.37276	0.18829
H	2.62862	4.72101	1.57048
H	4.69724	4.43927	2.95642
H	5.79146	2.20295	3.08279
H	4.87429	0.30107	1.79962
H	-1.96236	1.33509	0.69476
C	-2.59597	0.59841	-1.20676
C	-0.14134	-2.15069	0.46251
H	0.77521	-2.33543	1.02346
H	-1.08739	-2.38456	0.95333
C	-0.11894	-2.04113	-0.91989

C	-1.33775	-2.36713	-1.71961
H	0.82279	-2.10024	-1.47294
C	-2.97583	-0.58059	0.99772
H	-3.15322	-1.50787	0.43361
H	-2.44862	-0.83029	1.93250
C	-4.33090	0.05482	1.36048
H	-4.90030	0.28940	0.44992
H	-4.92693	-0.64152	1.97073
H	-4.19008	0.98309	1.93596
O	-1.94168	1.65341	-1.77364
C	-2.30721	1.93199	-3.14066
H	-1.68025	2.77786	-3.43621
H	-3.37277	2.18842	-3.20498
H	-2.10795	1.05817	-3.77334
O	-3.45088	-0.05386	-1.79231
C	4.76254	0.07303	-1.82059
C	5.30653	0.09012	-3.10786
C	4.47034	0.01205	-4.21976
C	3.09065	-0.07581	-4.06385
C	2.54816	-0.08007	-2.78033
O	5.51411	0.11702	-0.69023
H	6.38219	0.16726	-3.24973
H	4.91212	0.02893	-5.21666
H	2.43558	-0.12027	-4.93274
H	1.46684	-0.09740	-2.65384
C	3.98149	-2.45474	0.21265
C	4.40145	-3.60481	0.88241
C	4.07398	-3.77620	2.22387
C	3.31412	-2.81832	2.89683
C	2.88099	-1.67756	2.21818
H	4.24285	-2.32115	-0.83732
H	4.98598	-4.35766	0.35443
H	4.40281	-4.66666	2.76046

H	3.05517	-2.97212	3.94254
O	2.09502	-0.71134	2.76378
C	1.75854	-0.80816	4.15305
H	1.16297	0.08434	4.36712
H	2.66703	-0.80795	4.77312
H	1.16412	-1.71250	4.35032
C	6.91344	0.39250	-0.81945
H	7.28988	0.47631	0.20548
H	7.07475	1.34146	-1.35064
H	7.43167	-0.42960	-1.33515
O	-1.17040	-2.00238	-3.01532
O	-2.32101	-2.93689	-1.28426
C	-2.31072	-2.31586	-3.86048
H	-2.00944	-2.01648	-4.86842
H	-3.18135	-1.74683	-3.51489
H	-2.52227	-3.39144	-3.81576

2MA-rac-inser

E = -16.27185201 a.u.

Pd	0.00000	0.00000	0.00000
P	2.34127	0.00000	0.00000
C	3.05627	1.41754	0.95286
C	2.44637	2.68730	0.93894
S	0.92671	3.02723	0.00000
O	-0.07294	2.07128	0.66582
O	1.22215	2.63757	-1.38232
O	0.57725	4.41576	0.28592
C	2.99230	3.73449	1.68231
C	4.13370	3.53104	2.45255
C	4.72976	2.27281	2.48973
C	4.19356	1.22560	1.74606
H	2.49401	4.70320	1.64604
H	4.55190	4.35618	3.03043

H	5.61703	2.10213	3.10023
H	4.66367	0.24369	1.78054
C	3.11170	0.02053	-1.66532
C	3.00935	-1.48670	0.84979
H	-1.67781	-2.00218	1.13156
C	-1.49198	-1.81478	0.07259
C	-0.16957	-2.07718	-0.40232
H	-2.32272	-2.05502	-0.59563
C	-0.00359	-2.41198	-1.84047
C	-2.36799	0.17993	0.05510
H	-1.90648	1.17792	0.13068
H	0.54453	-2.55943	0.27345
C	-3.02148	0.03296	-1.28031
C	-3.27572	-0.07375	1.24092
H	-2.66218	-0.14956	2.15271
C	-4.29212	1.06325	1.41389
H	-3.81428	-1.02467	1.10514
C	4.50839	0.07365	-1.87682
C	5.01534	0.13823	-3.17794
C	4.14383	0.16690	-4.26509
C	2.76658	0.13654	-4.07084
C	2.26164	0.07126	-2.77481
O	5.29217	0.03624	-0.76678
H	6.08854	0.17708	-3.35005
H	4.55705	0.22678	-5.27270
H	2.08435	0.18889	-4.91830
H	1.18468	0.09206	-2.61177
C	3.75963	-2.46452	0.19500
C	4.17102	-3.62096	0.85860
C	3.82741	-3.80616	2.19439
C	3.05765	-2.85653	2.86748
C	2.63388	-1.70786	2.19611
H	4.02130	-2.32263	-0.85264

H	4.75890	-4.37136	0.33077
H	4.14995	-4.70206	2.72613
H	2.78441	-3.02187	3.90771
O	1.84659	-0.74553	2.74558
C	1.51406	-0.84581	4.13521
H	0.92961	0.05244	4.35634
H	2.42435	-0.85854	4.75261
H	0.91061	-1.74464	4.33032
C	6.69660	0.26729	-0.92882
H	7.10902	0.28426	0.08529
H	6.87549	1.23556	-1.41806
H	7.16678	-0.54489	-1.50314
O	-2.34689	0.71953	-2.23361
O	-4.02697	-0.62968	-1.49148
C	-2.84804	0.52725	-3.57850
H	-2.25773	1.20487	-4.20139
H	-3.91488	0.77696	-3.62545
H	-2.69420	-0.51736	-3.87503
O	-0.79441	-2.14270	-2.73116
O	1.16188	-3.08834	-2.03914
C	1.40295	-3.47199	-3.41362
H	2.28071	-4.12405	-3.38103
H	1.60733	-2.58135	-4.02079
H	0.53157	-4.00112	-3.81829
H	-4.94171	0.86527	2.28036
H	-4.93073	1.15108	0.52266
H	-3.78340	2.02545	1.57699

3-rac-KP

E -16.30274216 a.u.

Pd	0.00000	0.00000	0.00000
P	2.29179	0.00000	0.00000
C	3.24165	-1.46774	0.55988

C	3.09523	0.44668	-1.58876
C	2.84015	1.35233	1.14326
C	2.95271	-2.07439	1.80434
O	1.96042	-1.49753	2.53073
C	1.71929	-1.99741	3.85276
H	2.62497	-1.91202	4.47174
H	0.93108	-1.36071	4.26562
H	1.37889	-3.04280	3.82060
C	3.69298	-3.17819	2.23290
H	3.48602	-3.64328	3.19427
C	4.70894	-3.69145	1.42669
H	5.28340	-4.54931	1.77929
C	4.99334	-3.11530	0.19288
H	5.79170	-3.50956	-0.43522
C	4.25807	-2.00852	-0.23127
H	4.49186	-1.54087	-1.18777
C	2.66465	-0.12389	-2.80643
O	1.68495	-1.06034	-2.72917
C	1.12116	-1.53673	-3.96431
H	0.71709	-0.69580	-4.54628
H	1.87855	-2.07835	-4.55077
H	0.32385	-2.22029	-3.66099
C	3.26056	0.27425	-4.00743
H	2.93024	-0.15234	-4.95119
C	4.27861	1.22404	-4.00178
H	4.72791	1.52549	-4.94861
C	4.71334	1.78942	-2.80683
H	5.50008	2.54257	-2.80055
C	4.11272	1.40491	-1.61224
H	4.42868	1.87470	-0.68153
C	3.88914	1.10547	2.03850
H	4.38622	0.13602	2.03640
C	4.32602	2.08767	2.92457

H	5.14708	1.86853	3.60772
C	3.71752	3.33755	2.92932
H	4.04861	4.11154	3.62290
C	2.67918	3.60387	2.03985
H	2.18591	4.57583	2.01812
C	2.23283	2.62849	1.14835
S	0.90321	3.13525	0.00000
O	1.47271	2.98635	-1.33865
O	0.48485	4.46261	0.44306
O	-0.19436	2.11157	0.28575
C	-2.00216	-1.86194	-0.15067
C	-2.62932	-0.54603	0.40556
H	-2.07370	0.36675	0.07898
C	-3.98624	-0.39243	-0.27854
C	-2.77638	-0.54246	1.92834
H	-3.52302	-1.31134	2.18990
H	-1.81731	-0.84971	2.37476
C	-3.19422	0.81734	2.48580
H	-4.17146	1.12227	2.08099
H	-2.45594	1.59333	2.22956
H	-3.28547	0.78056	3.58147
O	-5.03383	-0.81644	0.17036
O	-3.85606	0.23024	-1.47262
C	-5.08805	0.35558	-2.22838
H	-5.81905	0.94085	-1.65822
H	-4.80490	0.87246	-3.14929
H	-5.50005	-0.63784	-2.44270
C	-0.51586	-2.03230	0.13853
H	-2.14568	-1.91182	-1.24098
H	-2.57418	-2.70607	0.28568
C	0.09892	-3.03626	-0.76201
H	-0.27222	-2.25518	1.18755
O	-0.30117	-3.33133	-1.88239

O	1.15215	-3.66114	-0.16649
C	1.79499	-4.66173	-0.98795
H	2.57606	-5.09400	-0.35497
H	2.23336	-4.19483	-1.87887
H	1.06783	-5.42419	-1.29687

Rac_3

E = -16.31797269 a.u.

Pd	0.00000	0.00000	0.00000
P	2.30478	0.00000	0.00000
C	3.13861	-0.15842	-1.63708
C	3.16226	-1.21514	1.09372
C	3.03047	1.58973	0.65720
C	2.65561	-1.42015	2.39788
O	1.54367	-0.71098	2.72161
C	1.06361	-0.77751	4.06992
H	0.73735	-1.79789	4.32046
H	1.83966	-0.44241	4.77373
H	0.21085	-0.09290	4.10541
C	3.30798	-2.29205	3.27554
H	2.92289	-2.45448	4.27980
C	4.47010	-2.94722	2.87064
H	4.97355	-3.61678	3.56903
C	4.99070	-2.74047	1.59638
H	5.90893	-3.23751	1.28450
C	4.33289	-1.87849	0.71944
H	4.75493	-1.69743	-0.26834
C	3.21885	-1.39151	-2.32505
O	2.77860	-2.48936	-1.65207
C	2.76255	-3.74286	-2.34086
H	3.77836	-4.04331	-2.63964
H	2.10093	-3.69038	-3.21760
H	2.36933	-4.46632	-1.61861

C	3.75845	-1.44424	-3.61137
H	3.83221	-2.39348	-4.13753
C	4.19822	-0.27631	-4.23337
H	4.61198	-0.33363	-5.24089
C	4.10598	0.94712	-3.57885
H	4.43595	1.86523	-4.06346
C	3.57794	0.99843	-2.28956
H	3.48951	1.96172	-1.78855
C	4.32749	1.54868	1.18778
H	4.87470	0.60802	1.21700
C	4.93661	2.69332	1.69503
H	5.94641	2.62828	2.10053
C	4.25302	3.90508	1.68888
H	4.71964	4.80458	2.09250
C	2.96262	3.96535	1.17246
H	2.39477	4.89578	1.16296
C	2.34820	2.82267	0.65702
S	0.66745	3.01131	0.00000
O	0.77710	2.62132	-1.41437
O	0.26068	4.38062	0.30919
O	-0.10745	1.99882	0.83307
C	-0.25960	-1.93510	-0.78010
H	0.70615	-2.44889	-0.79083
C	-1.24160	-2.65667	0.14336
H	-0.87620	-2.53284	1.17517
H	-1.16495	-3.74200	-0.05875
C	-2.74799	-2.29946	0.07745
H	-3.14992	-2.41357	1.10634
C	-2.98497	-0.83355	-0.21347
C	-3.57111	-3.25249	-0.81486
O	-2.18905	0.08474	0.01192
H	-3.10283	-3.28660	-1.81082
O	-4.22999	-0.56276	-0.61533

C	-4.49079	0.84301	-0.89556
H	-4.35770	1.43873	0.01397
H	-3.79941	1.19134	-1.67053
H	-5.52685	0.87078	-1.24362
C	-3.70292	-4.65655	-0.22642
H	-4.57543	-2.82724	-0.95389
C	-0.70676	-1.61100	-2.15669
O	-1.86251	-1.38563	-2.51295
O	0.34136	-1.54594	-3.02994
C	0.00686	-0.99230	-4.32342
H	-0.67759	-1.65996	-4.86278
H	0.96243	-0.89673	-4.84896
H	-0.46302	-0.00884	-4.19964
H	-4.30281	-5.29551	-0.89168
H	-4.20249	-4.63174	0.75552
H	-2.72761	-5.14897	-0.09317

3-meso

3MA-meso-cis

3MA-meso-isom

3MA-meso-trans

4MA-meso-inser

4-meso-KP

4-meso

3-meso

E = -16.32160953 a.u.

Pd	0.00000	0.00000	0.00000
P	2.30544	0.00000	0.00000
C	3.15439	-0.16667	1.62750
C	3.13133	-1.20960	-1.12203
C	3.03685	1.58693	-0.65692
C	2.60801	-1.36163	-2.42747
O	1.51510	-0.61024	-2.71684
C	1.02874	-0.60406	-4.06446
H	0.66074	-1.59957	-4.35392
H	1.81592	-0.27245	-4.75747
H	0.20431	0.11543	-4.06806
C	3.22417	-2.22704	-3.33614
H	2.82690	-2.34484	-4.34197
C	4.36598	-2.93272	-2.95852

H	4.84008	-3.60100	-3.67841
C	4.90486	-2.77659	-1.68455
H	5.80974	-3.31101	-1.39641
C	4.28477	-1.91688	-0.77754
H	4.72302	-1.77428	0.20918
C	3.23738	-1.39777	2.31838
O	2.79643	-2.49867	1.65029
C	2.79216	-3.75069	2.34220
H	3.81162	-4.04400	2.63581
H	2.13569	-3.69985	3.22283
H	2.39878	-4.47868	1.62465
C	3.78096	-1.44621	3.60342
H	3.85716	-2.39358	4.13235
C	4.22275	-0.27671	4.22083
H	4.63975	-0.33090	5.22721
C	4.12793	0.94481	3.56337
H	4.45800	1.86471	4.04448
C	3.59521	0.99224	2.27620
H	3.50266	1.95449	1.77416
C	4.33658	1.53885	-1.18021
H	4.88005	0.59565	-1.20223
C	4.95286	2.67997	-1.68674
H	5.96569	2.61155	-2.08397
C	4.27226	3.89370	-1.68973
H	4.74435	4.79042	-2.09316
C	2.97933	3.96030	-1.18066
H	2.41563	4.89332	-1.17517
C	2.35881	2.82140	-0.66365
S	0.68181	3.01993	0.00000
O	0.79958	2.63833	1.41563
O	0.28024	4.38934	-0.31604
O	-0.10466	2.00648	-0.82054
C	-0.24879	-1.94924	0.74561

H	0.72294	-2.45178	0.75502
C	-1.21710	-2.66067	-0.19846
H	-0.86343	-2.50658	-1.23347
H	-1.13173	-3.74960	-0.01734
C	-2.71328	-2.31900	-0.11866
H	-3.15148	-2.81015	0.76569
C	-2.98440	-0.84865	0.08928
C	-3.48278	-2.81144	-1.36759
O	-2.19068	0.08592	-0.04821
C	-3.40467	-4.32474	-1.56245
O	-4.26447	-0.61701	0.40017
H	-4.02734	-4.63514	-2.41484
C	-4.59231	0.77790	0.66366
H	-4.40187	1.38313	-0.22940
H	-3.98065	1.14456	1.49527
H	-5.65434	0.77143	0.92267
H	-3.08474	-2.29477	-2.25982
H	-4.53714	-2.50931	-1.26477
H	-2.37783	-4.66336	-1.76156
H	-3.77002	-4.85345	-0.66758
C	-0.72565	-1.68709	2.12774
O	-1.89275	-1.52851	2.47799
O	0.31338	-1.60068	3.01155
C	-0.06288	-1.13408	4.32662
H	-0.71275	-1.86640	4.82332
H	0.88116	-1.01092	4.86685
H	-0.58909	-0.17484	4.24816

3MA-meso-cis

E= -18.89057055 a.u.

Pd	0.00000	0.00000	0.00000
P	2.40785	0.00000	0.00000
C	3.10244	1.42444	-0.96720

C	2.49215	2.69249	-0.94818
S	0.98272	2.99342	0.00000
O	-0.00509	2.05372	-0.69972
O	1.28194	2.55487	1.36853
O	0.61921	4.39098	-0.22500
C	3.11301	0.05814	1.69577
C	3.21216	-1.45055	-0.79289
C	3.01903	3.74348	-1.69852
C	4.15070	3.54488	-2.48347
C	4.75094	2.28879	-2.52612
C	4.22969	1.23860	-1.77613
C	0.01355	-2.07069	0.59512
H	2.51370	4.70832	-1.65709
H	4.55714	4.37056	-3.06874
H	5.63128	2.12055	-3.14720
H	4.71550	0.26432	-1.81056
H	0.98220	-2.21427	1.09038
C	-1.07622	-2.22397	1.59301
C	-2.21599	-0.17586	-0.69510
H	-2.34952	-1.25575	-0.73035
H	-2.25854	0.40581	-1.61931
C	-2.27494	0.48009	0.50160
C	-2.50955	1.95750	0.55509
H	-2.40979	-0.06518	1.43754
C	-0.15112	-2.97746	-0.61396
H	0.59690	-2.73425	-1.37995
H	-1.14155	-2.82405	-1.06632
C	-0.02088	-4.48821	-0.29027
H	-0.77494	-4.76660	0.46512
C	1.38331	-4.86838	0.22107
C	-0.32118	-5.26670	-1.55755
C	4.15796	-2.24758	-0.14444
C	4.74589	-3.33534	-0.79053

C	4.37437	-3.63994	-2.09683
C	3.41274	-2.87819	-2.75927
C	2.83010	-1.78547	-2.11359
H	4.44446	-2.01275	0.88022
H	5.48981	-3.93892	-0.27115
H	4.82448	-4.48909	-2.61270
H	3.11276	-3.14854	-3.76926
O	1.88691	-0.98085	-2.66762
C	4.46922	0.35345	1.96478
C	4.92000	0.42039	3.28631
C	4.03693	0.18982	4.33885
C	2.69988	-0.10012	4.08844
C	2.24612	-0.14996	2.77291
O	5.27925	0.53067	0.88862
H	5.96084	0.65203	3.50047
H	4.40637	0.24488	5.36345
H	2.00433	-0.26656	4.90961
H	1.19237	-0.33944	2.57999
C	6.59030	1.06170	1.11720
H	7.00645	1.24867	0.12181
H	6.53191	2.00591	1.67728
H	7.22195	0.33703	1.65251
C	1.42924	-1.28644	-3.99455
H	0.67827	-0.52358	-4.22074
H	2.25815	-1.21480	-4.71392
H	0.97547	-2.28758	-4.02488
C	1.52671	-6.33262	0.63599
H	2.11587	-4.62327	-0.56686
H	1.61788	-4.22834	1.08669
O	-0.66525	-1.86967	2.85427
O	-2.21595	-2.60598	1.35921
C	-1.68605	-1.98885	3.87073
H	-1.19261	-1.72054	4.80952

H	-2.51877	-1.30452	3.66557
H	-2.06860	-3.01639	3.90885
H	2.53992	-6.52411	1.02028
H	0.80747	-6.59258	1.42876
H	1.35258	-7.01634	-0.20853
O	-2.17693	2.44037	1.77288
O	-2.99332	2.60621	-0.35196
C	-2.33645	3.87840	1.90632
H	-2.00852	4.10572	2.92415
H	-1.70496	4.38787	1.16884
H	-3.38821	4.15110	1.75451
O	0.08217	-4.97692	-2.67192
O	-1.08920	-6.35965	-1.29995
C	-1.38722	-7.17004	-2.46388
H	-1.98788	-8.00305	-2.08753
H	-1.94940	-6.58178	-3.19934
H	-0.45890	-7.53056	-2.92371

3MA-meso-isom

E= -18.87496679 a.u.

Pd	0.00000	0.00000	0.00000
P	2.73844	0.00000	0.00000
C	3.31732	1.53628	0.88443
C	2.58974	2.74167	0.83330
S	0.99133	2.84447	0.00000
O	0.12099	1.95504	0.90089
O	1.18243	2.21562	-1.31883
O	0.56935	4.23910	0.05957
C	3.68859	0.11404	-1.58110
C	3.68381	-1.30010	0.92551
C	3.05628	3.88795	1.47546
C	4.24603	3.85047	2.19677
C	4.96230	2.66037	2.28215

C	4.50190	1.51719	1.63105
C	-1.64589	-0.24673	1.35592
H	2.46361	4.79953	1.39874
H	4.60652	4.75028	2.69655
H	5.88992	2.61629	2.85336
H	5.08059	0.59638	1.70194
C	-2.95341	0.12140	0.74805
H	-1.28468	0.54213	2.02688
C	-0.10688	-1.91137	-1.09002
H	0.78902	-1.92692	-1.70974
H	-0.23835	-2.71606	-0.36655
C	-1.18290	-1.12637	-1.48867
H	-2.18937	-1.27933	-1.08977
C	-1.08995	-0.31784	-2.74226
C	-1.58934	-1.64250	1.92881
C	4.83178	-1.91072	0.41545
C	5.51005	-2.89977	1.12938
C	5.03082	-3.29447	2.37425
C	3.89085	-2.69898	2.91340
C	3.22032	-1.70105	2.19978
H	5.22005	-1.59017	-0.55123
H	6.40975	-3.35159	0.71210
H	5.54518	-4.07021	2.94309
H	3.53045	-3.01811	3.88877
O	2.12769	-1.04003	2.67140
C	4.39686	1.26262	-1.93935
C	5.03828	1.36216	-3.17416
C	4.96991	0.30160	-4.07027
C	4.26826	-0.85771	-3.73980
C	3.62652	-0.95181	-2.50510
H	4.44656	2.10054	-1.24489
H	5.58182	2.27106	-3.42917
H	5.46092	0.36657	-5.04168

H	4.21730	-1.67667	-4.45339
O	2.94474	-2.05935	-2.08830
C	1.72934	-1.29664	4.02840
H	0.94437	-0.56509	4.24051
H	2.57431	-1.13642	4.71503
H	1.32477	-2.31327	4.13603
C	2.85707	-3.17076	-2.98902
H	2.29081	-3.93821	-2.45123
H	3.85854	-3.55753	-3.23056
H	2.32230	-2.88482	-3.90649
O	-0.19081	-0.39377	-3.55978
O	-2.16543	0.50582	-2.85374
C	-2.12701	1.37728	-4.01181
H	-3.04516	1.96941	-3.95726
H	-2.09974	0.78162	-4.93246
H	-1.24054	2.02059	-3.96072
O	-3.14020	1.46531	0.74447
O	-3.77762	-0.67955	0.31829
C	-4.36767	1.89537	0.11307
C	-2.54813	-1.85876	3.13704
H	-0.56550	-1.87132	2.26015
H	-1.87760	-2.37553	1.15923
C	-2.24882	-3.22402	3.73038
H	-3.58617	-1.85395	2.76673
C	-2.39713	-0.79559	4.24141
H	-4.35534	2.98674	0.18062
H	-5.23457	1.47624	0.63965
H	-4.38297	1.56390	-0.93228
O	-3.36759	-3.98661	3.83064
O	-1.14580	-3.59181	4.10028
C	-3.15347	-5.28695	4.43846
C	-3.37562	-0.98519	5.40023
H	-2.55578	0.19878	3.79463

H	-1.35968	-0.82531	4.61529
H	-4.13870	-5.76129	4.45393
H	-2.75812	-5.16766	5.45447
H	-2.44383	-5.87088	3.84034
H	-3.25443	-0.18446	6.14461
H	-3.21826	-1.94684	5.91292
H	-4.41665	-0.96240	5.04152

3MA-meso-trans

E= -18.88139842 a.u.

Pd	0.00000	0.00000	0.00000
P	2.49842	0.00000	0.00000
C	3.21976	1.41689	-0.95073
C	2.59458	2.67747	-0.93410
S	1.06836	2.96072	0.00000
O	0.07648	2.03747	-0.72891
O	1.33599	2.48177	1.36227
O	0.71106	4.36035	-0.20630
C	3.31158	-0.03393	1.64743
C	3.13805	-1.47632	-0.88903
C	3.11524	3.73554	-1.67925
C	4.25323	3.54719	-2.45857
C	4.86465	2.29613	-2.50256
C	4.35062	1.24009	-1.75525
C	-2.13439	0.39254	-0.09530
H	2.60457	4.69738	-1.63739
H	4.65745	4.37817	-3.03784
H	5.74858	2.13880	-3.12150
H	4.83233	0.26409	-1.79598
H	-1.98157	1.42712	-0.42489
C	-2.75573	-0.41452	-1.17187
C	-0.31494	-2.18979	-0.28032
H	0.44759	-2.42264	-1.02635

H	-1.35961	-2.40384	-0.52280
C	0.03704	-2.00491	1.04440
C	-0.97084	-2.18428	2.13465
H	1.07833	-2.08778	1.36719
C	-2.77917	0.25543	1.26386
H	-2.05500	0.46773	2.06749
H	-3.13858	-0.77577	1.38727
C	-3.96455	1.23475	1.47053
C	-4.71237	0.80574	2.71812
C	-3.48260	2.68993	1.63916
H	-4.65667	1.16866	0.61351
O	-2.43692	0.08485	-2.41141
C	-3.00849	-0.65934	-3.50710
H	-2.69431	-0.13028	-4.41216
H	-2.63740	-1.69268	-3.50788
H	-4.10330	-0.67904	-3.42905
O	-3.45482	-1.40870	-1.02526
C	-4.61220	3.71758	1.69033
H	-2.87594	2.74308	2.56007
H	-2.80775	2.93227	0.80304
H	-4.20554	4.73261	1.80651
H	-5.20856	3.69330	0.76422
H	-5.29671	3.52750	2.53167
C	4.71217	0.01614	1.83694
C	5.24252	0.03493	3.13011
C	4.39298	0.00777	4.23459
C	3.01322	-0.03084	4.06475
C	2.48455	-0.03976	2.77632
O	5.47697	0.02156	0.71307
H	6.31828	0.07612	3.28407
H	4.82431	0.02485	5.23614
H	2.34634	-0.03296	4.92548
H	1.40508	-0.02762	2.64476

C	3.89591	-2.48017	-0.28284
C	4.26628	-3.62725	-0.98735
C	3.87984	-3.77293	-2.31638
C	3.10801	-2.79366	-2.94392
C	2.72246	-1.65788	-2.23040
H	4.20524	-2.36409	0.75600
H	4.85874	-4.39864	-0.49628
H	4.17164	-4.66007	-2.87957
H	2.80423	-2.92616	-3.98057
O	1.92995	-0.67077	-2.72427
C	1.52497	-0.73419	-4.09704
H	0.92437	0.16579	-4.25879
H	2.40257	-0.72452	-4.76028
H	0.91548	-1.63021	-4.28518
C	6.88244	0.25644	0.86115
H	7.27849	0.31469	-0.15791
H	7.06301	1.20685	1.38366
H	7.36673	-0.57333	1.39728
O	-0.55144	-1.58822	3.27837
O	-2.00723	-2.80927	2.01983
C	-1.48120	-1.70990	4.39172
H	-0.94485	-1.30558	5.25474
H	-2.38509	-1.12323	4.18591
H	-1.74199	-2.76383	4.54424
O	-6.05811	0.81330	2.52967
O	-4.18521	0.50462	3.77681
C	-6.82535	0.42240	3.69631
H	-7.87240	0.49569	3.38889
H	-6.57196	-0.60503	3.98483
H	-6.61210	1.09686	4.53449

3MA-meso-inser

E= -18.86074531 a.u.

Pd	0.00000	0.00000	0.00000
P	2.34499	0.00000	0.00000
C	3.09428	-1.52560	-0.70881
C	3.34927	0.33219	1.50473
C	2.94278	1.31416	-1.16569
C	2.58850	-2.02129	-1.93565
O	1.56983	-1.30834	-2.48109
C	0.97062	-1.78143	-3.69649
H	1.68225	-1.70534	-4.53188
H	0.11020	-1.12675	-3.86596
H	0.62903	-2.82069	-3.58294
C	3.13976	-3.16860	-2.51091
H	2.77158	-3.53830	-3.46579
C	4.17705	-3.84001	-1.86288
H	4.60555	-4.72922	-2.32689
C	4.66044	-3.38426	-0.64054
H	5.46545	-3.91311	-0.13104
C	4.11477	-2.23289	-0.07134
H	4.49491	-1.87200	0.88381
C	2.78339	0.32516	2.79898
O	1.48795	-0.05217	2.91079
C	0.80163	0.24879	4.13710
H	0.85316	1.32773	4.34102
H	1.22234	-0.32478	4.97702
H	-0.23125	-0.06938	3.97136
C	3.56844	0.69951	3.89585
H	3.13642	0.72133	4.89350
C	4.90014	1.06298	3.71898
H	5.49029	1.35572	4.58809
C	5.46881	1.07242	2.44811
H	6.50407	1.37728	2.30104
C	4.68405	0.72093	1.35324
H	5.11406	0.77428	0.35337

C	3.94123	1.03302	-2.10513
H	4.36857	0.03166	-2.16120
C	4.40443	2.01955	-2.97455
H	5.18588	1.77650	-3.69473
C	3.87011	3.30252	-2.92171
H	4.22548	4.07688	-3.60241
C	2.86812	3.59773	-2.00052
H	2.41718	4.58872	-1.94572
C	2.40305	2.61608	-1.12870
S	1.05612	3.06122	0.00000
O	1.52146	2.72293	1.34733
O	0.70361	4.44780	-0.29621
O	-0.05275	2.11893	-0.47916
C	-1.58011	-1.78242	0.03397
C	-2.34169	0.25142	-0.40288
H	-1.74964	1.11149	-0.73987
C	-3.00469	-0.25703	-1.63800
C	-3.17833	0.59812	0.81122
H	-2.52097	0.74666	1.68190
H	-3.86552	-0.22259	1.06848
C	-4.00033	1.89623	0.62228
H	-4.72165	1.75385	-0.20174
C	-4.82881	2.14621	1.87223
C	-3.13756	3.15271	0.30752
O	-2.44917	-0.41476	-2.71590
O	-4.32467	-0.53117	-1.43600
C	-5.03554	-0.94161	-2.62965
H	-4.97626	-0.15410	-3.39105
H	-6.06939	-1.09917	-2.30902
H	-4.60274	-1.86535	-3.03247
C	-0.22445	-2.07143	0.37232
H	-2.30822	-1.83843	0.84685
H	-1.90810	-2.12723	-0.94674

C	0.07943	-2.41461	1.78763
H	0.39987	-2.58551	-0.36524
O	-0.65638	-2.21893	2.74196
O	1.28738	-3.03302	1.86397
C	1.68597	-3.43181	3.19398
H	2.56211	-4.07183	3.05243
H	1.94947	-2.54415	3.78156
H	0.87297	-3.97608	3.68987
O	-4.69295	1.59664	2.94955
O	-5.75299	3.11943	1.63381
C	-6.52281	3.51851	2.79257
H	-7.15522	4.34172	2.44662
H	-7.13277	2.68104	3.15278
H	-5.85347	3.85089	3.59567
H	-3.56601	4.01942	0.83492
H	-2.12756	3.00047	0.71981
C	-3.04260	3.49881	-1.17900
H	-2.34146	4.33366	-1.32571
H	-2.66742	2.65986	-1.78269
H	-4.02830	3.79022	-1.57662

4-meso-KP

E = -18.89455172 a.u.

Pd	0.00000	0.00000	0.00000
P	2.28639	0.00000	0.00000
C	3.00860	-1.48483	-0.79763
C	3.24289	0.19520	1.55887
C	2.91366	1.39362	-1.04806
C	2.60743	-1.79175	-2.12088
O	1.72686	-0.92229	-2.67770
C	1.36274	-1.10207	-4.05177
H	2.25097	-1.04790	-4.69820
H	0.68691	-0.27231	-4.27919

H	0.84272	-2.06003	-4.19639
C	3.11583	-2.92034	-2.76594
H	2.82716	-3.14870	-3.78997
C	3.99792	-3.76461	-2.09059
H	4.39075	-4.64257	-2.60479
C	4.36802	-3.49823	-0.77568
H	5.04684	-4.16615	-0.24632
C	3.86764	-2.36432	-0.13536
H	4.15362	-2.15448	0.89457
C	2.63176	0.26532	2.83212
O	1.29928	0.06140	2.89948
C	0.61299	0.42239	4.10902
H	0.75835	1.49193	4.31619
H	0.95296	-0.19071	4.95708
H	-0.44110	0.20389	3.91755
C	3.42483	0.52197	3.95896
H	2.96437	0.60183	4.94072
C	4.80028	0.68601	3.83550
H	5.39484	0.88057	4.72888
C	5.41231	0.61682	2.58626
H	6.48664	0.76226	2.48066
C	4.62614	0.38847	1.46102
H	5.10043	0.37636	0.48050
C	4.01980	1.18921	-1.88180
H	4.48156	0.20323	-1.94190
C	4.54223	2.23158	-2.64412
H	5.40903	2.05034	-3.28004
C	3.95936	3.49384	-2.58962
H	4.36559	4.31477	-3.18152
C	2.84705	3.70905	-1.77994
H	2.35877	4.68241	-1.72958
C	2.32016	2.67105	-1.01329
S	0.85521	3.03582	0.00000

O	1.24041	2.68026	1.37084
O	0.49006	4.42009	-0.28842
O	-0.17917	2.06764	-0.57879
C	-1.64991	-2.27231	-0.12158
C	-2.59710	-1.01996	-0.17268
H	-2.08151	-0.14262	-0.63179
C	-3.68890	-1.39532	-1.17201
C	-3.22560	-0.64934	1.17536
H	-2.44399	-0.51682	1.93590
H	-3.82350	-1.51168	1.51072
C	-4.13637	0.58446	1.08711
H	-4.84284	0.44543	0.24828
C	-5.00348	0.69016	2.33055
C	-3.40176	1.92790	0.85011
O	-4.68026	-2.03896	-0.88831
O	-3.38839	-0.97514	-2.42771
C	-4.36277	-1.37012	-3.42939
H	-4.42460	-2.46393	-3.48320
H	-3.99583	-0.94816	-4.36901
H	-5.34894	-0.96418	-3.17468
C	-0.21535	-2.04472	0.36180
H	-2.15559	-3.02931	0.50385
H	-1.58575	-2.67355	-1.14548
C	0.01444	-2.35412	1.79687
H	0.51554	-2.57591	-0.26283
O	-0.80211	-2.22857	2.69841
O	1.27472	-2.85217	1.98814
C	1.58202	-3.21167	3.35187
H	2.51333	-3.78451	3.30033
H	1.72426	-2.30787	3.95667
H	0.77155	-3.81340	3.78167
O	-4.83154	0.10036	3.38055
O	-6.01956	1.57560	2.11979

C	-6.88654	1.77801	3.26028
H	-7.64095	2.49568	2.92412
H	-7.35168	0.82964	3.55597
H	-6.31535	2.17968	4.10635
H	-4.16992	2.70002	0.68076
C	-2.48282	2.35932	1.99155
H	-2.81995	1.86567	-0.08457
H	-2.03513	3.33870	1.76914
H	-3.03079	2.43641	2.94530
H	-1.64781	1.65841	2.13585

4-meso

E= -18.91609051 a.u.

Pd	0.00000	0.00000	0.00000
P	2.30899	0.00000	0.00000
C	3.17630	-0.21233	1.61306
C	3.12832	-1.15986	-1.17939
C	3.04815	1.60717	-0.60135
C	2.61345	-1.21018	-2.49634
O	1.53433	-0.42319	-2.73361
C	1.06986	-0.28267	-4.08155
H	0.68389	-1.23890	-4.46470
H	1.87544	0.09156	-4.73004
H	0.26262	0.45426	-4.02924
C	3.22521	-2.01403	-3.46198
H	2.83374	-2.05150	-4.47641
C	4.35523	-2.76006	-3.12864
H	4.82908	-3.37738	-3.89286
C	4.88304	-2.70766	-1.84167
H	5.77799	-3.27481	-1.58698
C	4.26690	-1.90871	-0.87739
H	4.69848	-1.84702	0.12024

C	3.27360	-1.46094	2.26810
O	2.81651	-2.54296	1.57953
C	2.81759	-3.81030	2.24327
H	3.84060	-4.11557	2.51172
H	2.17850	-3.77503	3.13750
H	2.40684	-4.51991	1.51728
C	3.84243	-1.54373	3.54060
H	3.93305	-2.50526	4.04093
C	4.28924	-0.39025	4.18404
H	4.72750	-0.47168	5.17954
C	4.17236	0.84970	3.56592
H	4.50393	1.75779	4.06806
C	3.61868	0.93042	2.28940
H	3.51318	1.90640	1.81689
C	4.36807	1.57479	-1.07301
H	4.91571	0.63390	-1.09340
C	5.00101	2.72891	-1.52609
H	6.02936	2.67222	-1.88340
C	4.31747	3.94122	-1.52643
H	4.80301	4.84871	-1.88771
C	3.00497	3.99226	-1.06869
H	2.43773	4.92309	-1.06474
C	2.36830	2.83970	-0.60356
S	0.66711	3.01937	0.00000
O	0.73605	2.63730	1.41867
O	0.26339	4.38521	-0.32943
O	-0.07633	1.99829	-0.85121
C	-0.28194	-1.92646	0.79232
H	0.67470	-2.45756	0.76881
C	-1.31416	-2.64274	-0.07989
H	-1.00202	-2.54846	-1.13543
H	-1.24940	-3.72385	0.15297
C	-2.79638	-2.25606	0.04929

H	-3.18714	-2.61048	1.01709
C	-3.02108	-0.76234	0.09386
C	-3.66327	-2.87771	-1.07402
O	-2.18334	0.12447	-0.08760
C	-3.69895	-4.41048	-1.05885
O	-4.29781	-0.45224	0.33414
C	-4.53766	-4.98670	-2.22526
C	-4.57673	0.97309	0.45227
H	-4.61374	-6.07806	-2.08128
H	-4.33413	1.48129	-0.48737
H	-3.97650	1.39593	1.26529
H	-5.64563	1.02988	0.67351
H	-3.28281	-2.53409	-2.05029
H	-4.69720	-2.51469	-0.96276
H	-2.68276	-4.83020	-1.13488
C	-4.32561	-4.91003	0.23188
H	-5.56195	-4.58264	-2.14795
C	-3.95652	-4.70388	-3.60985
C	-0.68834	-1.62047	2.18878
O	-1.83004	-1.39946	2.58250
O	0.38941	-1.57819	3.02955
C	0.08740	-1.07665	4.35131
H	-0.57877	-1.76967	4.88177
H	1.05609	-0.99494	4.85462
H	-0.39391	-0.09365	4.27883
O	-3.70628	-6.03910	0.67500
O	-5.28613	-4.40443	0.78129
C	-4.30821	-6.61645	1.86257
H	-4.55094	-5.21368	-4.38295
H	-3.95978	-3.63039	-3.84739
H	-2.92024	-5.06953	-3.68646
H	-3.70632	-7.50113	2.08889
H	-4.27691	-5.89594	2.68847

H	-5.35083	-6.89071	1.66100
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3-meso

3E-cis

3E-isom

3E-trans

4E-inser

4E-KP

4E

3-meso

E = -16.32160953 a.u.

Pd	0.00000	0.00000	0.00000
P	2.30544	0.00000	0.00000
C	3.15439	-0.16667	1.62750
C	3.13133	-1.20960	-1.12203
C	3.03685	1.58693	-0.65692
C	2.60801	-1.36163	-2.42747
O	1.51510	-0.61024	-2.71684
C	1.02874	-0.60406	-4.06446
H	0.66074	-1.59957	-4.35392
H	1.81592	-0.27245	-4.75747
H	0.20431	0.11543	-4.06806
C	3.22417	-2.22704	-3.33614
H	2.82690	-2.34484	-4.34197
C	4.36598	-2.93272	-2.95852

H	4.84008	-3.60100	-3.67841
C	4.90486	-2.77659	-1.68455
H	5.80974	-3.31101	-1.39641
C	4.28477	-1.91688	-0.77754
H	4.72302	-1.77428	0.20918
C	3.23738	-1.39777	2.31838
O	2.79643	-2.49867	1.65029
C	2.79216	-3.75069	2.34220
H	3.81162	-4.04400	2.63581
H	2.13569	-3.69985	3.22283
H	2.39878	-4.47868	1.62465
C	3.78096	-1.44621	3.60342
H	3.85716	-2.39358	4.13235
C	4.22275	-0.27671	4.22083
H	4.63975	-0.33090	5.22721
C	4.12793	0.94481	3.56337
H	4.45800	1.86471	4.04448
C	3.59521	0.99224	2.27620
H	3.50266	1.95449	1.77416
C	4.33658	1.53885	-1.18021
H	4.88005	0.59565	-1.20223
C	4.95286	2.67997	-1.68674
H	5.96569	2.61155	-2.08397
C	4.27226	3.89370	-1.68973
H	4.74435	4.79042	-2.09316
C	2.97933	3.96030	-1.18066
H	2.41563	4.89332	-1.17517
C	2.35881	2.82140	-0.66365
S	0.68181	3.01993	0.00000
O	0.79958	2.63833	1.41563
O	0.28024	4.38934	-0.31604
O	-0.10466	2.00648	-0.82054
C	-0.24879	-1.94924	0.74561

H	0.72294	-2.45178	0.75502
C	-1.21710	-2.66067	-0.19846
H	-0.86343	-2.50658	-1.23347
H	-1.13173	-3.74960	-0.01734
C	-2.71328	-2.31900	-0.11866
H	-3.15148	-2.81015	0.76569
C	-2.98440	-0.84865	0.08928
C	-3.48278	-2.81144	-1.36759
O	-2.19068	0.08592	-0.04821
C	-3.40467	-4.32474	-1.56245
O	-4.26447	-0.61701	0.40017
H	-4.02734	-4.63514	-2.41484
C	-4.59231	0.77790	0.66366
H	-4.40187	1.38313	-0.22940
H	-3.98065	1.14456	1.49527
H	-5.65434	0.77143	0.92267
H	-3.08474	-2.29477	-2.25982
H	-4.53714	-2.50931	-1.26477
H	-2.37783	-4.66336	-1.76156
H	-3.77002	-4.85345	-0.66758
C	-0.72565	-1.68709	2.12774
O	-1.89275	-1.52851	2.47799
O	0.31338	-1.60068	3.01155
C	-0.06288	-1.13408	4.32662
H	-0.71275	-1.86640	4.82332
H	0.88116	-1.01092	4.86685
H	-0.58909	-0.17484	4.24816

3E-cis

E= -17.48945993 a.u.

Pd	0.00000	0.00000	0.00000
P	2.40144	0.00000	0.00000
C	3.09205	1.44683	-0.93594

C	2.46914	2.70952	-0.90933
S	0.92909	3.00071	0.00000
O	-0.03442	2.05520	-0.72810
O	1.18527	2.55930	1.37695
O	0.56678	4.39533	-0.23744
C	3.10763	0.02366	1.69568
C	3.19675	-1.43467	-0.82878
C	3.00354	3.77483	-1.63505
C	4.14712	3.59582	-2.40724
C	4.75331	2.34328	-2.46473
C	4.22925	1.28006	-1.73551
C	-0.03236	-2.06228	0.58184
H	2.49195	4.73602	-1.58642
H	4.55661	4.43374	-2.97277
H	5.64004	2.18844	-3.08015
H	4.71760	0.30756	-1.78159
H	0.93378	-2.23991	1.07101
C	-1.12525	-2.22568	1.57654
C	-2.24385	0.01368	-0.54881
H	-2.57795	-1.02063	-0.64724
H	-2.18460	0.63171	-1.44795
C	-2.13167	0.58134	0.69043
H	-1.96815	1.65413	0.80598
H	-2.37461	0.00769	1.58564
C	-0.22256	-2.91978	-0.65885
H	0.52533	-2.66144	-1.42012
H	-1.21478	-2.72626	-1.09338
C	-0.11398	-4.44412	-0.39519
H	-0.87509	-4.74341	0.34506
C	1.28338	-4.86132	0.10792
C	-0.41258	-5.17169	-1.69263
C	4.13445	-2.25962	-0.20445
C	4.69400	-3.34759	-0.87545

C	4.30366	-3.62222	-2.18304
C	3.35204	-2.82939	-2.82312
C	2.79794	-1.73733	-2.15234
H	4.43625	-2.04725	0.82086
H	5.43032	-3.97529	-0.37413
H	4.73110	-4.47131	-2.71795
H	3.03703	-3.07534	-3.83482
O	1.86588	-0.90403	-2.68286
C	4.46629	0.29869	1.97387
C	4.91227	0.34534	3.29776
C	4.02250	0.11053	4.34386
C	2.68399	-0.16476	4.08485
C	2.23506	-0.19258	2.76694
O	5.28255	0.47758	0.90263
H	5.95444	0.56367	3.51919
H	4.38809	0.15075	5.37055
H	1.98403	-0.33786	4.90085
H	1.18130	-0.37372	2.56509
C	6.60104	0.98528	1.14064
H	7.02354	1.17550	0.14852
H	6.55583	1.92477	1.70984
H	7.21949	0.24535	1.67042
C	1.38442	-1.18138	-4.00749
H	0.64700	-0.39955	-4.21272
H	2.20506	-1.11635	-4.73696
H	0.90941	-2.17236	-4.04544
C	1.39815	-6.33532	0.49700
H	2.02127	-4.61481	-0.67492
H	1.53100	-4.24231	0.98485
O	-0.70710	-1.91099	2.84708
O	-2.26929	-2.58944	1.33746
C	-1.72505	-2.05901	3.86181
H	-1.23753	-1.79009	4.80358

H	-2.57332	-1.39199	3.66272
H	-2.08727	-3.09451	3.89096
H	2.40917	-6.55402	0.87172
H	0.67769	-6.59163	1.29006
H	1.20204	-7.00119	-0.35682
O	-0.01345	-4.83562	-2.79554
O	-1.16694	-6.28366	-1.47715
C	-1.44148	-7.06157	-2.66842
H	-2.03033	-7.91641	-2.32354
H	-2.00776	-6.46045	-3.39020
H	-0.50313	-7.39150	-3.13106

3E-isom

E = -17,47352517 a.u.

Pd	0.00000	0.00000	0.00000
P	2.57406	0.00000	0.00000
C	3.16929	1.46272	0.98937
C	2.51088	2.70614	0.94304
S	0.98520	2.92431	0.00000
O	0.02792	2.01533	0.78291
O	1.27591	2.39242	-1.33956
O	0.60454	4.32651	0.13432
C	3.68903	0.07193	-1.47374
C	3.31539	-1.37584	0.99397
C	2.98990	3.79367	1.67185
C	4.11887	3.65594	2.47437
C	4.76248	2.42475	2.55445
C	4.29221	1.33965	1.81730
C	-1.93118	-0.06375	0.95120
H	2.45200	4.73887	1.59765
H	4.48875	4.50940	3.04374
H	5.63814	2.30168	3.19214
H	4.81075	0.38439	1.89101

C	-3.08121	0.40634	0.13435
H	-1.65038	0.69628	1.69122
C	-0.08829	-1.98460	-1.02685
H	0.93322	-2.17680	-1.34995
H	-0.53510	-2.71766	-0.35383
C	-0.87937	-1.07734	-1.71447
H	-1.96738	-1.07510	-1.60394
H	-0.47334	-0.50983	-2.55709
C	-2.10246	-1.45608	1.51418
C	4.50738	-2.01539	0.64748
C	5.05809	-3.01328	1.45314
C	4.40125	-3.38973	2.62082
C	3.20876	-2.76983	2.99268
C	2.66952	-1.75856	2.19191
H	5.03658	-1.70442	-0.25358
H	6.00057	-3.48226	1.17124
H	4.81774	-4.16847	3.26123
H	2.70763	-3.07391	3.90904
O	1.54323	-1.06461	2.50970
C	4.45441	1.20961	-1.74081
C	5.26543	1.29056	-2.87261
C	5.31421	0.22190	-3.75946
C	4.55368	-0.92358	-3.52451
C	3.73731	-0.99808	-2.39507
H	4.41896	2.05153	-1.05095
H	5.85273	2.19005	-3.05278
H	5.94474	0.26879	-4.64775
H	4.59782	-1.75000	-4.22985
O	2.97688	-2.09100	-2.08838
C	0.95729	-1.28530	3.80450
H	0.18049	-0.52098	3.90051
H	1.70975	-1.14481	4.59488
H	0.49972	-2.28271	3.86782

C	3.06132	-3.23277	-2.94960
H	2.42470	-3.99517	-2.48902
H	4.09542	-3.60375	-3.00627
H	2.68731	-2.99347	-3.95578
O	-3.26402	1.74731	0.27167
O	-3.80823	-0.30742	-0.54963
C	-4.38446	2.28919	-0.46407
C	-3.21517	-1.59220	2.59743
H	-1.15922	-1.79063	1.96973
H	-2.36110	-2.15384	0.70214
C	-3.03491	-2.95539	3.24107
H	-4.20083	-1.55861	2.10409
C	-3.15786	-0.50901	3.68936
H	-4.33469	3.36978	-0.30291
H	-5.32532	1.87860	-0.07492
H	-4.29769	2.04659	-1.52971
O	-4.14937	-3.72427	3.14004
O	-2.01072	-3.32625	3.79278
C	-4.01795	-5.03819	3.74211
C	-4.26745	-0.64686	4.73186
H	-3.23410	0.47800	3.20618
H	-2.17211	-0.55846	4.18223
H	-4.99014	-5.51836	3.59947
H	-3.77594	-4.94299	4.80758
H	-3.22203	-5.60235	3.24028
H	-4.20777	0.16439	5.47243
H	-4.19769	-1.60231	5.27526
H	-5.26038	-0.60147	4.25710

3E-trans

E = -17.48039179 a.u.

Pd	0.00000	0.00000	0.00000
P	2.47144	0.00000	0.00000

C	3.20683	1.44673	-0.88768
C	2.56551	2.70017	-0.87019
S	0.99364	2.96729	0.00000
O	0.03081	2.02753	-0.74526
O	1.21699	2.50681	1.37755
O	0.63452	4.36197	-0.23323
C	3.25233	-0.06558	1.66201
C	3.11639	-1.45303	-0.92100
C	3.11953	3.78206	-1.55520
C	4.30107	3.62583	-2.27476
C	4.92508	2.38166	-2.32337
C	4.38005	1.30084	-1.63607
C	-2.13228	0.32989	0.01189
H	2.59984	4.73910	-1.51456
H	4.72863	4.47719	-2.80568
H	5.84202	2.24888	-2.89834
H	4.86763	0.32835	-1.68102
H	-2.14930	1.07708	-0.79227
C	-2.88892	-0.88468	-0.35616
C	-0.13759	-2.21187	-0.17622
H	0.82266	-2.55339	-0.56885
H	-1.00986	-2.41202	-0.80037
C	-0.28390	-1.88341	1.15895
H	-1.28138	-1.82939	1.60145
H	0.56374	-1.96320	1.84340
C	-2.47838	0.87790	1.38198
H	-1.72388	1.60347	1.72417
H	-2.50617	0.05217	2.10823
C	-3.86313	1.58534	1.38663
C	-4.35927	1.68081	2.81665
C	-3.78294	2.99537	0.77165
H	-4.58553	0.97360	0.81982
O	-2.98426	-1.03166	-1.72103

C	-3.72707	-2.19856	-2.13614
H	-3.70085	-2.18443	-3.23006
H	-3.26552	-3.11527	-1.74635
H	-4.76075	-2.14417	-1.77071
O	-3.36721	-1.70126	0.42275
C	-5.14937	3.63960	0.54130
H	-3.16827	3.62385	1.43883
H	-3.23875	2.92775	-0.18423
H	-5.03737	4.64661	0.11295
H	-5.75679	3.03819	-0.15416
H	-5.71632	3.73318	1.48071
C	4.64822	-0.10710	1.88533
C	5.14645	-0.12306	3.19126
C	4.27070	-0.08015	4.27470
C	2.89628	-0.01279	4.07264
C	2.40117	0.00272	2.77123
O	5.43913	-0.14627	0.78023
H	6.21818	-0.15834	3.37231
H	4.67874	-0.08721	5.28601
H	2.21113	0.05001	4.91698
H	1.33171	0.11180	2.60270
C	3.82915	-2.49809	-0.32980
C	4.16272	-3.64342	-1.05560
C	3.78100	-3.74727	-2.39009
C	3.05107	-2.72703	-3.00211
C	2.70578	-1.59029	-2.26923
H	4.12263	-2.42160	0.71701
H	4.71837	-4.44844	-0.57547
H	4.04090	-4.63449	-2.96864
H	2.74465	-2.82936	-4.04134
O	1.95176	-0.56668	-2.74535
C	1.50696	-0.61191	-4.10636
H	0.94181	0.31332	-4.25295

H	2.36506	-0.63951	-4.79385
H	0.85389	-1.48056	-4.27425
C	6.85676	-0.06047	0.96692
H	7.28427	-0.04695	-0.04087
H	7.12253	0.86630	1.49550
H	7.23638	-0.93573	1.51498
O	-5.65328	1.26453	2.92593
O	-3.70053	2.08402	3.75801
C	-6.18849	1.34017	4.27016
H	-7.21713	0.97625	4.19121
H	-5.59961	0.70826	4.94642
H	-6.16366	2.37517	4.63262

3E-insert

E = -17.45304088 a.u.

Pd	0.00000	0.00000	0.00000
P	2.33877	0.00000	0.00000
C	3.11507	-1.46915	-0.79414
C	3.27382	0.18866	1.57841
C	2.97961	1.39508	-1.03695
C	2.57148	-1.93365	-2.01607
O	1.53741	-1.20786	-2.50830
C	0.90245	-1.63863	-3.71995
H	1.59409	-1.54597	-4.57045
H	0.04615	-0.96907	-3.84561
H	0.55051	-2.67666	-3.62820
C	3.10843	-3.06359	-2.63867
H	2.70083	-3.41976	-3.58256
C	4.18610	-3.73041	-2.05492
H	4.59980	-4.60814	-2.55316
C	4.73561	-3.28013	-0.85802
H	5.58473	-3.79511	-0.40952
C	4.19544	-2.15348	-0.23573

H	4.63256	-1.79009	0.69460
C	3.13180	-0.73944	2.63418
O	2.33722	-1.82380	2.39013
C	2.19599	-2.79428	3.43469
H	1.73089	-2.34655	4.32512
H	3.17015	-3.23436	3.69520
H	1.54263	-3.57334	3.02800
C	3.80511	-0.54182	3.84120
H	3.70023	-1.25472	4.65551
C	4.61130	0.58251	4.01448
H	5.12354	0.72776	4.96605
C	4.75361	1.50953	2.98899
H	5.37149	2.39660	3.12185
C	4.08329	1.30886	1.78425
H	4.18306	2.04839	0.99161
C	4.09457	1.18321	-1.85756
H	4.58945	0.21219	-1.85875
C	4.58608	2.19848	-2.67533
H	5.45768	2.00919	-3.30222
C	3.96414	3.44288	-2.68806
H	4.34005	4.24039	-3.33015
C	2.85519	3.67172	-1.87713
H	2.34877	4.63695	-1.86304
C	2.35869	2.66150	-1.05393
S	0.93226	3.06678	0.00000
O	1.36383	2.72144	1.35939
O	0.59159	4.45669	-0.29524
O	-0.14400	2.11948	-0.52439
C	-1.49450	-1.78192	0.60069
C	-2.38991	0.10412	-0.00783
H	-1.89857	1.07560	-0.16761
C	-2.89009	-0.36369	-1.32850
C	-3.32607	0.17001	1.18236

H	-2.72899	0.33657	2.09317
H	-3.85691	-0.78450	1.31943
C	-4.37284	1.30062	1.12206
H	-5.05041	1.13322	0.26606
C	-5.23091	1.20528	2.37532
C	-3.76307	2.72551	0.99322
O	-2.25689	-0.32280	-2.37320
O	-4.14942	-0.89092	-1.24466
C	-4.68324	-1.35349	-2.50843
H	-4.73425	-0.52327	-3.22356
H	-5.68298	-1.73334	-2.27778
H	-4.04808	-2.14609	-2.92337
C	-0.12981	-2.06967	0.32516
H	-1.78209	-1.66191	1.64682
H	-2.26338	-2.24325	-0.02412
H	0.53669	-2.26438	1.16579
H	0.12496	-2.58674	-0.60550
O	-4.97657	0.54227	3.36459
O	-6.34035	1.98624	2.26363
C	-7.17243	2.00445	3.44981
H	-8.00503	2.67112	3.20758
H	-7.53083	0.99314	3.67748
H	-6.60114	2.38506	4.30553
H	-4.35282	3.42150	1.61096
H	-2.74463	2.71612	1.41901
C	-3.72942	3.26061	-0.43880
H	-3.26154	4.25588	-0.46412
H	-3.14584	2.61648	-1.11242
H	-4.75095	3.34665	-0.84319

4E-KP

E = -17.49024538 a.u.

Pd	0.00000	0.00000	0.00000
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P	2.28272	0.00000	0.00000
C	3.09511	-1.41833	-0.84315
C	3.19183	0.15991	1.58960
C	2.88425	1.45234	-0.98220
C	2.60443	-1.82410	-2.10738
O	1.58281	-1.08407	-2.60929
C	1.09160	-1.40056	-3.91746
H	1.88781	-1.28664	-4.66799
H	0.29428	-0.67600	-4.10814
H	0.68413	-2.42183	-3.94722
C	3.18063	-2.91250	-2.76709
H	2.80992	-3.22838	-3.73991
C	4.24793	-3.59387	-2.18224
H	4.69255	-4.43762	-2.71129
C	4.74891	-3.19793	-0.94559
H	5.59387	-3.71942	-0.49689
C	4.16719	-2.11634	-0.28361
H	4.57120	-1.79359	0.67580
C	3.08429	-0.83494	2.58736
O	2.31318	-1.91264	2.27451
C	2.18328	-2.94961	3.25426
H	1.73090	-2.55979	4.17785
H	3.16033	-3.40649	3.47343
H	1.52155	-3.69629	2.80403
C	3.76818	-0.69315	3.79666
H	3.70010	-1.46126	4.56356
C	4.53643	0.44699	4.03098
H	5.05849	0.54917	4.98291
C	4.62987	1.44580	3.06781
H	5.21680	2.34452	3.25301
C	3.95586	1.29898	1.85709
H	4.01841	2.09057	1.11201
C	4.04501	1.29975	-1.75269

H	4.56783	0.34374	-1.76218
C	4.55041	2.35743	-2.50536
H	5.45829	2.21387	-3.09148
C	3.89779	3.58602	-2.50205
H	4.28641	4.41879	-3.08966
C	2.74140	3.75354	-1.74484
H	2.20906	4.70466	-1.71938
C	2.22805	2.70077	-0.98700
S	0.73467	3.04252	0.00000
O	1.12078	2.68324	1.37158
O	0.37590	4.43078	-0.28001
O	-0.27951	2.07263	-0.59240
C	-1.25647	-2.51696	-0.47733
C	-2.53944	-1.63646	-0.48060
H	-2.26762	-0.59794	-0.75144
C	-3.44352	-2.14898	-1.59282
C	-3.28472	-1.67375	0.85765
H	-2.58167	-1.53946	1.69182
H	-3.72429	-2.67787	0.97515
C	-4.39449	-0.61959	0.96152
H	-5.13025	-0.77549	0.15093
C	-5.15694	-0.80306	2.26357
C	-3.88700	0.84216	0.85073
O	-4.13196	-3.14933	-1.51253
O	-3.36005	-1.37522	-2.70782
C	-4.17400	-1.84289	-3.81523
H	-3.85925	-2.84924	-4.11721
H	-4.00966	-1.11930	-4.61854
H	-5.23002	-1.86901	-3.52060
C	-0.14397	-2.01649	0.42839
H	-1.55536	-3.54186	-0.17472
H	-0.88036	-2.59623	-1.51158
H	-0.40500	-2.02423	1.49974

H	0.78267	-2.58316	0.27138
O	-4.77253	-1.42966	3.23377
O	-6.34730	-0.14215	2.21528
C	-7.12920	-0.22495	3.43153
H	-8.03836	0.34847	3.22813
H	-7.36773	-1.27153	3.65692
H	-6.57237	0.20864	4.27113
H	-4.74896	1.51059	1.01023
C	-2.76768	1.19588	1.82694
H	-3.55273	1.02685	-0.18385
H	-2.49246	2.25586	1.73641
H	-3.05462	0.99211	2.87157
H	-1.84329	0.62145	1.63152

4E

E= -17.50649847 **a.u.**

Pd	0.00000	0.00000	0.00000
P	2.28657	0.00000	0.00000
C	3.21701	0.13179	1.58718
C	3.07429	-1.44106	-0.84425
C	2.95385	1.42386	-0.98288
C	2.58696	-1.82198	-2.11751
O	1.59826	-1.04244	-2.62611
C	1.11784	-1.32601	-3.94391
H	0.66077	-2.32583	-3.98895
H	1.93174	-1.24777	-4.68006
H	0.36237	-0.56046	-4.14566
C	3.13020	-2.92639	-2.77866
H	2.75977	-3.22114	-3.75828
C	4.16453	-3.65144	-2.18616
H	4.58284	-4.50902	-2.71466
C	4.66516	-3.28021	-0.94242
H	5.48556	-3.83429	-0.48705

C	4.11391	-2.18152	-0.28034
H	4.51798	-1.88129	0.68627
C	3.08724	-0.85801	2.58622
O	2.30011	-1.92518	2.26945
C	2.14881	-2.95743	3.24723
H	3.11821	-3.42374	3.48199
H	1.68800	-2.56365	4.16557
H	1.48737	-3.69961	2.78846
C	3.76382	-0.72838	3.80073
H	3.67372	-1.49315	4.56870
C	4.55357	0.39640	4.03906
H	5.06944	0.49098	4.99514
C	4.67452	1.38896	3.07339
H	5.27679	2.27705	3.26063
C	4.00562	1.25231	1.85798
H	4.08895	2.04114	1.11210
C	4.11424	1.23585	-1.74529
H	4.61303	0.26686	-1.74325
C	4.64864	2.27284	-2.50643
H	5.55518	2.10129	-3.08725
C	4.02546	3.51709	-2.51861
H	4.43667	4.33384	-3.11349
C	2.87217	3.72105	-1.76565
H	2.36316	4.68509	-1.75068
C	2.33128	2.68893	-0.99765
S	0.85506	3.07359	0.00000
O	1.26315	2.74763	1.37369
O	0.52158	4.46376	-0.30973
O	-0.18493	2.11431	-0.54837
C	-0.11260	-2.03147	0.38585
H	0.80938	-2.53827	0.06934
C	-1.31650	-2.63458	-0.32471
H	-1.31983	-2.36680	-1.39740

H	-1.20242	-3.73564	-0.29691
C	-2.69507	-2.31436	0.27229
H	-2.65725	-2.46762	1.37080
C	-3.02291	-0.84203	0.12167
C	-3.81170	-3.22347	-0.28815
O	-2.20272	0.05512	-0.07964
C	-3.74260	-4.67619	0.19266
O	-4.32327	-0.56011	0.25465
C	-4.67333	-5.60724	-0.62326
C	-4.65549	0.85938	0.19869
H	-4.74150	-6.57233	-0.09617
H	-4.36370	1.27075	-0.77371
H	-4.12638	1.39438	0.99475
H	-5.73840	0.89687	0.34187
H	-3.75564	-3.20156	-1.38891
H	-4.79186	-2.82200	0.00590
H	-2.71913	-5.07900	0.10096
C	-4.12853	-4.76820	1.66236
H	-5.68822	-5.17116	-0.62820
C	-4.19660	-5.85348	-2.05376
H	-0.20543	-2.11102	1.48267
O	-3.71736	-5.95177	2.19382
O	-4.74693	-3.92723	2.28819
C	-4.12601	-6.16042	3.56950
H	-4.88057	-6.54067	-2.57383
H	-4.15296	-4.92593	-2.64301
H	-3.19351	-6.30873	-2.05931
H	-3.71726	-7.13636	3.84620
H	-3.72043	-5.36731	4.20893
H	-5.22043	-6.15804	3.64187

3-meso-4-membered chelate

E= -16.31303952 a.u.

C	-3.283902	2.469771	0.428228
C	-3.004186	1.161921	0.015077
C	-3.977229	0.455348	-0.718983
C	-5.211976	1.047788	-0.984508
C	-5.489428	2.335938	-0.534245
C	-4.520304	3.052411	0.162342
P	-1.389951	0.387208	0.467310
C	-0.257097	1.810953	0.725841
C	0.466009	2.015935	1.904417
C	1.425581	3.025607	1.996321
C	1.664863	3.845804	0.898737
C	0.964337	3.660527	-0.294477
C	0.016976	2.640233	-0.391098
O	-0.686730	2.350135	-1.512925
C	-0.528216	3.189111	-2.663768
S	-3.695089	-1.223515	-1.371308
O	-4.860014	-1.529893	-2.197644
Pd	-0.579876	-0.961057	-1.173347

O	0.833942	-2.121268	-2.523079
C	1.475493	-2.199964	-1.444463
O	2.079146	-3.334653	-1.050023
C	1.917174	-4.458850	-1.960221
O	-2.448577	-1.035254	-2.237155
C	1.445434	-1.070621	-0.516998
C	1.833533	-1.255627	0.927576
C	3.362361	-1.370620	1.204440
C	3.488681	-1.570062	2.704322
C	-1.697952	-0.250178	2.167334
C	-2.181573	0.633877	3.140076
C	-2.507587	0.203855	4.421845
C	-2.371392	-1.146115	4.737812
C	-1.912884	-2.050577	3.786837
C	-1.566214	-1.617708	2.499502
O	-1.091047	-2.454643	1.549424
C	-1.357420	-3.855912	1.696306
O	-3.436174	-2.057464	-0.190193
C	4.143149	-0.137586	0.747082
H	-2.319487	1.683801	2.886213
H	-2.880619	0.914859	5.157932
H	-2.631603	-1.506180	5.733778
H	-1.823780	-3.102796	4.047460
H	0.285177	1.373198	2.766087
H	1.982660	3.158924	2.922994
H	2.409529	4.640471	0.958513
H	1.168481	4.305813	-1.146630
H	-5.941931	0.475588	-1.557027
H	-6.462599	2.783512	-0.739632
H	-4.721563	4.068835	0.501311
H	-2.522101	3.046889	0.954215
H	-1.065083	-4.306501	0.742864
H	-0.757170	-4.289623	2.510211

H	-2.430384	-4.021910	1.865229
H	-1.218447	2.783246	-3.409380
H	-0.801776	4.227669	-2.426268
H	0.503100	3.142047	-3.042135
H	1.793871	-0.142457	-0.992173
H	1.473905	-0.387442	1.502635
H	1.335740	-2.148805	1.332048
H	3.739826	-2.276376	0.700744
H	2.428288	-5.293213	-1.472374
H	0.852829	-4.674356	-2.108055
H	2.379678	-4.225691	-2.926584
C	5.648875	-0.250321	0.985288
H	3.954247	0.011192	-0.328361
H	3.743038	0.744974	1.274164
H	6.171489	0.645484	0.617968
H	5.871217	-0.351623	2.058146
H	6.068581	-1.124020	0.460719
O	3.352765	-2.884439	3.038287
O	3.626939	-0.680328	3.523943
C	3.334206	-3.132076	4.466182
H	3.214896	-4.214506	4.569670
H	4.272853	-2.795554	4.922747
H	2.495763	-2.597328	4.929342

3MA-meso-sqpy-6

E = -18.88190039 a.u.

Pd	0.174402	-0.580803	-1.192052
P	1.938892	-0.162116	0.579633
C	3.294802	0.985036	0.070486
C	1.429906	0.532293	2.221145
C	2.700978	-1.779078	1.117150
C	0.389426	-0.101994	2.942150
O	-0.167283	-1.190137	2.346452
C	-1.130000	-1.943145	3.091481
H	-2.025160	-1.338564	3.301465
H	-0.693319	-2.314169	4.031081
H	-1.398230	-2.790537	2.453418
C	0.020465	0.364261	4.205894
H	-0.767966	-0.131501	4.768788
C	0.668621	1.469387	4.758219
H	0.372064	1.821254	5.747377
C	1.682972	2.112598	4.057604
H	2.196755	2.972355	4.487210
C	2.057106	1.638361	2.798332
H	2.869502	2.128591	2.262263
C	2.882168	2.251835	-0.359236
H	1.827796	2.522427	-0.284090

C	3.785292	3.188005	-0.857546
H	3.432772	4.169818	-1.172590
C	5.130555	2.844729	-0.961089
H	5.852763	3.554283	-1.367225
C	5.570092	1.593586	-0.538518
H	6.625885	1.342487	-0.615026
C	4.671009	0.664922	0.002841
O	5.059571	-0.532318	0.494231
C	2.984301	-1.998825	2.469924
H	2.810215	-1.207291	3.197572
C	3.511618	-3.210844	2.909612
H	3.729033	-3.347184	3.969528
C	3.760291	-4.235263	2.001611
H	4.165941	-5.189683	2.339989
C	3.489287	-4.034910	0.650676
H	3.677786	-4.811678	-0.090577
C	2.966038	-2.820589	0.206356
S	2.707863	-2.631157	-1.573709
O	3.473489	-1.435466	-1.938931
O	3.079774	-3.908062	-2.184493
O	1.199113	-2.435000	-1.670680
C	-1.100519	1.124995	-1.085040
C	-0.911808	2.057852	0.060239
C	-1.099213	1.810181	-2.455142
H	-1.365440	1.061684	-3.218698
H	-1.932009	2.542986	-2.435112
C	0.148215	2.581805	-2.911474
H	0.513935	3.168787	-2.050800
C	1.272571	1.635578	-3.270640
C	-0.170814	3.586081	-4.039903
O	1.333177	0.454184	-2.942390
H	-0.901951	4.309747	-3.641400
O	2.245539	2.214190	-3.990870

C	3.388947	1.344706	-4.254834
H	3.071610	0.490758	-4.864570
H	3.799626	0.976735	-3.307622
H	4.101684	1.976891	-4.791838
C	-0.710560	2.949191	-5.320760
H	0.744352	4.153753	-4.267175
H	-2.082008	0.656695	-0.937085
C	-1.486741	-1.848561	-0.543534
C	-1.709016	-1.649355	-1.907593
H	-1.022343	-2.779101	-0.211200
H	-2.033752	-1.264752	0.198276
C	-1.412576	-2.630227	-2.982000
H	-2.381226	-0.862439	-2.253456
C	6.357920	-1.024000	0.144257
H	6.387626	-2.049849	0.527316
H	6.481258	-1.031575	-0.948309
H	7.150519	-0.428075	0.622148
O	-1.729497	1.722915	1.100683
O	-0.194645	3.052155	0.088966
C	-1.699763	2.667595	2.199431
H	-2.360003	2.243961	2.962186
H	-0.678779	2.782071	2.580582
H	-2.072516	3.643306	1.859312
O	-1.135216	-3.860833	-2.494318
O	-1.458597	-2.345696	-4.169637
C	-0.693206	-4.814064	-3.491291
H	-0.643473	-5.773658	-2.969014
H	-1.405499	-4.849405	-4.324189
H	0.299804	-4.521739	-3.854020
H	-0.876375	3.716644	-6.092105
H	0.001243	2.214386	-5.728776
H	-1.668996	2.435085	-5.154237

3E-sqpy-6

E = -17.47432298 a.u.

Pd	0.120262	-0.559380	-1.117597
P	1.909289	-0.146191	0.561105
C	3.273902	0.987469	0.043110
C	1.438886	0.528375	2.220988
C	2.659465	-1.780954	1.066394
C	0.381143	-0.083171	2.936571
O	-0.215221	-1.140938	2.325396
C	-1.250813	-1.827704	3.034335
H	-2.103816	-1.159358	3.225364
H	-0.871154	-2.240430	3.981359
H	-1.561964	-2.646784	2.379160
C	0.035126	0.373510	4.210399
H	-0.768845	-0.102483	4.768355
C	0.727877	1.441995	4.780045
H	0.449724	1.785298	5.777591
C	1.761748	2.060911	4.086299
H	2.308635	2.892912	4.529548
C	2.109483	1.599256	2.814906
H	2.932732	2.072379	2.279571
C	2.870338	2.254498	-0.393701

H	1.818704	2.534881	-0.314412
C	3.780073	3.176434	-0.906821
H	3.435055	4.157664	-1.231268
C	5.120934	2.819184	-1.015375
H	5.847343	3.517586	-1.433316
C	5.551391	1.567833	-0.584114
H	6.603799	1.304598	-0.666510
C	4.645893	0.652709	-0.032298
O	5.023601	-0.548386	0.460543
C	2.948979	-2.031749	2.412339
H	2.780812	-1.257139	3.159131
C	3.477493	-3.254733	2.820858
H	3.700346	-3.415580	3.876144
C	3.721704	-4.258252	1.888725
H	4.130561	-5.219435	2.203438
C	3.439800	-4.028663	0.544535
H	3.620905	-4.789392	-0.215348
C	2.913576	-2.804889	0.133087
S	2.611150	-2.576995	-1.633124
O	3.317463	-1.336635	-1.975694
O	3.020695	-3.814412	-2.294806
O	1.092851	-2.427673	-1.680753
C	-1.153185	1.137984	-0.963597
C	-0.924509	2.086016	0.161026
C	-1.218945	1.841125	-2.326915
H	-1.550046	1.114157	-3.086550
H	-2.030721	2.588102	-2.237356
C	0.010734	2.578379	-2.873692
H	0.466337	3.166990	-2.059466
C	1.060787	1.591299	-3.343287
C	-0.369219	3.562194	-4.005327
O	0.992713	0.375827	-3.197450
C	-1.190462	4.760636	-3.531452

O	2.098613	2.183633	-3.956627
H	-1.359317	5.461618	-4.362821
C	3.164282	1.265262	-4.346614
H	2.789864	0.569596	-5.107335
H	3.503924	0.698114	-3.472636
H	3.951732	1.907196	-4.751201
H	-0.920787	3.010564	-4.788772
H	0.560794	3.922004	-4.469529
H	-2.178346	4.466944	-3.147086
H	-0.666061	5.302286	-2.728827
H	-2.123785	0.658040	-0.778364
C	-1.594496	-1.904263	-0.626469
C	-1.669341	-1.649020	-1.985027
H	-1.067473	-2.789315	-0.264100
H	-2.244823	-1.387723	0.082020
H	-1.200456	-2.324125	-2.702445
H	-2.385288	-0.926016	-2.379457
C	6.315241	-1.054760	0.107833
H	6.334654	-2.080523	0.492174
H	6.436678	-1.064585	-0.985019
H	7.116149	-0.467385	0.582607
O	-1.708534	1.780404	1.236655
O	-0.201987	3.076630	0.143451
C	-1.632013	2.752165	2.309276
H	-2.272511	2.357618	3.103939
H	-0.598065	2.862553	2.655561
H	-2.002161	3.724660	1.956899

E = -1.15478621 a.u.

MA = -2.56344510 a.u.

XII. Full list of authors for ref. [6c] in the manuscript

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