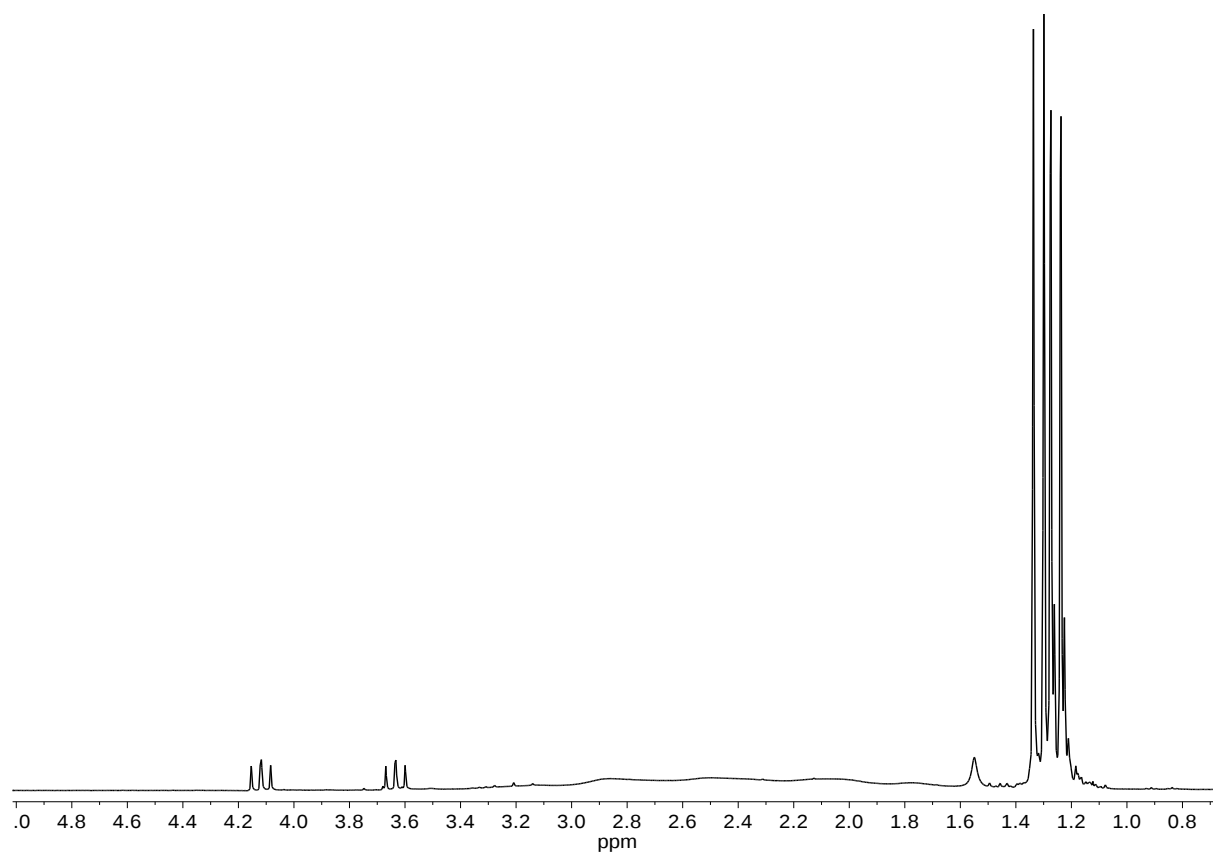


Table of Contents

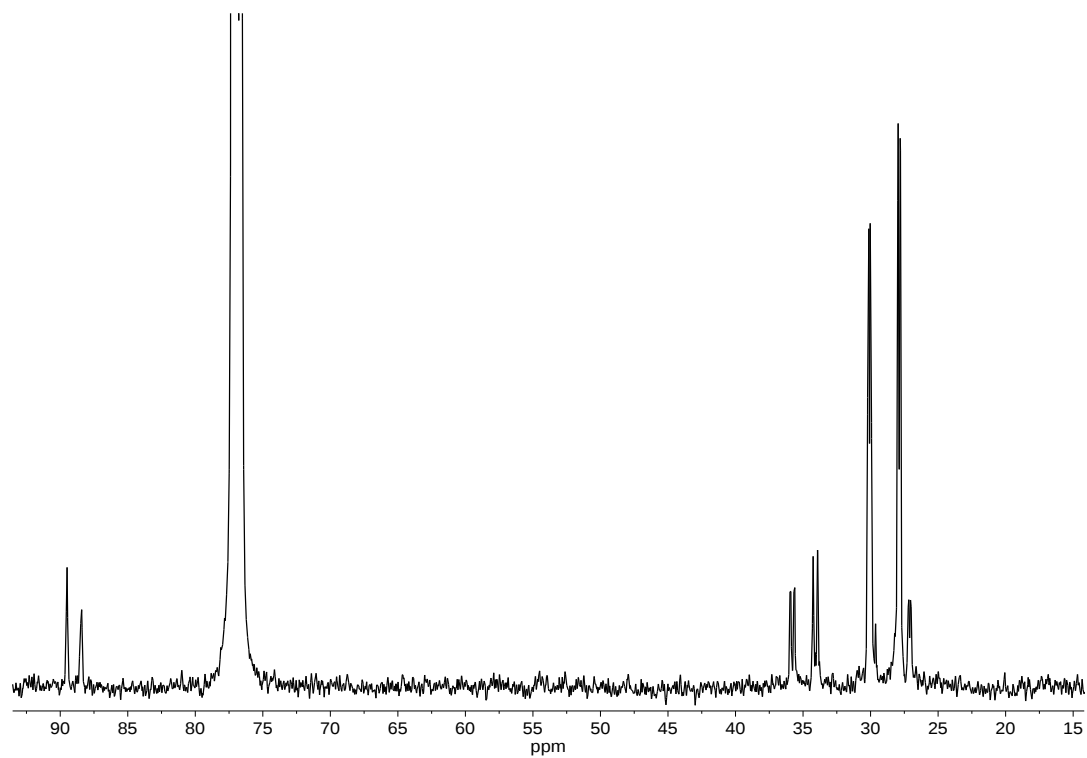
1. NMR Spectra of <i>rac</i> / <i>meso</i> -1-H, <i>meso</i> -1-Cl and <i>meso</i> -3	2
2. Experimental Section	9
2.1 General Methods	9
2.2 Procedures	10
3. Computational Details	12
3.1. General Methods	12
3.2. Mechanism of the Reaction of Diphosphetane 2 with NaOCP	13
3.3. Investigations on the Stereochemistry of Selected Triphospholane Derivatives.....	16
3.4. Trough-space Interactions in <i>meso</i> -3	17
4. NMR Investigations.....	18
4.1. Formation of an Equilibrium Between <i>rac</i> -1-H and <i>meso</i> -1-H.....	18
4.2. Investigations on <i>meso</i> -3.....	19
5. Cartesian coordinates of calculated molecular structures.....	22
References.....	147

1. NMR Spectra of *rac*/*meso*-1-H, *meso*-1-Cl and *meso*-3

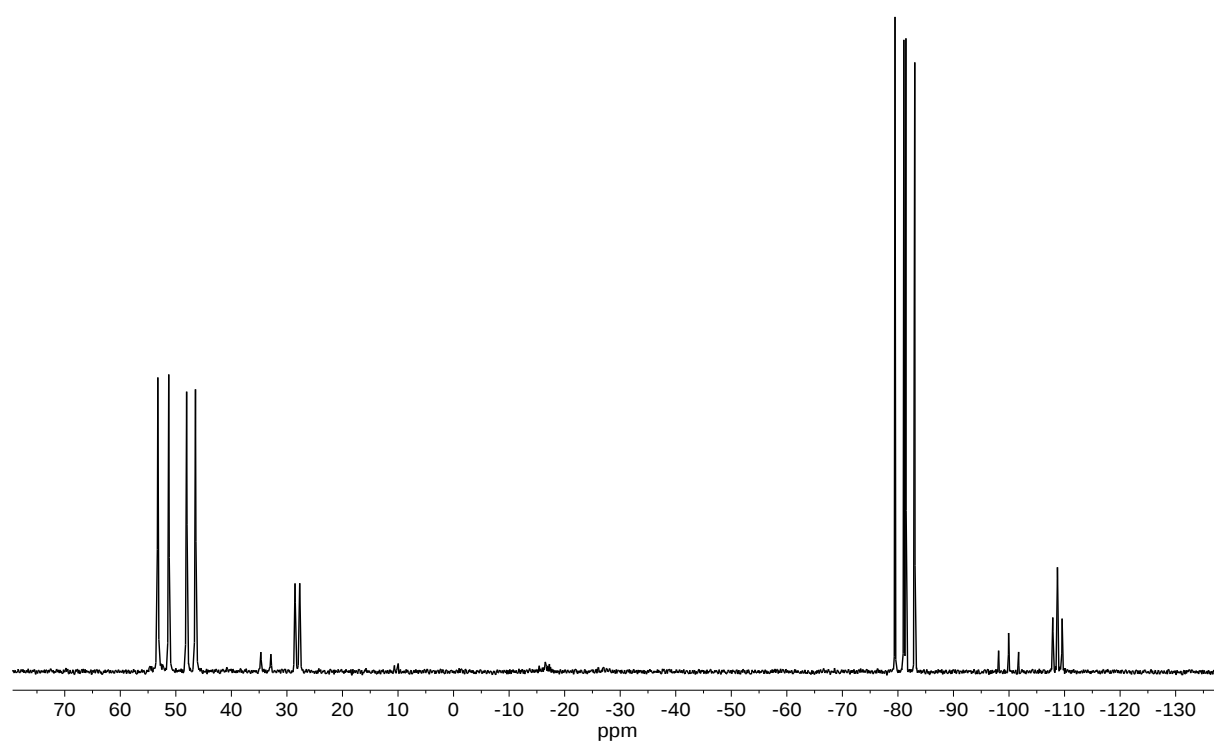
^1H NMR spectrum of *rac*/*meso*-1-H



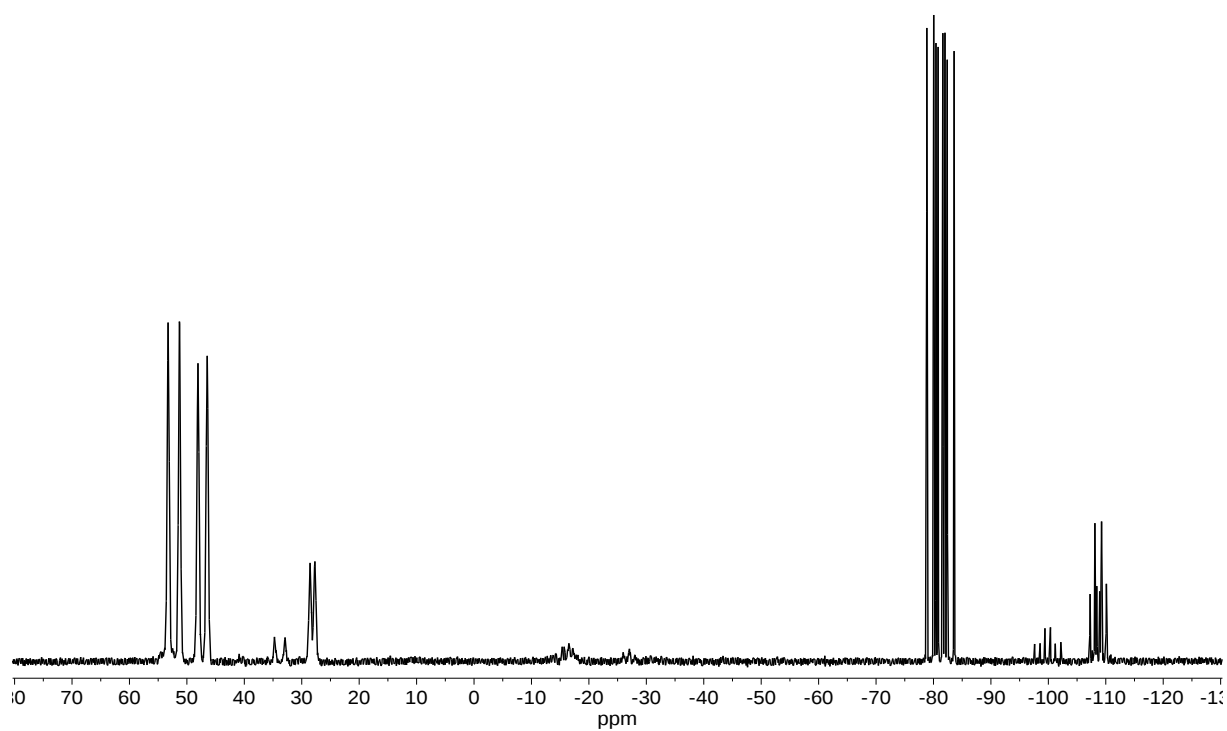
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of *rac*/*meso*-1-H



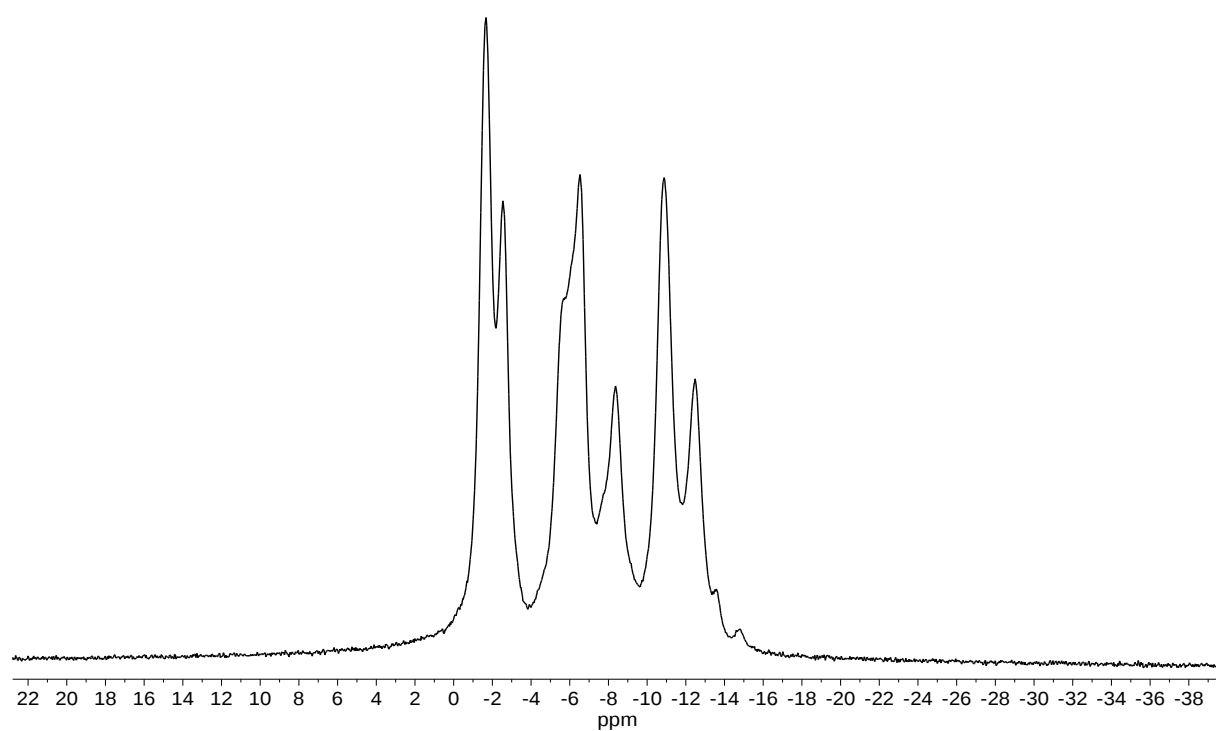
$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of *rac/meso*-1-H



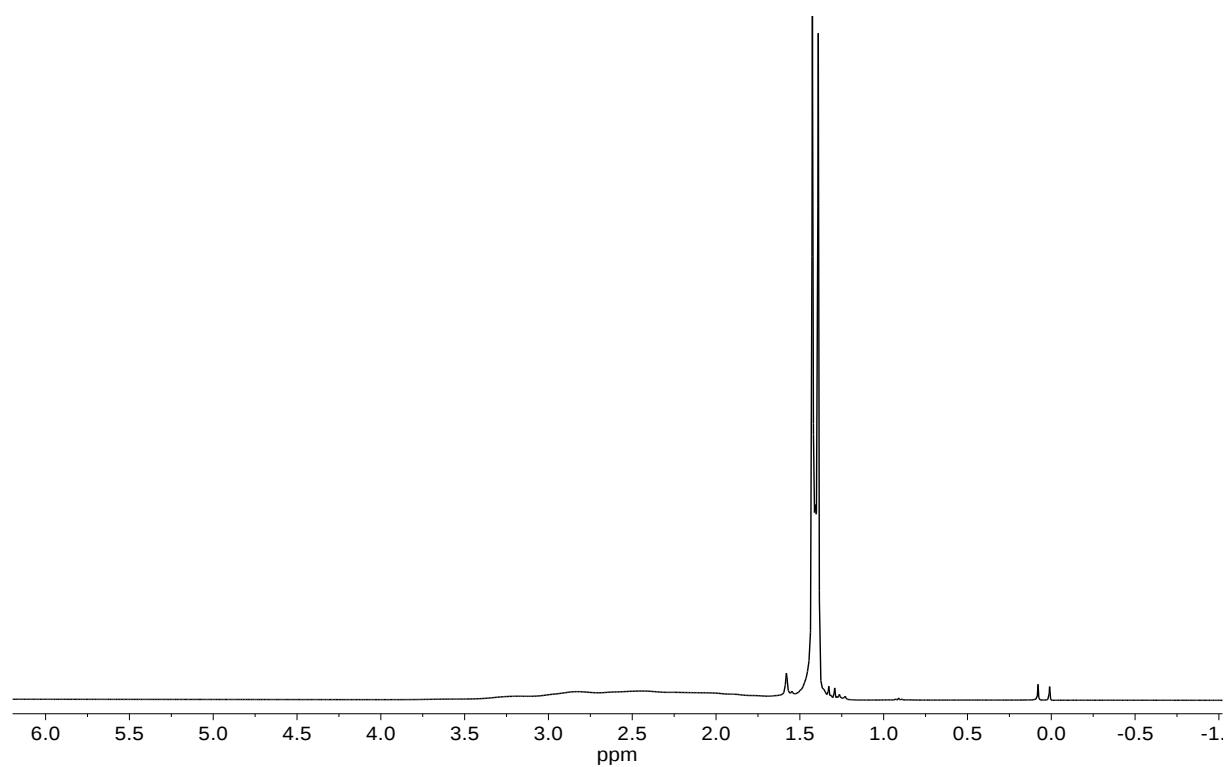
^{31}P NMR spectrum of *rac/meso*-1-H



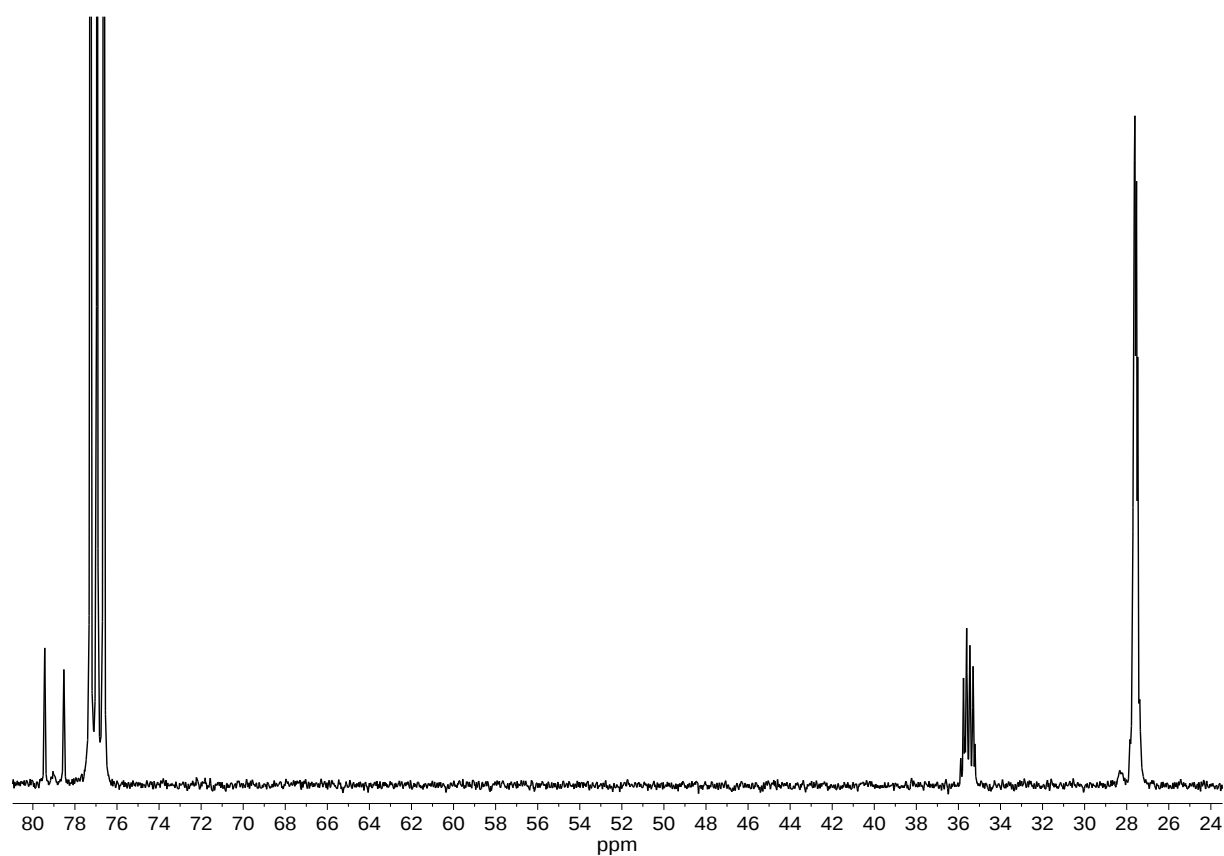
$^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of *rac/meso*-1-H



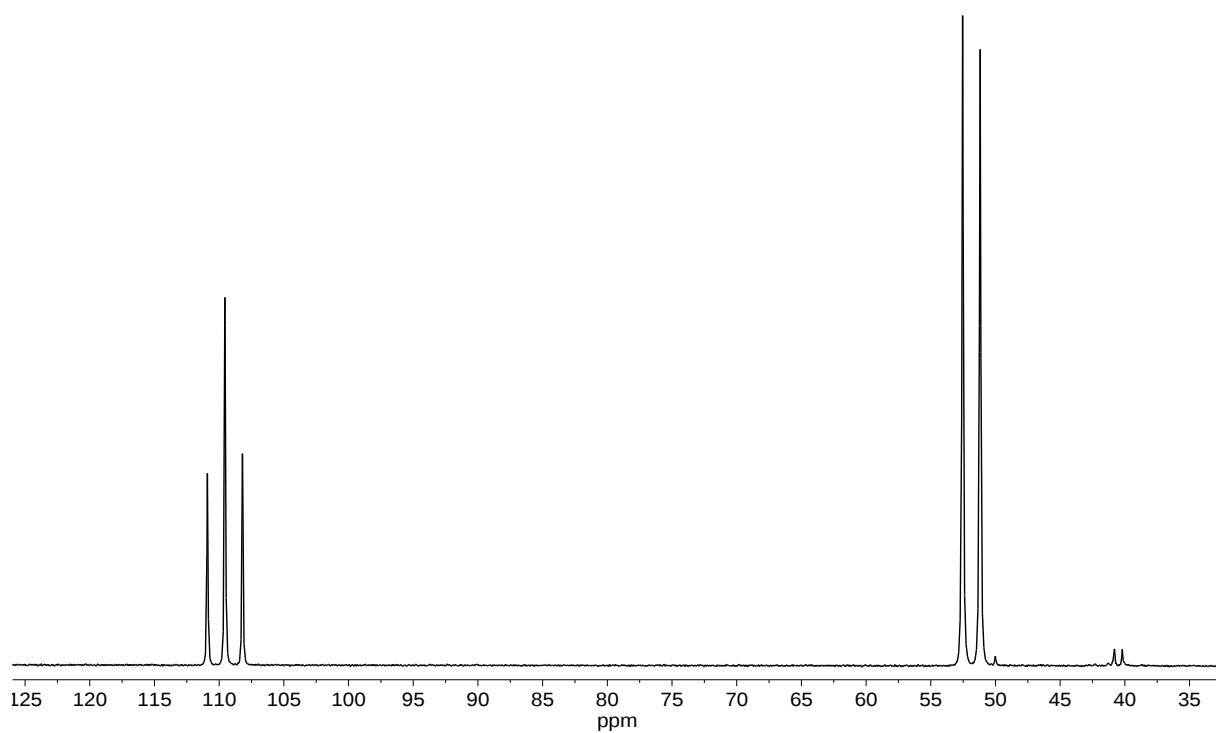
^1H NMR spectrum of *meso*-1-Cl



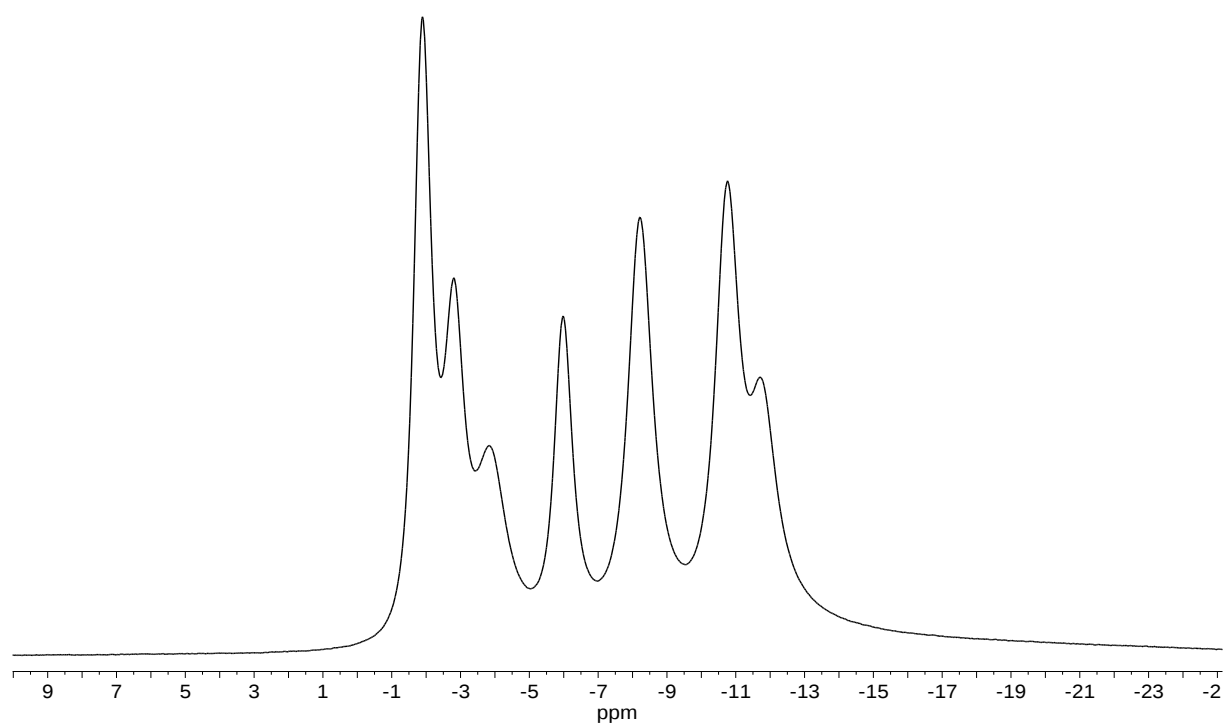
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of *meso*-1-Cl



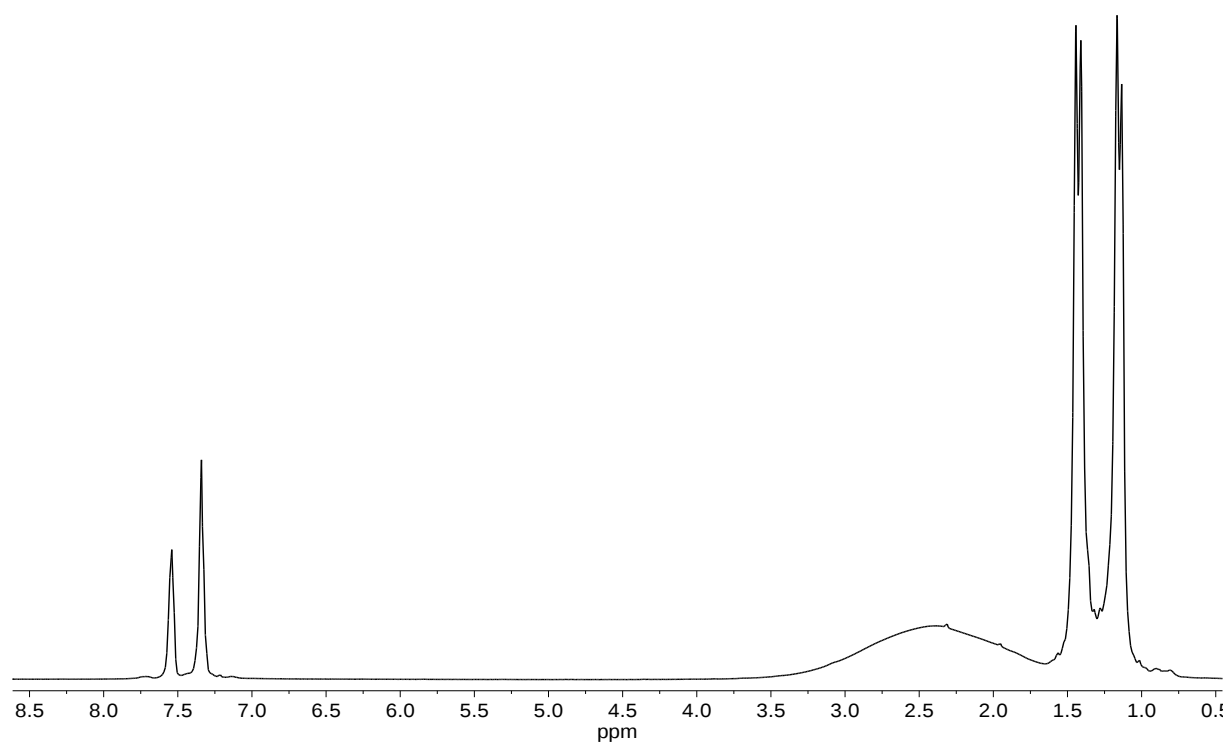
$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of *meso*-1-Cl



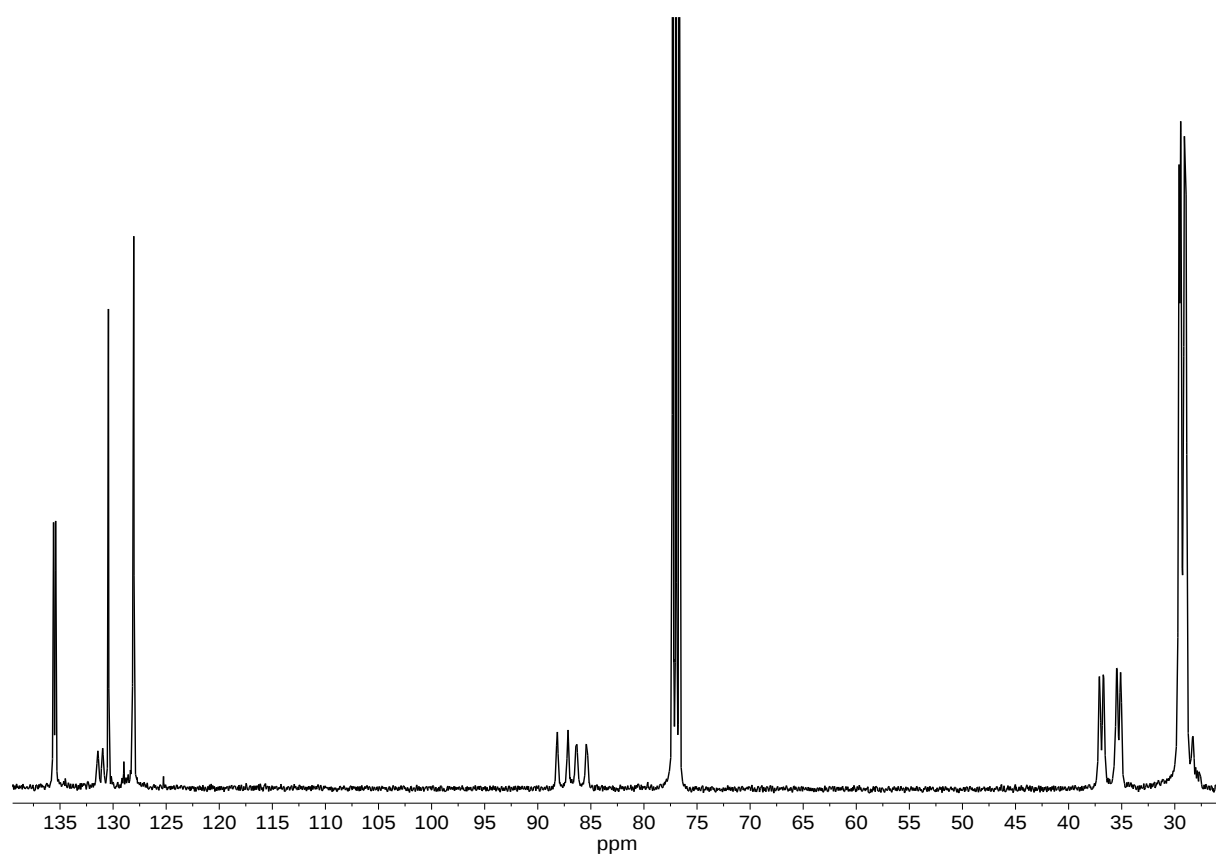
$^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of *meso*-1-Cl



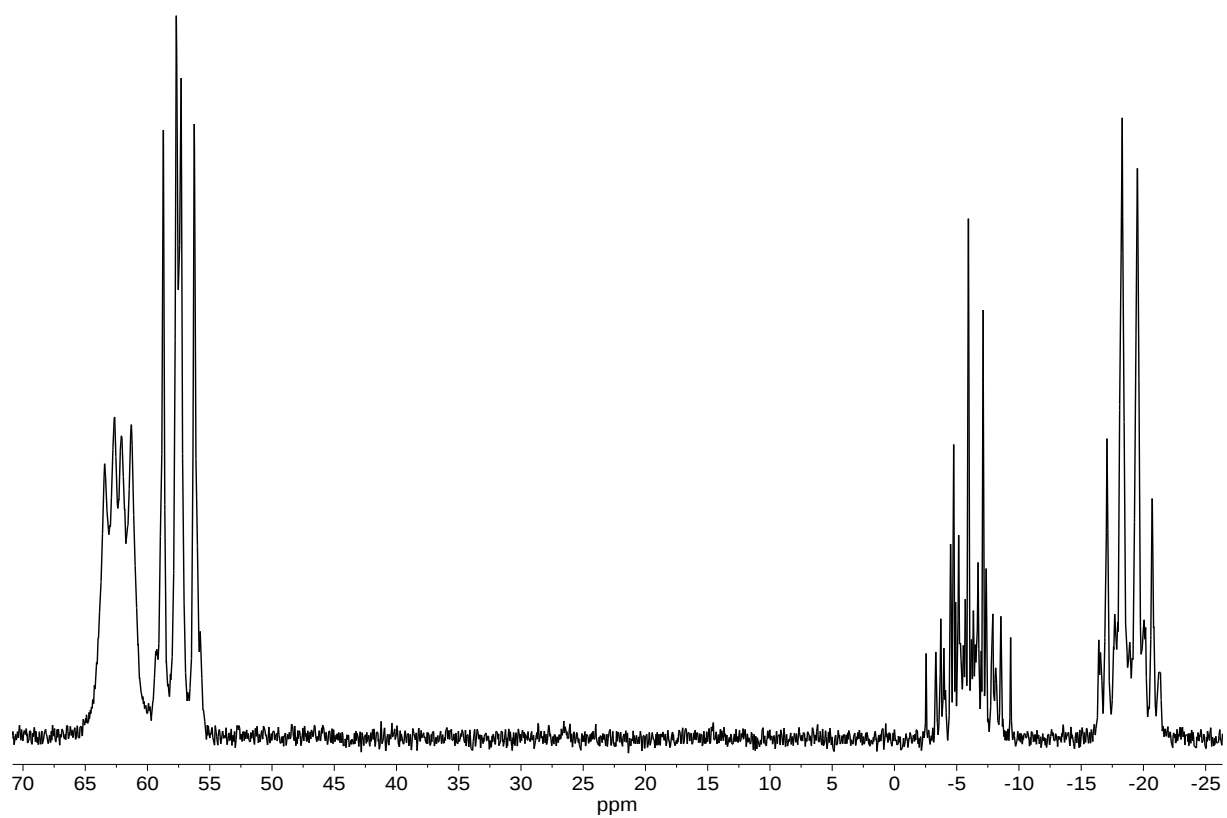
^1H NMR spectrum of *meso*-3



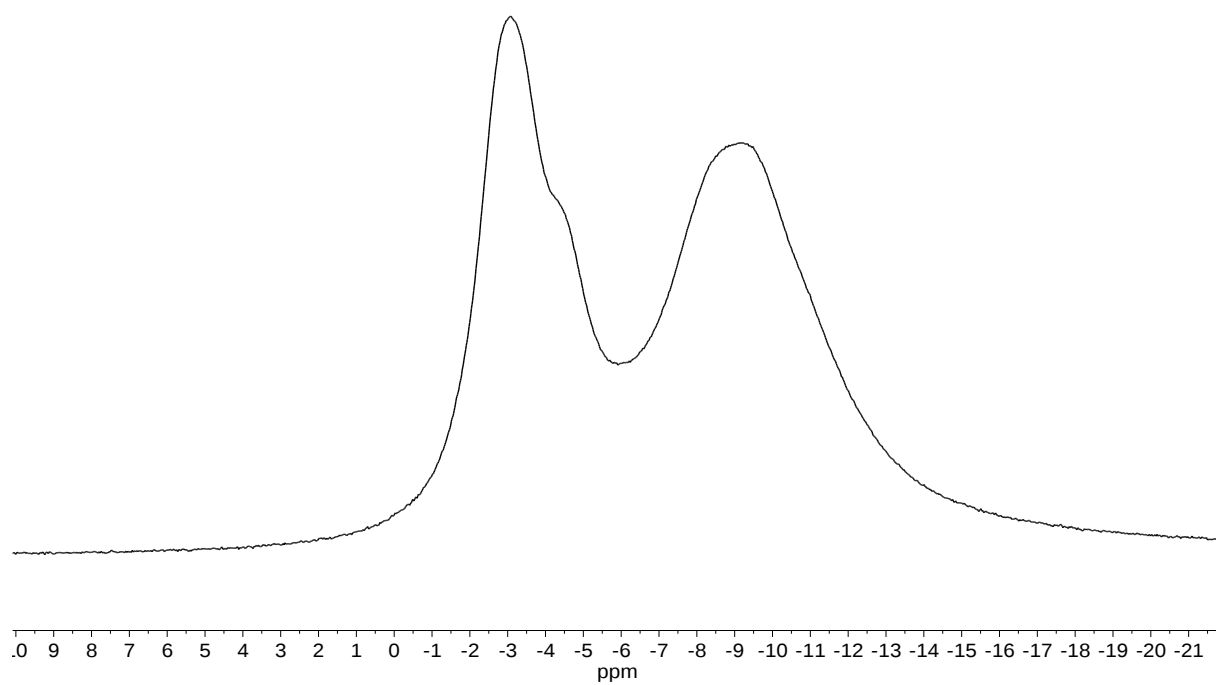
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of *meso*-3



$^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of *meso*-3



$^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of *meso*-**3**



2. Experimental Section

2.1 General Methods

All reactions and manipulations were carried out under a nitrogen atmosphere by using standard Schlenk techniques unless stated otherwise. Solvents were either obtained from an MBraun Solvent Purification System, or dried and stored according to common procedures.^[1] Hexachloroethane, chlorodiphenylphosphane and *n*BuLi are commercially available compounds and were used as obtained (the concentration of *n*BuLi was determined by titration prior to use). Diphosphetane **1** and NaOCP(dioxane)_{2.84} were synthesized according to literature procedures.^[2–3] NMR spectra were recorded with a Bruker AVANCE DRX 400 MHz NMR spectrometer at room temperature in deuterated chloroform. Tetramethylsilane was used as internal standard for ¹H and ¹³C{¹H} NMR spectra. 85% H₃PO₄ was used as external standard for ³¹P{¹H} NMR spectra, and BF₃·OEt₂ was used as external standard for ¹¹B{¹H} NMR spectra. NMR spectra were recorded at the following frequencies: ¹H: 400.13 MHz, ¹³C: 100.63 MHz, ¹¹B: 128.38 MHz, ³¹P: 161.99 MHz. Mass spectra were recorded with a Micromass LCT. Elemental analyses (C, H, and N) were carried out with a Heraeus VARIO EL oven. IR spectra were recorded as KBr disks in the range of 4000–400 cm^{−1} with a PerkinElmer System 2000 IR spectrometer. X-ray diffraction studies were performed with an Oxford Diffraction CCD Xcalibur-S diffractometer using Mo-K α radiation and ω -scan rotation. Data were collected using ω steps accumulating area detector frames (data reduction was carried out with CrysAlis Pro).^[4] All data were corrected for Lorentz polarization and long-term intensity fluctuations. Absorption effects were corrected based on multiple equivalent reflections. Structures were solved by direct methods and refined by full-matrix least-squares techniques against F² by using the SHELX program package.^[5] Hydrogen atoms were assigned riding isotropic displacement parameters and constrained to idealised geometries. Structure figures were generated with DIAMOND.^[6] CCDC 1888315 (*rac*-1-H), 1888316 (*meso*-1-Cl), and 1888317 (*meso*-3) contain the supplementary crystallographic data for this paper. These data are provided free of charge by Cambridge Crystallographic Data Centre.

Compound	<i>rac</i> -1-H	<i>meso</i> -1-Cl·0.5 toluene	<i>meso</i> -3·0.5 toluene
empirical formula	C ₁₀ H ₂₉ B ₁₀ P ₃	C _{13.5} H ₃₂ B ₁₀ ClP ₃	C _{27.50} H ₆₄ B ₂₀ P ₇
formula weight	350.34	430.85	827.77
T [K]	130	130	130
crystal system	Monoclinic	Monoclinic	Triclinic
space group	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> $\bar{1}$
a [Å]	9.9771(4)	28.5977(9)	15.4923(3)
b [Å]	21.9776(7)	12.0510(5)	17.3312(3)

c [Å]	10.1920(4)	16.6081(5)	18.8760(3)
α	90	90	105.834(1)
β	117.372(5)	124.396(3)	104.446(1)
γ	90	90	93.690(1)
V [Å ³]	1984.6(2)	4722.9(3)	4673.8(1)
Z	4	8	4
ρ_{calcd} [g·cm ⁻³]	1.173	1.212	1.176
θ_{max}	30.679	32.301	28.282
F(000)	736	1800	1736
reflns collected	34632	12209	141264
independent reflns	5765	6305	23181
R1/wR2 [$I > 2\sigma(I)$]	6.72 %/15.90 %	4.47 %/9.29 %	3.93 %/8.88 %
R1/wR2 (all data)	9.05 %/17.05 %	7.14 %/10.47 %	5.51 %/9.59 %
Largest diff. peak/hole/(e·Å ⁻³)	0.846/−0.452	0.337/−0.267	0.855/−0.302

2.2 Procedures

Synthesis of 1,3-Di-*tert*-butyl-1,2,3-triphospholane-4,5-dicarba-closo-dodecaborane(12) (*rac*/*meso*-1-H). Diphosphetane **2** (1.44 g, 4.58 mmol, 1.15 eq.) and NaOCP(dioxane)_{2.84} (1.28 g, 3.98 mmol, 1.00 eq) were dissolved in DME (10 mL) and the mixture was stirred for 6 h at room temperature. Afterwards, volatiles were removed *in vacuo* and the residue was washed with *n*-hexane (3 x 5 mL). The resulting red oil was suspended in *n*-hexane (10 mL) and water (1 mL) was added. After stirring for 15 h, the mixture was filtered and the residue was extracted with *n*-hexane (2 x 5 mL). Volatiles were removed from the collected *n*-hexane fractions *in vacuo*. Recrystallisation of the residue by adding acetonitrile to a concentrated toluene solution (4:1 v/v) afforded a mixture of *rac*-1-H and *meso*-1-H (9:1) as an air-stable colourless solid (1.00 g, 72%). Crystals suitable for single-crystal X-ray diffraction experiments were obtained from slow solvent evaporation from an *n*-hexane solution. The reaction can also be carried out using THF instead of DME, which results in higher amounts of *meso*-1-H in the final product. IR (KBr): $\tilde{\nu}$ = 2990 (w, vC-H), 2952 (2, vC-H), 2893 (m, vC-H), 2861 (m, vC-H), 2615 (s, vB-H), 2573 (vs, vB-H), 2302 (w), 2271 (w), 1635 (w), 1459 (s), 1394 (m), 1364 (s), 1261 (w), 1172 (s), 1070 (s), 1012 (m), 934 (w), 875 (w), 798 (m), 733 (m), 673 (w), 626 (w), 578 (w), 555 (w), 471 (w) cm⁻¹. ¹H NMR: δ = 1.29 (d, ³J_{HP} = 14.4 Hz, 2H, *meso*, -CH₃), 1.30 (dd, ³J_{HP} =

14.4 Hz, $^4J_{\text{HP}} = 1.2$ Hz, 9H, *rac*, -CH₃), 1.36 (d, $^3J_{\text{HP}} = 15.2$ Hz, 9H, *rac*, -CH₃), 1.28 – 3.60 (m, 11H, BH), 3.49 (dt, $^1J_{\text{HP}} = 189$ Hz, $^2J_{\text{HP}} = 27.4$ Hz, 0.11H, *meso*, -PH), 3.92 (ddd, $^1J_{\text{HP}} = 194$ Hz, $^2J_{\text{HP}} = 14.7$ Hz, $^2J_{\text{HP}} = 13.2$ Hz, 1H, *rac*, -PH) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR: $\delta = 27.2$ (d, $^2J_{\text{CP}} = 12.2$ Hz, *meso*, -CH₃), 27.9 (dd, $^2J_{\text{CP}} = 16.0$ Hz, $^3J_{\text{CP}} = 3.8$ Hz, *rac*, -CH₃), 30.1 (dd, $^2J_{\text{CP}} = 17.2$ Hz, $^3J_{\text{CP}} = 3.9$ Hz, *rac*, -CH₃), 34.2 (dd, $^1J_{\text{CP}} = 32.5$ Hz, $^2J_{\text{CP}} = 3.8$ Hz, *rac*, -C(CH₃)₃), 35.9 (dd, $^1J_{\text{CP}} = 29.4$ Hz, $^2J_{\text{CP}} = 6.5$ Hz, *rac*, -C(CH₃)₃), 88.5 – 89.5 (m, C_{cluster}) ppm. $^{11}\text{B}\{^1\text{H}\}$ NMR: $\delta = -12.5$ (bs, 1B), -11.0 (bs, 2B), -8.9 (bs, 1B), -6.1 (bs, 3B), -2.6 (bs, 1B), -1.7 (bs, 2B) ppm. $^{31}\text{P}\{^1\text{H}\}$ NMR: $\delta = -108.7$ (t, $^1J_{\text{PP}} = 136$ Hz, *meso*, PH), -99.9 (t, $^1J_{\text{PP}} = 292$ Hz, *meso*, PH), -81.3 (dd, $^1J_{\text{PP}} = 318$ Hz, $^1J_{\text{PP}} = 258$ Hz, *rac*, PH), 28.1 (d, $^1J_{\text{PP}} = 136$ Hz, *meso*, PtBu), 33.8 (d, $^1J_{\text{PP}} = 292$ Hz, *meso*, PtBu), 47.3 (d, $^1J_{\text{PP}} = 258$ Hz, *rac*, PtBu), 52.3 (d, $^1J_{\text{PP}} = 318$ Hz, *rac*, PtBu) ppm. ^{31}P NMR: $\delta = -108.7$ (dt, $^1J_{\text{PP}} = 136$ Hz, $^1J_{\text{PH}} = 188$ Hz, *meso*, PH), -99.9 (dt, $^1J_{\text{PP}} = 292$ Hz, $^1J_{\text{PH}} = 156$ Hz, *meso*, PH), -81.3 (ddd, $^1J_{\text{PP}} = 318$ Hz, $^1J_{\text{PP}} = 258$ Hz, $^1J_{\text{PH}} = 194$ Hz, *rac*, PH), 28.1 (bd, $^1J_{\text{PP}} = 136$ Hz, *meso*, PtBu), 33.8 (bd, $^1J_{\text{PP}} = 292$ Hz, *meso*, PtBu), 47.3 (bd, $^1J_{\text{PP}} = 258$ Hz, *rac*, PtBu), 52.3 (bd, $^1J_{\text{PP}} = 318$ Hz, *rac*, PtBu) ppm. Elemental analysis: C₁₀H₂₉B₁₀P₃, calculated (%): C 31.21; H, 7.33; found (%): C 31.37, H, 7.35.

Synthesis of 2-Chloro-1,3-di-*tert*-butyl-1,2,3-triphospholane-4,5-dicarba-*closo*-dodecaborane(12) (*meso*-1-Cl). Triphospholane **1-H** (235 mg, 0.67 mmol, 1.00 eq.) was dissolved in *n*-hexane and *n*BuLi (0.48 mL of a 1.54 M solution in *n*-hexane, 0.74 mmol, 1.10 eq) was added at 0 °C. The resulting yellow suspension was stirred for 2 h at 0 °C. Afterwards, hexachloroethane (159 mg, 0.67 mmol, 1.00 eq) was added under nitrogen flow, and the reaction mixture was stirred for 15 h whilst being allowed to warm to room temperature slowly. Subsequently, the suspension was filtered through celite to afford a pale-yellow solution. Volatiles were removed *in vacuo* and the resulting solid was recrystallised by layering a concentrated toluene solution with acetonitrile (1:4 v/v) to afford ***meso*-1-Cl** (100 mg, 39% yield) as colourless crystals suitable for single crystal X-ray diffraction experiments. IR (KBr): $\tilde{\nu} = 2997$ (w, $\nu\text{C-H}$), 2955 (m, $\nu\text{C-H}$), 2894 (m, $\nu\text{C-H}$), 2861 (m, $\nu\text{C-H}$), 2632 (m, $\nu\text{B-H}$), 2607 (m, $\nu\text{B-H}$), 2575 (vs, $\nu\text{B-H}$), 1633 (w), 1458 (m), 1394 (w), 1366 (m), 1261 (w), 1171 (m), 1071 (s), 931 (w), 877 (w), 849 (w), 797 (m), 733 (m), 626 (w), 575 (w), 481 (s), 454 (w), 438 (w) cm⁻¹. ^1H NMR: $\delta = 1.39 - 1.42$ (m, 18H, -CH₃), 1.28 – 3.60 (m, 10H, BH) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR: $\delta = 27.4 - 27.8$ (m, -CH₃), 35.2 – 35.9 (m, -C(CH₃)₃), 78.5 – 79.3 (m, C_{cluster}) ppm. $^{11}\text{B}\{^1\text{H}\}$ NMR: $\delta = -11.7$ (bs, 1B), -10.8 (bs, 2B), -8.2 (bs, 2B), -6.0 (bs, 1B), -3.8 (bs, 1B), -2.8 (bs, 1B), -1.9 (bs, 2B) ppm. $^{31}\text{P}\{^1\text{H}\}$ NMR: $\delta = 51.9$ (d, $^1J_{\text{PP}} = 219$ Hz, PtBu), 109.6 (t, $^1J_{\text{PP}} = 219$ Hz, PCl) ppm. Elemental analysis: C₁₀H₂₈B₁₀ClP₃, calculated (%): C 34.28; H, 8.34; found (%): 34.63, H, 8.36.

Synthesis of 2,2'-(Phenylphosphanediyl)bis(1,3-di-*tert*-butyl-1,2,3-triphospholane-4,5-dicarba-*closo*-dodecaborane(12)) (*meso*-3). Triphospholane **1-H** (150 mg, 0.43 mmol, 1.00 eq.) was dissolved in diethyl ether and *n*BuLi (0.28 mL of a 1.56 M solution in *n*-hexane, 0.43 mmol, 1.00 eq) was added at 0 °C. The resulting orange solution was stirred for 2 h at 0 °C. Afterwards, the solution was cooled to -80 °C and dichlorophenylphosphane (0.43 mL of a 0.49 M solution in *n*-hexane, 0.22 mmol, 0.51 eq) was added and the reaction mixture was stirred

for 15 h whilst being allowed to warm to room temperature slowly. Subsequently, the mixture was filtered through celite to afford a pale-yellow solution. Volatiles were removed *in vacuo* and the resulting solid was recrystallised by adding acetonitrile to a concentrated toluene solution (4:1 v/v) to afford **meso-3** as a colourless solid (110 mg, 63%). Crystals suitable for single-crystal X-ray diffraction experiments were obtained from slow solvent evaporation from an *n*-hexane solution. IR (KBr): $\tilde{\nu}$ = 3065 (w, ν C-H), 2995 (m, ν C-H), 2954 (m, ν C-H), 2891 (m, ν C-H), 2859 (m, ν C-H), 2678 (w, ν B-H), 2614 (s, ν B-H), 2583 (vs, ν B-H), 2567 (vs, ν B-H), 2554 (vs, ν B-H), 1631 (w), 1456 (m), 1436 (m), 1390 (w), 1362 (s), 1261 (w), 1207 (w), 1169 (m), 1069 (s), 1020 (m), 931 (w), 876 (w), 842 (w), 799 (m), 736 (s), 695 (m), 628 (w), 573 (w), 495 (w), 477 (w), 462 (w), 435 (w) cm^{-1} . ^1H NMR: δ = 1.15 (d, $^3J_{\text{HP}}$ = 13.7 Hz, 9H, -CH₃), 1.43 (d, $^3J_{\text{HP}}$ = 14.1 Hz, 9H, -CH₃), 1.28 – 3.60 (m, 10H, BH), 7.28 – 7.39 (m, 3H, phenyl-H), 7.51 – 7.59 (m, 2H, phenyl-H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR: δ = 28.4 – 30.1 (m, -CH₃), 35.3 (d, $^1J_{\text{CP}}$ = 37 Hz, -C(CH₃)₃), 36.9 (d, $^1J_{\text{CP}}$ = 38 Hz, -C(CH₃)₃), 85.9 (d, $^1J_{\text{CP}}$ = 92 Hz, C_{cluster}), 87.7 (d, $^1J_{\text{CP}}$ = 101 Hz, C_{cluster}), 128.1 (d, $^2J_{\text{CP}}$ = 7 Hz, *meta*-C in Ph), 130.4 (s, *para*-C in Ph), 131.2 (d, $^1J_{\text{CP}}$ = 46 Hz, *ipso*-C in Ph), 135.5 (dt, $^2J_{\text{CP}}$ = 20 Hz, $^2J_{\text{CP}}$ = 4 Hz, *ortho*-C in Ph) ppm. $^{11}\text{B}\{^1\text{H}\}$ NMR: δ = -13.2 to -6.0 (bs, 6B), -5.2 to -0.8 (m, 4B) ppm. $^{31}\text{P}\{^1\text{H}\}$ NMR: δ = -22.1 to -15.4 (m, *P* in P₃), -9.6 to -2.2 (m, PPh), 55.6 – 59.6 (m, PtBu), 60.3 – 64.4 (m, PtBu) ppm. Elemental analysis: C₂₀H₆₁B₂₀P₇, calculated (%): C 38.71; H, 7.62; found (%): C 38.72 H, 7.64.

3. Computational Details

3.1. General Methods

All calculations except the NBO (natural bond orbital) calculations were carried out with the ORCA program package.^[7,8] All calculations were carried out in the gas phase. Frequency calculations were performed to confirm the nature of stationary points found by geometry optimisations. Density fitting techniques, also called resolution-of-identity approximation (RI), were used for GGA and coupled-cluster calculations (hereby, the Hartree-Fock part of the latter was sped up with the RIJCOSX^[9] approximation). Atom-pairwise dispersion corrections with the Becke-Johnson damping (D3BJ)^[10,11] were used throughout, except for NBO analyses and coupled-cluster calculations. NBO analyses were carried out using the build-in NBO3.1^[12] module of Gaussian09^[13] on the geometries obtained with ORCA (using the same functional and basis set). Relaxed surface scans were carried out to find approximate minima and transition states for the investigation of the reaction between **2** and OCP⁻ (or Na(dme)₂OCP, respectively). Subsequent geometry optimisations were performed to locate the minima and transition states. The same strategy was used to investigate the isomerisation of the compounds **1**, **1-H**, **1-Cl**, **1-Me** and **1-*t*Bu**.

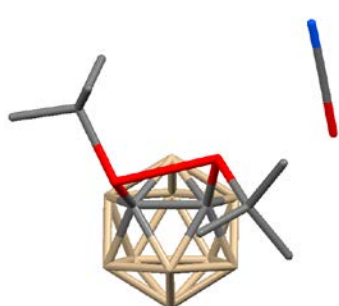
3.2. Mechanism of the Reaction of Diphosphetane **2** with NaOCP

Figure S1 shows the located minima and transition states for the reaction mechanism of diphosphetane **2** with the OCP[−] anion. Here, the reactive van-der-Waals complex (**RC**) between **2** and OCP[−] and the respective transition state leading to the phosphanido-phosphaketene **A** are included (which have been omitted in the main text for clarity). To obtain a more realistic insight, we incorporated counterion effects by including the [Na(dme)₂]⁺ (dme = 1,2 dimethoxyethane) cation into the calculations. To save computational costs, these calculations were carried out at the TPSS-D3BJ/def2-SVP^[10,11,14,15] level of theory. Hereby, initial relaxed surface scans were carried out similarly to the reaction between **2** and OCP[−]. Whilst we were able to locate the phosphanido-phosphaketene [Na(dme)₂]**A**, we have not been able to find either a reactive van-der-Waals complex or a transition state leading to [Na(dme)₂]**A**. However, the subsequent mechanism was calculated to proceed similarly to the one without the counterion included. Finally, the geometries of [Na(dme)₂]**A**, [Na(dme)₂]**B** and [Na(dme)₂]**C** were optimised at the TPSS-D3BJ/def2-TZVP^[10,11,14,15] level of theory (Figure S2) and their energies were calculated at the DLPNO-CCSD(T)/def2-QZVPP^[15-17] level of theory for comparison with the calculations without counterion effects. The calculated energies are summarised in Table S1. Comparing the DFT (TPSS) and *ab initio* (DLPNO-CCSD(T)) results, it is obvious that the *meta*-GGA functional underestimates the kinetic barriers, however, the overall result of the TPSS-D3BJ/def2-TZVP calculations is qualitatively the same. The underestimation of barrier heights is well documented for pure GGA and *meta*-GGA functionals.^[18,19] It is also noteworthy that incorporation of the [Na(dme)₂]⁺ cation rises all transition states in energy, presumably due to steric effects. As for the calculations without counterion effects, transition states [Na(dme)₂]**B** and [Na(dme)₂]**C** have very similar energies and therefore a mixture of *rac*-**1** and *meso*-**1** is predicted by these calculations as well.

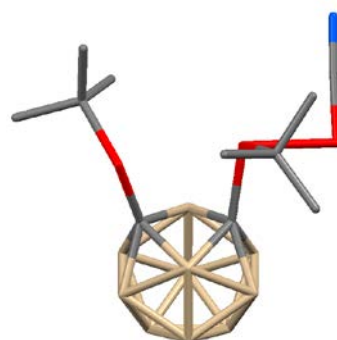
Table S1: Comparison of the energy profile of the reaction mechanism between OCP[−] and diphosphetane **2**. Energies are given in kcal·mol^{−1}.

	TPSS- D3BJ/def2- TZVP	DLPNO- CCSD(T)/def2- QZVPP	TPSS- D3BJ/def2-SVP (+[Na(dme) ₂] ⁺)	TPSS-D3BJ/def2- TZVP (+[Na(dme) ₂] ⁺)	DLPNO- CCSD(T)/def2- QZVPP (+[Na(dme) ₂] ⁺)
RC	1.9	3.3	...	...	...
TS1	6.1	10.1	...	...	...
A	0.0	0.0	0.0	0.0	0.0
B	8.9	11.6	12.7	13.4	18.3
<i>meso</i> - 1 + CO	−1.9	−16.6	2.5	...	...

C	8.3	13.7	10.3	12.4	18.7
D	-8.2	-11.8	-19.2	...	...
E	9.7	9.5	-1.4	...	...
F	-7.3	-11.6	-20.0	...	...
G	6.3	10.6	-0.6	...	...
H	-1.1	-0.9	-6.7	...	...
I	2.3	6.2	9.3	...	...
<i>rac</i>-1 + CO	-2.1	-17.0	-7.7	...	...



RC



TS1

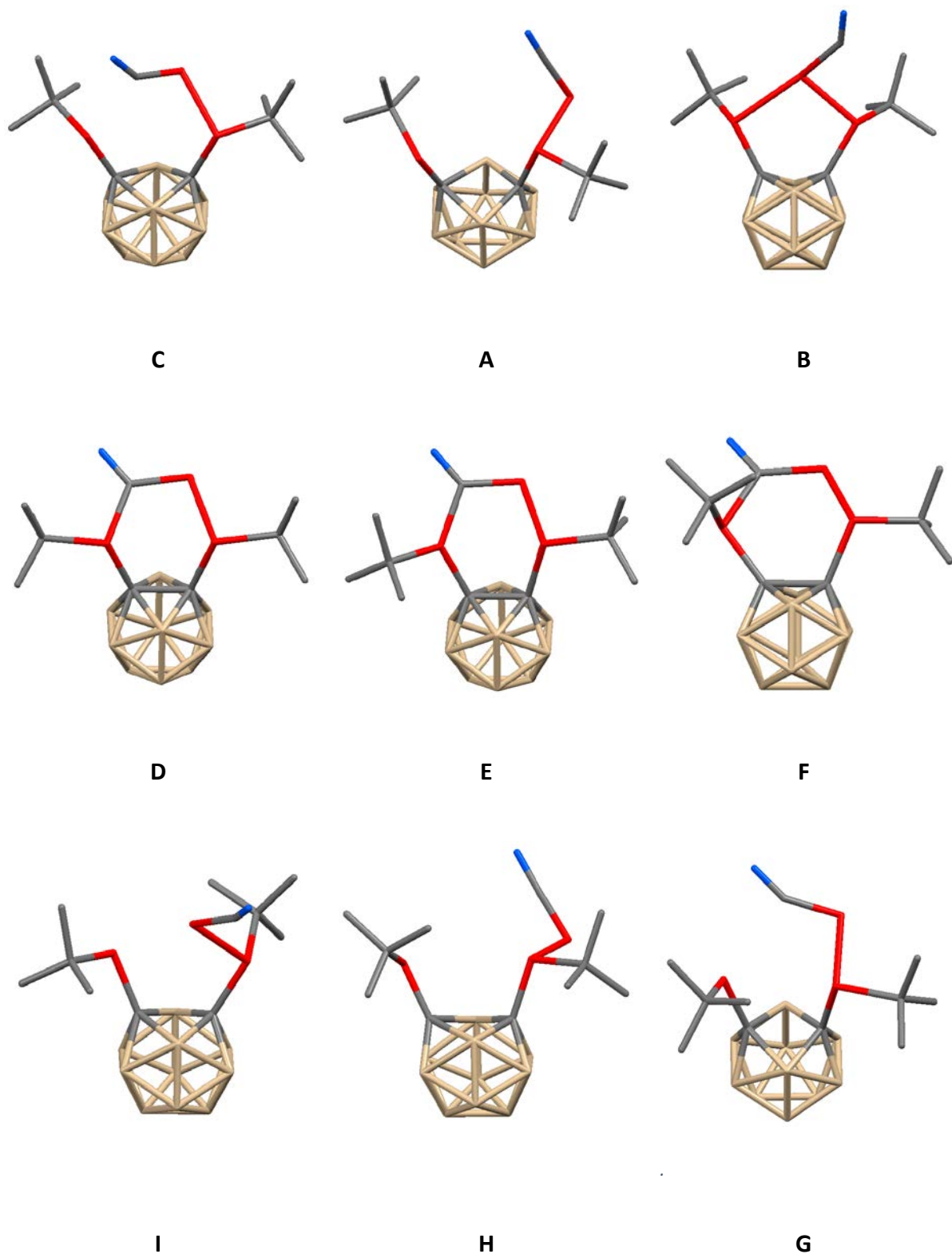


Figure S1: Graphical representation of located transition states and minima for the reaction mechanism between OCP⁻ and diphosphetane 2 at the TPSS-D3BJ/def2-TZVP level of theory.

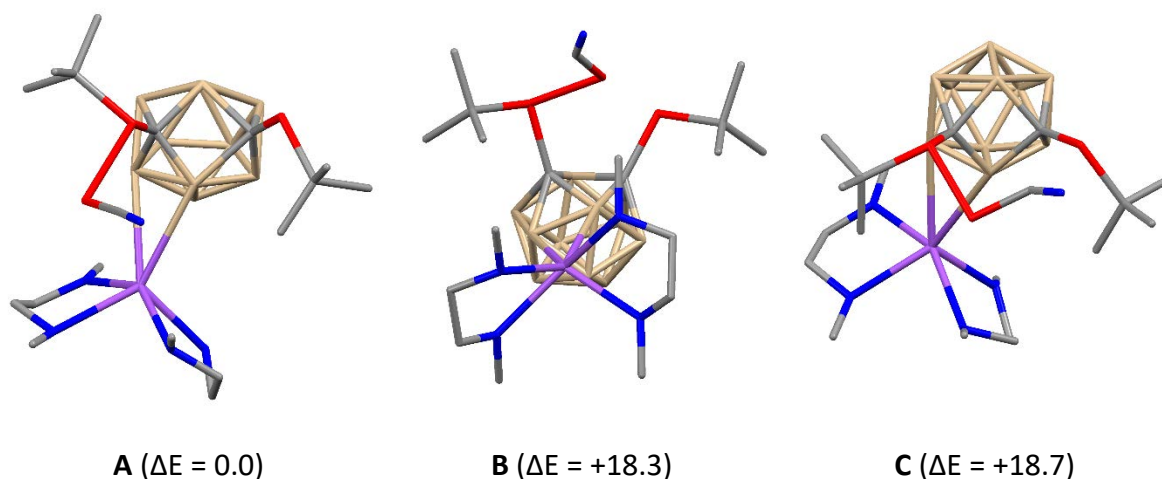


Figure S2: Molecular structures of **A**, **B** and **C** with $[\text{Na}(\text{dme})_2]^+$ at the TPSS-D3BJ/def2-TZVP level of theory (energies are given in $\text{kcal}\cdot\text{mol}^{-1}$ and were obtained at the DLPNO-CCSD(T)/def2-QZVPP level of theory).

3.3. Investigations on the Stereochemistry of Selected Triphospholane Derivatives

The stereochemistry of a series of triphospholanes (**1-H**, **1-Me**, **1-*t*Bu** and **1-Cl**) was examined by means of quantum mechanical calculations at the TPSS-D3BJ/def2-TZVP level of theory (Table S2). Similar to the ferrocenophanes **IIa-f**,^[20] four diastereomers (two *rac* isomers and two *meso* isomers) can be possibly formed which are exemplarily shown for **1-H** in Figure S3 (see below for the Cartesian coordinates of the four isomers of the other investigated triphospholanes). Our calculations revealed that the *rac2* configuration is thermodynamically favoured over the *rac1* configuration in all investigated cases (Table S2). Additionally, the transition between these isomers proceeds almost barrier free indicating that only one *rac* isomer should be observed experimentally. The calculations also showed that the *meso1* configuration is the most favoured for all investigated triphospholanes (Table S2). This can be explained by the steric repulsion between the *tert*-butyl groups and the substituent on the central phosphorus atom which is present in all other diastereomers. Increasing steric repulsion also decreases the epimerisation barrier between *rac2* and *meso1*, and *rac1* and *meso2*, respectively (Table S2). These isomers transform into each other *via* inversion of one *tert*-butylphosphanyl moiety. For **1-Me**, **1-*t*Bu** and **1-Cl** these epimerisation barriers are readily accessible at room temperature indicating the formation of an equilibrium between all four diastereomers which is strongly shifted towards the *meso1* isomer. This agrees with the exclusively observed all-*trans* (*meso1*) configuration of the triphospholanes **Ia-d**.^[21] The situation is different for **1-H**. Here, the epimerisation barrier between the *rac2* and the *meso1* isomer is higher than for the other triphospholane derivatives. However, it is still accessible and corresponds to a half-life of the *rac2* isomer of 5.5 d at room temperature. Together with the small energy difference between the *rac2* and the *meso1* isomer these results indicate the slow formation of an equilibrium between these isomers. In contrast, the epimerisation barriers between ***rac1-1-H*** and ***meso2-1-H*** as well as between ***meso1-1-H*** and ***meso2-1-H*** are high and thus do not indicate the formation of an equilibrium between these isomers.

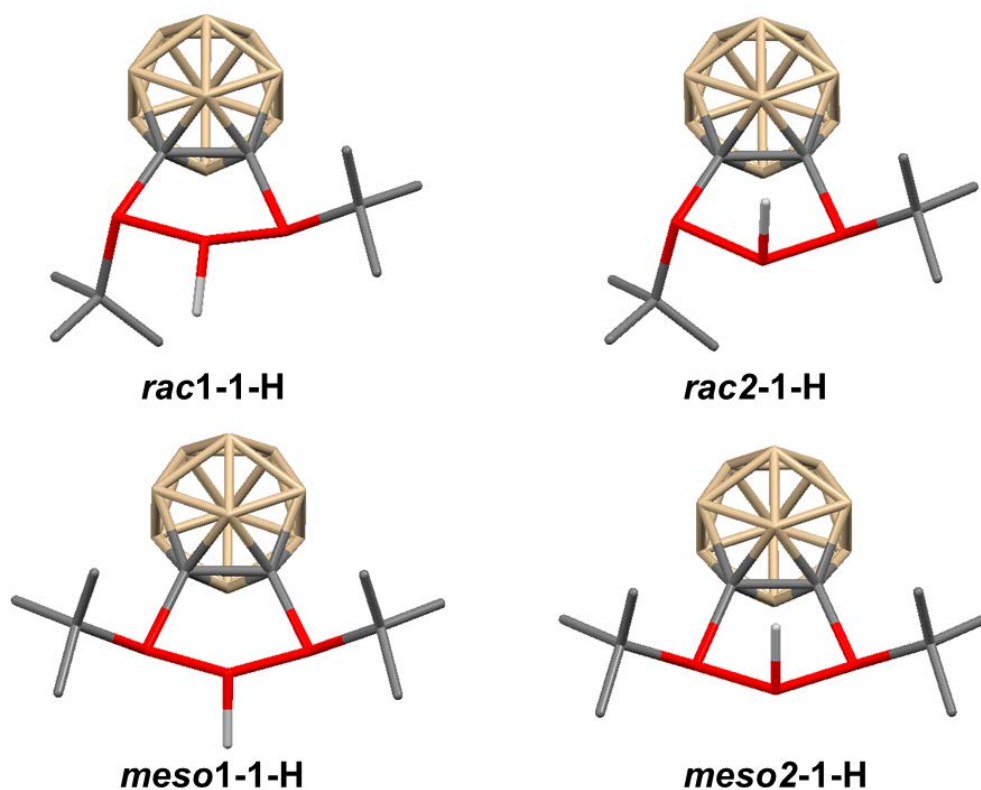


Figure S3. Calculated geometries of the four possible diastereomers of **1-H** at the TPSS-D3BJ/def2-TZVP level of theory. Colour code: tan = B, grey = C, white = H, red = P. All hydrogen atoms except the one binding to the central phosphorus atom have been omitted for clarity.

Table S2. Relative free enthalpies and inversion barriers ($\Delta G^\ddagger$) of the four possible diastereomers for a series of triphospholane derivatives **1-R** (in kcal·mol⁻¹) at the TPSS-D3BJ/def2-TZVP level of theory.

	R = H	R = Me	R = <i>t</i> Bu	R = Cl
ΔG_{rac1}	0.0	0.0	0.0	0.0
ΔG_{rac2}	-2.3	-1.9	-4.5	-2.3
ΔG_{meso1}	-3.5	-8.0	-15.0	-6.1
ΔG_{meso2}	-2.4	1.9	-5.8	-2.2
$\Delta G^\ddagger_{rac1-rac2}$	1.5	2.0	4.3	2.5
$\Delta G^\ddagger_{rac1-meso2}$	32.3	20.7	16.8	14.0
$\Delta G^\ddagger_{rac2-meso1}$	25.4	20.6	16.7	17.8
$\Delta G^\ddagger_{meso1-meso2}$	28.5	28.0	26.4	35.2

3.4. Trough-space Interactions in *meso*-3

The geometry of heptaphosphane **meso-3** was optimised at the TPSS-D3BJ/def2-SVP^[10,,11,14,15] level of theory. Subsequently, an NBO^[13] analysis was performed at the BP86/def2-TZVP^[15,22,23] level of theory. The P-P distances and Wiberg Bond Indices (WBI) between the phosphorus atoms listed in Figure S4 show significant through-space interactions. This is in accordance with the simulated coupling constants in solution (see the main text).

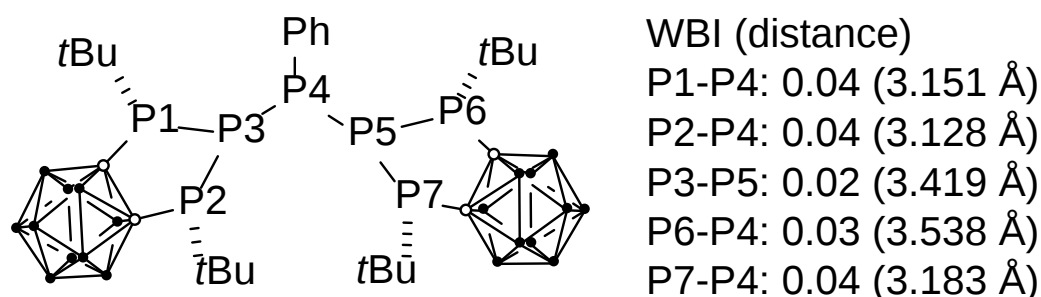


Figure S4: Compound **meso-3** with calculated Wiberg Bond Indices (WBI) and distances between phosphorus atoms (numbering scheme according to the main text).

4. NMR Investigations

4.1. Formation of an Equilibrium Between *rac*-1-H and *meso*-1-H

Figure S5 shows the time-dependent $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **1-H** (CDCl_3 , 65 °C). The initial starting material was obtained from the reaction of phosphaehtynolate with **2** in THF and therefore contained a significant amount of one of the *meso* diastereomers. Although the ^{31}P NMR shifts of the stereoisomers of **1-H** are similar in solution (*rac*-**1-H**: -81.3 (dd), 47.3 (d) and 52.3 (d) ppm, *meso***1,2-1-H**: -108.7 (t) and 28.1 (d) ppm; -99.9 (t) and 33.8 (d) ppm), their $^1J_{\text{PP}}$ coupling constants markedly differ from each other (*rac*-**1-H**: 318 and 258 Hz, *meso***1,2-1-H**: 136 and 292 Hz). Similar differences have been found for the two *meso* isomers in ferrocenophanes **Ila-e** which were attributed to the different dihedral angles of the lone pairs of electrons on the phosphorus atoms within the stereoisomers.^[9] The equilibrium between *rac*-**1-H** and *meso*-**1-H** is reached between 10 and 22 h with the *meso* isomers being the major components (*rac*-**1-H**/*meso*-**1-H** $\approx$ 1:4, derived from the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum). The isomeric ratio could not be deduced from the ^1H NMR spectrum due to signal overlap. Additionally, the formation of decomposition products is clearly visible indicating that **1-H** is not thermally stable for extended periods of time. Thus, our calculations slightly overestimate the epimerisation barrier between *meso***1-1-H** and *meso***2-1-H**. This might be caused by the exclusion of solvent effects in the calculations.

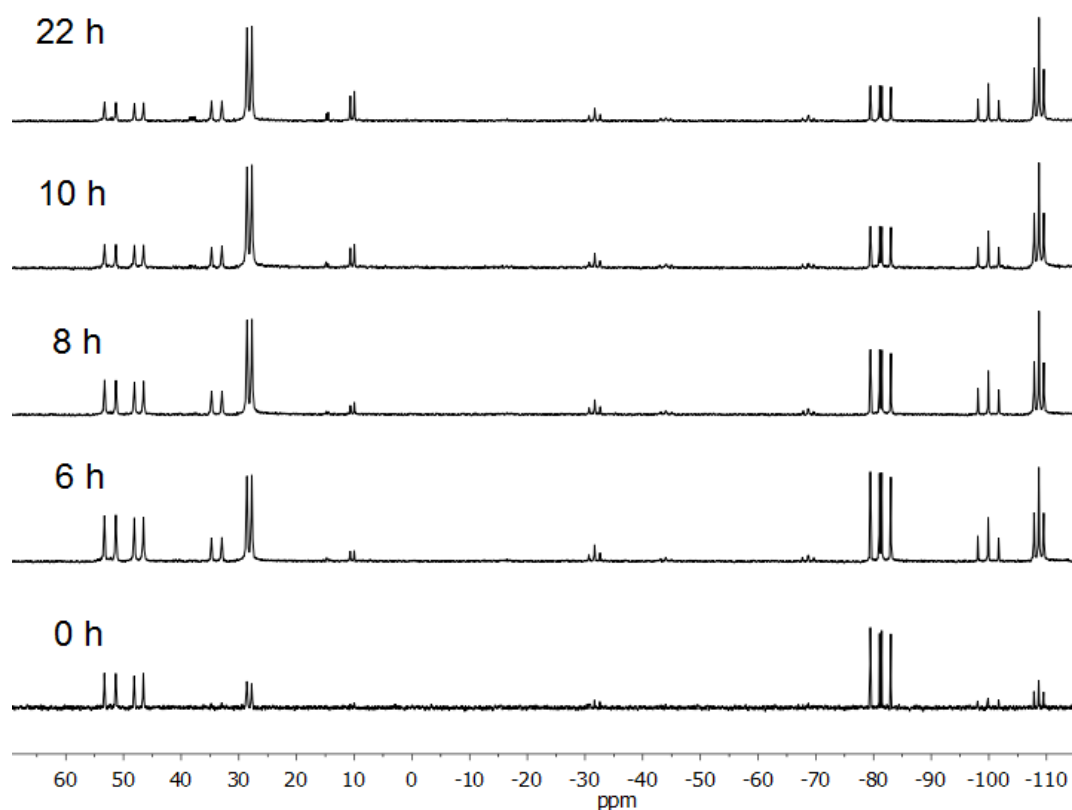


Figure S5: Time-dependent $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of **1-H** (CDCl_3 , 65°C).

4.2. Investigations on *meso-3*

Figure S6 and S7 show the temperature-dependent ^1H NMR and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of *meso-3*, respectively. At 25°C , the resonances for the methyl groups of the two distinct *tert*-butyl groups are well separated in the ^1H NMR spectrum and split into doublets due to coupling to ^{31}P . At elevated temperatures, the signals broaden, and the chemical shifts of the methyl groups become almost identical at 60°C . These findings clearly support the assumption of dynamic processes like hindered rotations in *meso-3*. These assumptions are underpinned by the temperature-dependent $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of *meso-3*. Especially the multiplet at 62.8 ppm corresponding to either the AA' or the BB' part of the AA'BB'XYY' spin system shows a comparably large linewidth, and the multiplet corresponding to P4 (-5.9 ppm) exhibits a very complex pattern. The multiplet corresponding to the bridging P4 atom becomes remarkably simple at elevated temperatures allowing for the simulation of the respective coupling constants (see the main text). Figure S8 shows a section of the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of *meso-3* simulated with the values given in the main text. For comparison, the experimental spectrum is plotted below with a phase shift of 180° . The simulated spectrum is in reasonable agreement with the experimental one. Figure S9 contains the ^{31}P - ^{31}P COSY NMR spectrum of *meso-3* with the couplings between the AA'BB' part and the XYY' part clearly visible. However, large through-space interactions are not unambiguously proven by this experiment since cross peaks could also arise from simple scalar coupling between the respective phosphorus atoms.

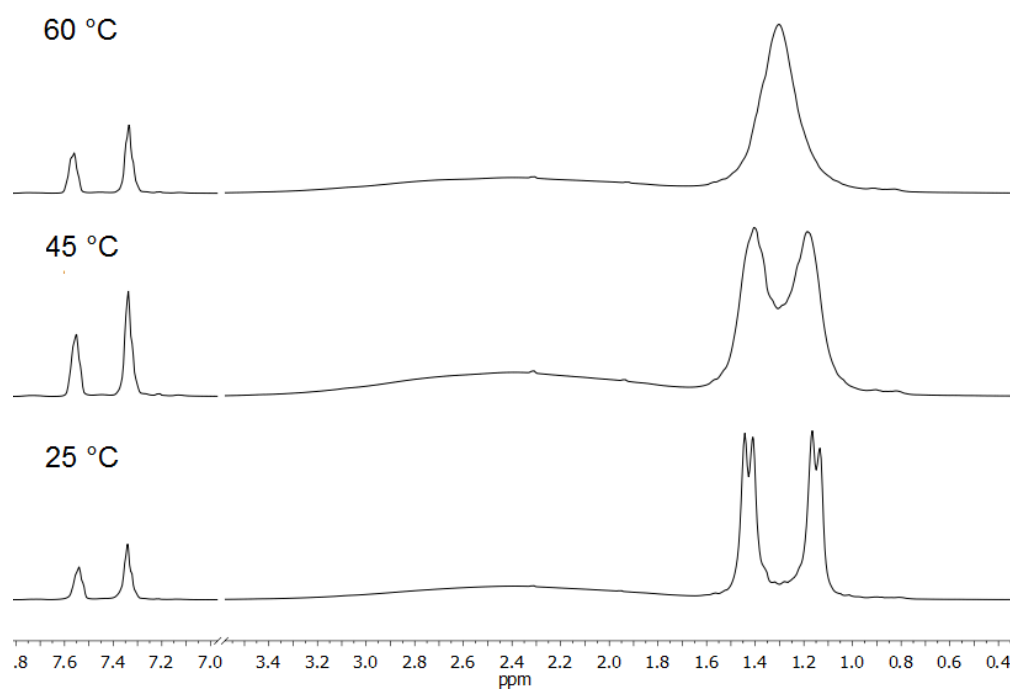


Figure S6: Temperature-dependent ^1H NMR spectra of *meso-3* (CDCl_3).

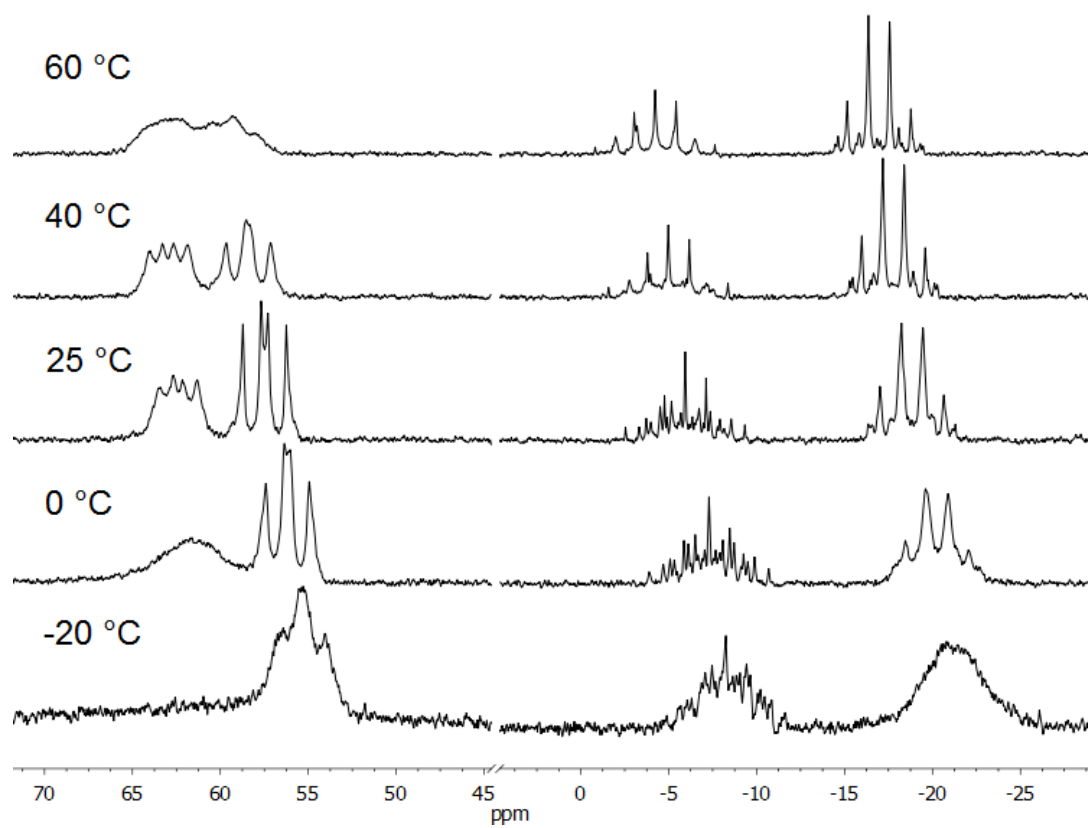


Figure S7. Temperature-dependent $^{31}\text{P}\{^1\text{H}\}$ NMR spectra (400 MHz, CDCl_3) of *meso-3*.

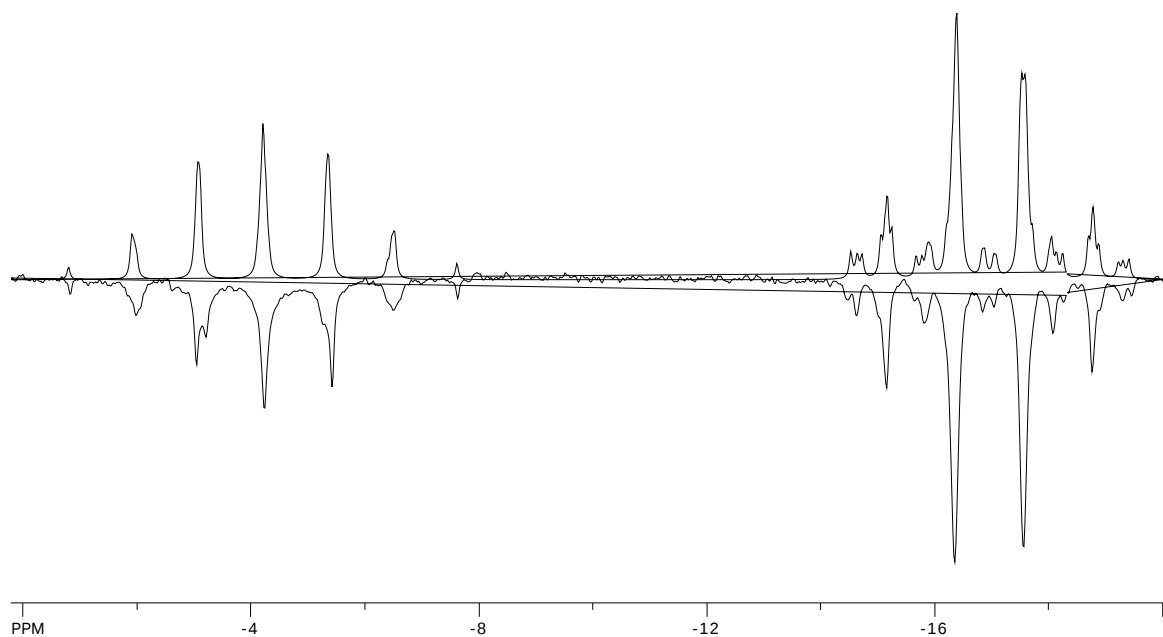


Figure S8: Comparison between simulated (top) and measured (bottom) $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of *meso-3* (CDCl_3 , 60 °C).

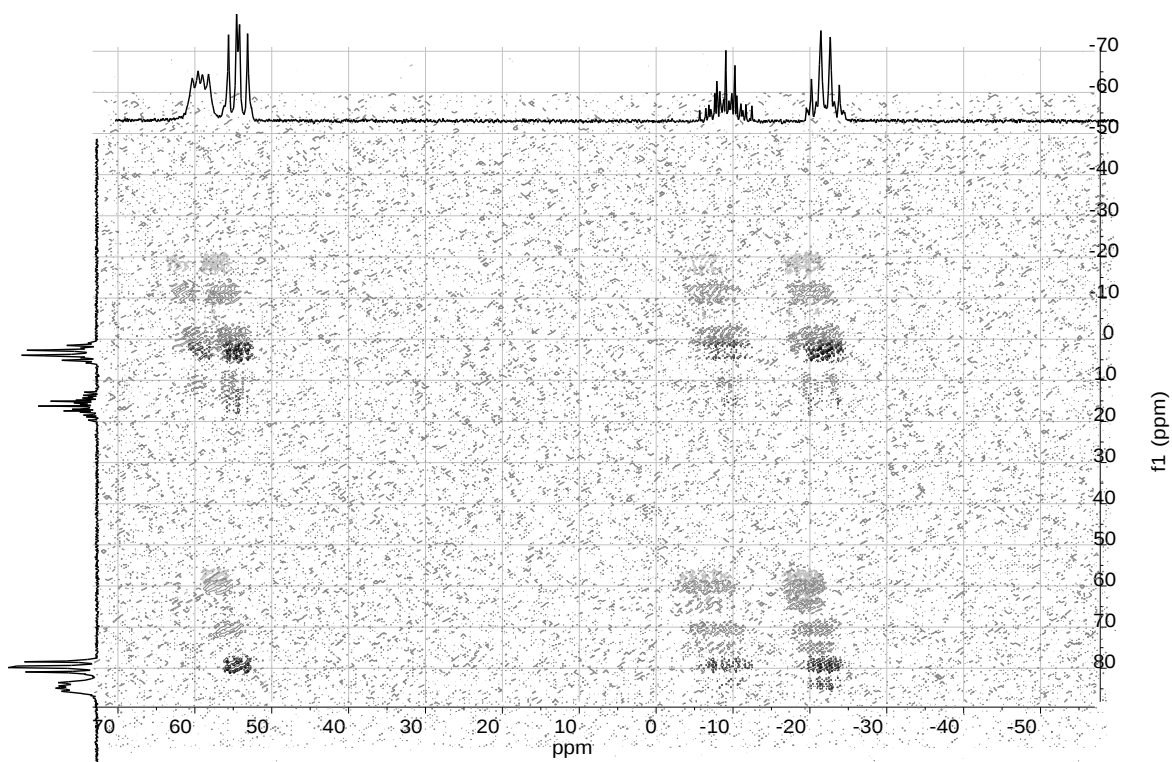


Figure S9: ^{31}P - ^{31}P COSY spectrum of *meso-3*.

5. Cartesian coordinates of calculated molecular structures

Cartesian coordinates of **2** (TPSS-D3BJ/def2-TZVP)

P	9.41174600240687	10.37823961182705	9.36616855938974
P	7.29128181138985	11.14892434137147	9.36693333836560
C	9.17546488280047	10.70104911041148	11.21187175294325
C	10.49458737440663	11.71479394063354	8.60265875321508
B	8.25734920251511	9.32460584794196	11.67613358492445
C	7.52745036444205	10.82275747454353	11.21203774891383
C	6.20798445480378	9.81398151498923	8.60100661166604
B	8.44568180521154	12.19807663754756	11.67925280952382
C	10.25714800102069	13.17269529975244	9.00126917279526
C	6.44458726481941	8.35520881573941	8.99741799781281
B	9.85779883715011	11.54633757062177	12.51946182906876
B	9.73305309071012	9.77524801878801	12.53444689361259
C	11.93986727856149	11.30172196373587	8.94845355385634
C	10.24361289849295	11.54166145843510	7.09085645020983
H	12.14675065188067	10.27045711799934	8.64355543487404
H	12.12971989550642	11.38848239652527	10.02329619288785
B	6.84545701115930	9.97458600164356	12.51793148157364
B	8.24954223738867	9.32119526993281	13.41873497384870
H	8.23486315384731	8.43061929536438	10.91444157811487
H	10.69070141471984	9.10113576941609	12.36724571439269
B	6.97012760926660	11.74566315745161	12.53685599160737
C	4.76285602734580	10.22717084204399	8.94728901869327
C	6.45931163754398	9.98954921106667	7.08956151499519
H	4.55660238980239	11.25908292801584	8.64414067458726
H	4.57280349805740	10.13867874746023	10.02195641399174
B	8.45390915544063	12.19773551507897	13.42186365055106
H	6.01227265999960	12.41989798464962	12.37137198622221
H	10.91331911220265	13.81421739350805	8.39833786686089

H	10.49397719449991	13.34666314908586	10.05315922255035
H	9.22208892347146	13.47605374189718	8.82033529558314
H	5.78748695636677	7.71531423328878	8.39388156082927
H	7.47941927379510	8.05151265182216	8.81593131480934
H	6.20812820283733	8.18052040950328	10.04929689939498
B	9.24392962209020	10.69610041272438	13.96462022470407
H	10.90221183794476	12.08176244472557	12.37201283354575
H	12.64253496899637	11.96287522881334	8.42617031511101
H	10.39220515150311	10.50384698920468	6.77122357103057
H	10.94465841858073	12.17329230154936	6.53225568730742
H	9.22635345351472	11.84783638766753	6.82189564432672
H	8.52704290849211	13.22688593020868	14.00385394472650
B	7.45960088705591	10.82162842225002	13.96487408403743
H	5.80089748652709	9.43964576475176	12.36973237011160
H	8.17616385438785	8.29085361783116	13.99858200708040
H	4.05992241629009	9.56727942892621	8.42377130817384
H	6.31128289382011	11.02796198230213	6.77161010115765
H	5.75805067479266	9.35916465391739	6.52982123193965
H	7.47648324281636	9.68336803018008	6.82029419513251
H	9.88045639503437	10.65083188472557	14.96311292886290
H	6.82252995047668	10.86459402168107	14.96312447057868
H	8.46848556381399	13.09395507644892	10.91970923950800

Cartesian coordinates of **OCP⁻** (TPSS-D3BJ/def2-TZVP)

O	-7.93679666313051	1.71019627389455	-0.00000000314703
C	-6.72828206302128	1.73852408413777	0.00000000628806
P	-5.10298127384821	1.77661964196768	-0.00000000314103

Cartesian coordinates of **RC** (TPSS-D3BJ/def2-TZVP)

O	5.89651945573532	14.45240520437108	7.78169831468503
---	------------------	-------------------	------------------

C	5.50364325557459	13.81312181940398	8.70642463573638
P	4.99102237608994	12.91906542840273	9.97829700615979
P	9.47285298731799	10.25969024172076	9.50622165511681
P	7.32939458501353	11.35207158095315	9.35293300239837
C	9.13882411851233	10.66185970095974	11.28955159964602
C	10.64767505029186	11.53204045666158	8.73298611437707
B	7.97602670214520	9.47227042232616	11.70866105105138
C	7.49747573148459	11.05645793049802	11.23754870810719
C	6.26343423886842	9.95168361516568	8.55571835493113
B	8.60990632328905	12.24534964550075	11.73953384800977
C	10.47657930159455	13.01709228720179	9.06450722913931
C	7.10749013424915	8.77592535095744	8.03916339698979
B	9.89208505137443	11.37860293570038	12.62272885367792
B	9.48697286973074	9.65308896171562	12.61761119413439
C	12.08308943498717	11.09069175063783	9.07070430178391
C	10.37735170531862	11.32465174144491	7.22827608780099
H	12.24885923279372	10.04203576216936	8.80066933380775
H	12.28335269272624	11.20110309801267	10.14188354207971
B	6.67441030127623	10.32338802462742	12.54297794213340
B	7.93482640430822	9.43749260587335	13.45858042149261
H	7.80313582366699	8.59205837567349	10.94228986824137
H	10.32574477833860	8.83008454789086	12.46815655986300
B	7.07406054880802	12.04416690762602	12.59022298779624
C	5.17014821760664	9.41179633361399	9.48523920154343
C	5.60533778694655	10.62933642218256	7.33560195383486
H	4.53698739188835	10.22149970711786	9.85723257670165
H	5.59350169712385	8.87179041227034	10.33545849616465
B	8.59976755003971	12.23711787667539	13.49296754546794
H	6.24938037742371	12.87695557267259	12.47571685442161
H	11.14618974169096	13.60447703709817	8.41847582517894
H	10.74351493631898	13.22913900893699	10.10265200155121
H	9.45012952751270	13.35137720080755	8.89090210301020

H	6.44422601593104	8.08955818895150	7.49193171380525
H	7.89079281786139	9.10996326652065	7.35048993849536
H	7.58895555174738	8.22278282380858	8.84842651439500
B	9.12331733261893	10.62587028227867	14.04686095302415
H	11.01436907681665	11.74238733423029	12.51041539698895
H	12.80697201886286	11.71207360128936	8.52237134454011
H	10.47505123177901	10.26939132462218	6.94435968490906
H	11.09767573983425	11.90678989367892	6.63785534653396
H	9.36845440005471	11.66459953442994	6.96686851126911
H	8.82636605473558	13.23693595721785	14.09199484797421
B	7.38997498180782	11.03848022024207	14.01008344349543
H	5.56135051693076	9.95639234002940	12.39569479814578
H	7.68188605939372	8.42444721327967	14.02493736574557
H	4.54138652136745	8.70992790433240	8.91743293008650
H	4.92580671039306	11.42458580543519	7.65159894485404
H	5.04077952728530	9.87398023318098	6.77101198801644
H	6.35819944748753	11.06265316172107	6.66637275278597
H	9.72245034639389	10.47460951854170	15.06219656149758
H	6.74611942859374	11.17608975465622	14.99898417857594
H	8.79923289005800	13.14686667468306	11.01273021782771

Cartesian coordinates of **TS1** (TPSS-D3BJ/def2-TZVP)

O	5.75831660387218	14.49819915257136	7.68475967355953
C	5.60000038703073	13.78263776242040	8.60619104970993
P	5.31610651142689	12.84548257220345	9.94730703983087
P	9.69269575062332	10.18393545351543	9.48420186164720
P	7.12164591857578	11.38517224974814	9.37846472558549
C	9.28840478745333	10.59123482253862	11.18009762076181
C	10.83249240608210	11.52973813375388	8.76077754854729
B	7.97245438612227	9.54322316852535	11.59152019785506
C	7.33154319664879	11.08552226100332	11.22264353198332
C	6.04506513495428	9.98050196566235	8.61948055928471

B	8.56354444989171	12.16014508438855	11.63442463090130
C	10.50222389452910	12.99908954610886	9.03715858222732
C	6.94670005537415	8.85434258377771	8.08003017972308
B	9.89921719784851	11.35930801902848	12.52878019457103
B	9.49648390347842	9.62559052562468	12.52604996720957
C	12.27200539665704	11.23746955072626	9.22191999923082
C	10.72048402922732	11.27452756018913	7.24455064957081
H	12.55430687863110	10.20322377110127	8.99638902394170
H	12.37072868182056	11.38595957179959	10.30199237970943
B	6.64829764966454	10.30231905919352	12.52828280652609
B	7.94822549522203	9.42098621644321	13.36848648827453
H	7.75074560311906	8.63610649334012	10.86686180761232
H	10.29757319158773	8.75847154799132	12.42825950739726
B	7.03549582634053	12.02808743461924	12.57587235514485
C	5.00175328393496	9.39406401297574	9.57399222421888
C	5.33453129376515	10.61649287999729	7.40773738858019
H	4.34896161680958	10.17503124493769	9.97743207577131
H	5.47253953983264	8.86900019291626	10.40753225856364
B	8.60887038757565	12.21022761478553	13.39821236029476
H	6.22573075559188	12.89035558590843	12.54754062199679
H	11.16028243730636	13.63881881619231	8.42812057817549
H	10.66647320821346	13.25498764182579	10.08642627223916
H	9.46380129218185	13.23086869724657	8.78460103107402
H	6.30808872763320	8.12248377439625	7.56250752855364
H	7.68200575051150	9.23982512273295	7.36806116600606
H	7.49333379367517	8.34572458363265	8.87460419032324
B	9.13578513177623	10.60009059250961	13.96104835748269
H	11.00695574223691	11.77812817023012	12.45710602943969
H	12.98094180241210	11.91217003151624	8.71494875133119
H	10.91528350914891	10.22200014631176	7.00322391782510
H	11.45061261255180	11.89188592750366	6.70180596825770
H	9.71735812976179	11.52787272665253	6.88317993589225

H	8.85805687839398	13.20873474872959	13.99305529186265
B	7.41245815084659	11.01034771586328	13.97308388063673
H	5.54652680735107	9.87851500836289	12.43654729451224
H	7.71016442264423	8.39689209630242	13.92334335019373
H	4.37643355190480	8.67363088574716	9.02589996494527
H	4.56949825561343	11.33047455188334	7.72227956121040
H	4.85618284844661	9.82095559060537	6.82022048824077
H	6.04512207597336	11.13882998033728	6.75554874836839
H	9.74894427269183	10.44523307940610	14.96869275408003
H	6.80338523883379	11.13940578819592	14.98623726839697
H	8.72822114619990	13.09394828602086	10.93671836072156

Cartesian coordinates of **A** (TPSS-D3BJ/def2-TZVP)

O	7.31261481745973	13.55404305352507	6.77772074343549
C	6.76158785405485	13.27540351210460	7.77190206414427
P	5.94518479252819	12.98569681046737	9.20402623250128
P	10.40473785599529	10.38480253246504	9.30186972637089
P	6.80510555274509	10.90960797530222	9.16495985662898
C	9.70199455443325	10.55487690397930	10.86705546291087
C	11.37370240500758	11.98689236689252	8.91643856550443
B	8.36924707327428	9.40963008710392	11.11179127807967
C	7.33304585197235	10.75456887076213	10.89082576494401
C	5.19936072000070	9.90721468886399	8.95953863245362
B	8.41878116749255	11.91848174140906	11.32334440724038
C	10.67986561185077	13.31135125419360	9.24450779191907
C	5.57671534714329	8.42130761861925	9.10750015232903
B	9.89882150029867	11.39000675549308	12.25756324925905
B	9.82344929976898	9.58420369064441	12.18846136550616
C	12.71692052983994	11.91115626508598	9.66808007702316
C	11.63679510350860	11.92032870949217	7.39956281250858
H	13.24813591497359	10.98112327993954	9.43498461938639
H	12.55890953529193	11.95030676457678	10.74982227005266

B	6.85405054233326	9.77708715266183	12.12490558864282
B	8.28703882133743	9.09975216433622	12.89789872531573
H	8.30692170697633	8.52380880562370	10.32265619308127
H	10.74993183798206	8.84368663001886	12.18907647455481
B	6.90689005955293	11.54231307609952	12.28480861462635
C	4.08774462281620	10.29387217129619	9.94025371498082
C	4.72922074920884	10.15960172785919	7.51709578890746
H	3.78257609993988	11.33556639664495	9.78804078113953
H	4.40483577794685	10.17231849183998	10.97780343055662
B	8.42608118197506	11.94402067542382	13.09858811190218
H	5.94951673785706	12.24907050393759	12.26912833011348
H	11.30356599226603	14.14623506842429	8.88794624512612
H	10.53592560407708	13.43129127130491	10.32004894064645
H	9.70283742028368	13.38353048635959	8.75855127320529
H	4.69909796072465	7.80585405216577	8.86424869186555
H	6.38738201782271	8.15176285969709	8.42227031051102
H	5.89405712216879	8.18277820691499	10.12379890361641
B	9.22535261790911	10.43347329094141	13.62246538873269
H	10.88219783133711	12.04995941921978	12.35649901132543
H	13.36099748934299	12.75714662783962	9.37906990056545
H	12.10468085405036	10.96868757098281	7.11814806848153
H	12.31005817050343	12.73556873358679	7.09747572904074
H	10.70184310122219	12.01705260329311	6.83674445028899
H	8.52290273232018	12.94115148478457	13.74080568851569
B	7.46439621471209	10.51844894954566	13.61382172349424
H	5.86403007655310	9.13069016808431	12.03067856819454
H	8.22322275416188	8.01394027037619	13.38112630393202
H	3.20688712478810	9.65740882427151	9.77048533607359
H	4.44830122053124	11.20808836333598	7.37213213378961
H	3.85155412925419	9.53329735523556	7.30635209102595
H	5.51381165606678	9.90905171278340	6.79415770052483
H	9.82947451292601	10.33730186317675	14.64422620950395

H	6.84531497458247	10.46072075467912	14.62891138496316
H	8.46538479683033	12.90272938633480	10.67403512055737

Cartesian coordinates of **B** (TPSS-D3BJ/def2-TZVP)

O	7.69542989454787	8.64401377560065	5.47282668351090
C	7.60106664726731	9.13615490102402	6.54279504563118
P	8.51561045119027	10.10060179173734	7.81632287992106
P	10.38863520166261	10.75240834154119	9.34507069771758
P	6.90651476509538	9.54897470076571	9.23017783620915
C	9.57974551398805	10.42910618600309	10.94009715042246
C	10.54292841658031	12.62970341190330	9.01322634453795
B	9.06131458357605	8.77294236742043	11.03774304005080
C	7.72180351230981	9.82869225733223	10.88041700745731
C	5.46184186106899	10.81076212064555	9.11188457745181
B	8.25104073200615	11.30813876769634	11.57975649823629
C	9.25179615990603	13.43757854587733	8.85458417742672
C	4.29592548288586	10.16474594133273	9.88687844322137
B	9.79808334115616	11.10651744063089	12.46097698398950
B	10.32338899838492	9.45522066449531	12.09993411412911
C	11.46413770392530	13.29514478940876	10.04577109722303
C	11.25865938508781	12.60045266599636	7.64424261456849
H	12.38171013174165	12.71368714908900	10.18905278927422
H	10.96950601190595	13.39279039342111	11.01520543305119
B	7.56449917288868	8.58596372671015	12.00298743259623
B	9.13427875345864	8.33891999913467	12.77611259320208
H	9.31845938475900	8.05700116069558	10.13337649163545
H	11.45419504438527	9.17153637836227	11.89641688403299
B	7.03173155416406	10.23872163599936	12.34320206410052
C	5.69992279812649	12.23879748474184	9.60152472667230
C	5.08257515186459	10.85200949863640	7.62284690470076
H	6.57630201996207	12.67810624793146	9.11931898497305
H	5.83923044199558	12.27976140451395	10.68348708183308

B	8.27143773229008	11.01611106945285	13.33951313146568
H	5.89896062308542	10.57866519302721	12.36465945083091
H	9.49144692245193	14.44042231069126	8.46879619431246
H	8.73177834957453	13.56005987198983	9.80633527777263
H	8.57745741940979	12.94568926176624	8.14603213704023
H	3.39138202829759	10.77837334866592	9.76638273026968
H	4.08476976919714	9.16039678721935	9.50394406061579
H	4.51177607542844	10.08344648252612	10.95511628656207
B	9.55527537513327	9.82163267671156	13.66224059367913
H	10.53955862795930	12.02319962837992	12.54884597536213
H	11.74294957100185	14.30332929688094	9.70120169441069
H	12.20245723310831	12.04589461992211	7.69945987807823
H	11.47569540321534	13.62890271261331	7.32327399658527
H	10.62505898408053	12.12694192230458	6.88494321299182
H	7.97120711329650	11.87233402858372	14.10711866373991
B	7.87192686005454	9.29287136972537	13.59647847847884
H	6.81620747444690	7.71319914452463	11.72004931356580
H	9.46616924180067	7.25385076759414	13.12787166267770
H	4.82542270481946	12.85826213626527	9.35041290955042
H	5.85913480327734	11.34556509605168	7.03163070688543
H	4.13984481206127	11.40740274638345	7.51451646297279
H	4.94218985436421	9.84546217481943	7.21327300842989
H	10.19181259043427	9.81719105241436	14.66657642548583
H	7.28341433551816	8.90605577232099	14.55437428374450
H	7.95539697980232	12.33455378051858	11.09492588671540

Cartesian coordinates of carbon monoxide (TPSS-D3BJ/def2-TZVP)

C	-8.01074072549693	1.62644243410453	0.00000000000000
O	-6.89344927450307	1.82353756589547	0.00000000000000

Cartesian coordinates of carbon monoxide (TPSS-D3BJ/def2-SVP)

C	-8.01326264237434	1.62599755686245	0.00000000000000
---	-------------------	------------------	------------------

O -6.89092735762565 1.82398244313755 0.000000000000000

Cartesian coordinates of **meso-1** (TPSS-D3BJ/def2-TZVP)

C	1.40309305346086	6.55238643830763	2.60238714307583
H	1.51962168928642	7.06174613170137	1.64020872636721
H	0.32994362795706	6.45137979285156	2.82038898107797
H	1.83294077347726	5.54773540438166	2.51043031149947
C	6.11415317928926	9.14089790235881	3.87093051068198
C	5.77051786055747	11.46699286963763	1.29962434561353
H	6.05725044192303	12.27960122263442	0.61459931303449
H	5.85552750439672	11.84015377063191	2.32228978877345
H	4.72273212286171	11.20314560704697	1.12118066462640
C	6.67614908991613	10.25408503471561	1.06569588843135
C	8.13478075831264	10.58129069083676	1.42325427799131
H	8.78127225540311	9.71228115578322	1.25537584536390
H	8.23436717787279	10.88180501236461	2.46960183723096
H	8.49482421108257	11.40902084040899	0.79451318889628
C	2.08512638794551	7.34826421879049	3.73281583432011
C	1.86533248807070	6.61393088071075	5.06510914468454
H	0.78773127333582	6.52942745152864	5.26936059469758
H	2.32804674077316	7.14764818825638	5.89943740957397
H	2.29101650556799	5.60459304241126	5.02827563510858
C	1.49443018671977	8.76062727038079	3.78279925210779
H	1.72722975481124	9.30633075725822	2.86226246526149
H	1.89159735595627	9.33227677541137	4.62413079230316
H	0.40121698470561	8.70002912499719	3.89677152428887
C	6.60250076682815	9.84418310549885	-0.41850747463071
H	6.98530056050903	10.66294635964403	-1.04499876395037
H	5.57038678919255	9.62896472408461	-0.71385555153337
H	7.20611547097743	8.94949445946519	-0.61272696856563
C	4.85611533893058	8.34423099023393	4.60209147819076
B	4.31315965991087	9.20736861943857	5.96949827560882

H	3.16771241190486	9.17569440951628	6.26443173807924
B	5.32386413140496	7.76747921217810	6.14254692379176
H	4.85221600525546	6.74252683382230	6.50709035663231
B	6.48095836154018	10.58036713393969	4.70954403017960
H	6.87328620274780	11.52255889319595	4.11083806379691
B	7.02516385410982	10.07155901090008	6.31812938251831
H	7.82372031905882	10.71294971632794	6.92297308329993
B	5.35032021803981	10.63804786908679	6.06988983623858
H	4.94359763493271	11.67112582468726	6.49574475116498
B	7.00723581701174	8.29229754339419	6.36469314403936
H	7.78192290866726	7.64765746752360	6.99492627049336
B	7.49374176811194	9.14176329208616	4.88155667964168
H	8.55497769779998	9.08761936183053	4.35557234598235
B	5.67729982610452	9.21782548745444	7.10156073582870
H	5.49450049530542	9.23766913277629	8.27675527223313
B	4.80595064401954	10.04951068574453	4.49217042196069
H	4.05362200515612	10.52670505181787	3.71823658616115
B	6.45025684653408	7.72828472281458	4.79177749477971
H	6.72745198225468	6.74643163809270	4.19856108740534
P	6.18228835396088	8.65762980086289	1.98696369790453
P	3.93818664527259	7.23700399107523	3.29080634551098
P	4.05422486077514	8.56435007910109	1.57967328222765

Cartesian coordinates of **C** (TPSS-D3BJ/def2-TZVP)

O	9.75161861379757	10.57944427490719	6.30825878992145
C	8.99872156331740	10.72536065922941	7.21757243310977
P	7.44978844322018	11.32173487156523	7.70316366398846
P	10.50900560568894	10.69353261889077	9.17206943929007
P	6.74850021398427	9.68757193115552	9.04723084930940
C	9.65025613804877	10.54312813901086	10.70836307662726
C	11.08227272860845	12.51466999325433	9.04707908482382
B	8.86230236582269	9.00774649763123	10.89762267350012

C	7.45877745868412	10.00632313904613	10.71058234117424
C	4.94686422911822	10.30715542722435	9.13276943603136
B	8.13690693386098	11.45797101504262	11.21313037766503
C	10.07804669303457	13.59619797092714	9.45458728288630
C	4.21554430185281	9.40346350219810	10.14151239496752
B	9.70103684689276	11.33441870775714	12.14225179499362
B	10.18402504385418	9.61090596538978	11.96587799759543
C	12.34300529398781	12.60241108599688	9.93352065378247
C	11.51254037015869	12.75608670087038	7.58827768244103
H	13.09877618413660	11.87727919148404	9.61123686522185
H	12.11039121762738	12.40953791104268	10.98366124854647
B	7.34839276174568	8.86891520348356	11.89058730673587
B	8.91153866432692	8.63005369507234	12.67980258073823
H	9.06680506550554	8.19423823221715	10.05923133732459
H	11.29600913271478	9.21412929938768	11.86870624579303
B	6.86041020560869	10.56766182099850	12.14121175026883
C	4.77494992340199	11.78592560953074	9.49955912667670
C	4.35476373545696	10.04613478012323	7.73403001064090
H	5.23945997056039	12.43285780206377	8.74718284526896
H	5.22048006583482	12.01596262857289	10.46907448085851
B	8.16288497672474	11.36813278556982	13.00928156569908
H	5.74339750973020	10.95762313550302	12.20011455692697
H	10.51246287824407	14.58599180238881	9.24570564642515
H	9.84374654996256	13.54963947232110	10.51944534762539
H	9.14534834200228	13.49777156905316	8.89113395677836
H	3.14140361830734	9.63656234715151	10.12061909171299
H	4.34332665980425	8.34706821053486	9.88045495815399
H	4.57780327452348	9.55046817359353	11.16039831084876
B	9.39330270373058	10.15310019299752	13.45724964290959
H	10.43983713988365	12.25524352156031	12.24184301595526
H	12.77705133184120	13.61119552024656	9.85441340050703
H	12.12522809426770	11.93283474153541	7.20324797498418

H	12.10766953785993	13.67917961248523	7.54096479336429
H	10.65041301099276	12.87176339271610	6.92733853679534
H	7.93388833922135	12.30575980970643	13.70431792358219
B	7.69679236150759	9.68719222822372	13.43371940213264
H	6.60309801489709	7.96280125394486	11.70391232062679
H	9.19194157504412	7.55828074195745	13.11121322430896
H	3.70377185776218	12.03331343437481	9.54398313346849
H	4.84708686073199	10.65317752842456	6.96782877155895
H	3.28498870757904	10.29753779612731	7.74558867059872
H	4.45945305712557	8.99159398099869	7.45490590662100
H	10.02056939755385	10.21375222583518	14.46668084254665
H	7.10683318080790	9.39694094773184	14.42552776789828
H	7.86957124904231	12.44052690094448	10.61616746778902

Cartesian coordinates of **D** (TPSS-D3BJ/def2-TZVP)

C	6.70393076454749	10.65355791356488	10.21559250600724
C	8.13781985169860	11.39818022374969	10.68535985200098
C	10.47634466740384	13.27359868869813	10.00623208424497
P	9.19234872092159	12.08379899106742	9.24133439752442
P	6.52988885683023	10.72599071276091	8.29769927013276
P	6.42939097535197	12.83411255458953	7.79567281675708
O	8.56513410926033	14.42204281699932	7.95915343617237
C	8.07770536212566	13.31703071257926	8.26478451178171
B	8.05980131044608	9.66951207622313	10.61737583446570
C	4.71510807896026	10.27142711877825	7.87484187413176
B	6.63904632672683	12.09506731067757	11.15705052851808
C	9.93151887679130	14.58445705739294	10.59547142116264
C	3.64732604853150	11.27808784316504	8.32290192196621
B	7.99302319758980	11.98261891897921	12.28882318993340
B	8.87094952294093	10.48235623569879	11.94768084384502
C	11.34698011417672	12.56796987397974	11.05655494681855
C	11.37797837114592	13.59001308631234	8.78887033239999

H	11.69690274619267	11.59105685926241	10.70604443606166
H	10.81726202291365	12.42768628640164	12.00047246925783
B	6.44081812650536	9.23431424823605	11.14299557208159
B	7.79184691462061	9.12213243370016	12.27162773236246
H	8.62921702381287	9.13880524796066	9.73161479170593
H	10.04774161718711	10.41597230721495	11.98963043370813
B	5.55590181922745	10.73294652267058	11.47342182703266
C	4.73580461133176	10.20975471504493	6.33219941005177
C	4.36552330381701	8.87692291458059	8.41231557472487
H	5.47064179097285	9.47845671014450	5.97715737835089
H	4.98531191212588	11.18449560665291	5.90162483620921
B	6.35869472152070	11.55851103967300	12.81983043655983
H	4.41194322666599	10.83777515054863	11.19477582635931
H	10.78285979089063	15.19449100336079	10.93405483600152
H	9.28962869276118	14.39854857492536	11.45877418528198
H	9.37278686654600	15.14375116253093	9.84504257476937
H	2.66022747302892	10.93452402484344	7.97775932449448
H	3.61508422215765	11.37097743426006	9.41041920777858
H	3.83671141767176	12.26994132319147	7.90264322236641
B	7.74853664455786	10.56026709367873	13.31552122246752
H	8.56911061300801	12.96733917782079	12.59063300924721
H	12.22674785714630	13.19853370145936	11.25198140408517
H	11.82281964405785	12.67307975790265	8.38479461912172
H	12.19146464666929	14.25075285976987	9.12141672752324
H	10.81131092238788	14.09406232526857	8.00340009435254
H	5.75506832458045	12.25369021930928	13.57044859422292
B	6.22978565143626	9.78233823814417	12.81292866463452
H	5.92642767587882	8.30907897146653	10.62012813278744
H	8.22047793322740	8.07068977101164	12.62110797332762
H	3.74185746305142	9.90743264779634	5.97272485294405
H	5.15421633969363	8.15018868219044	8.18867851341827
H	3.43470138642836	8.53444359821353	7.93731646043833

H	4.20754981026923	8.89053788759517	9.49262142903858
H	8.14845655536442	10.54631367519322	14.43481413217408
H	5.51893171997596	9.19672161524253	13.56476241924759
H	6.29920335686774	13.09221407751794	10.63090790794784

Cartesian coordinates of E (TPSS-D3BJ/def2-TZVP)

C	6.59890930347163	10.84854672977251	10.37143385293806
C	7.78600604721018	11.90277123343749	10.97079766745635
C	10.49865980344877	13.03478157626651	9.87979915892288
P	8.62030266798711	12.96586846248435	9.71412785734946
P	6.64737576170308	11.06610062470182	8.43596878072518
P	6.08434096740182	13.10586192124939	7.97953604600049
O	8.13377657627666	14.90734527475021	7.87232090621821
C	7.67816128394818	13.86139160122600	8.33032821202177
B	8.09561727949555	10.20169787547927	10.89923229507601
C	5.04476673348560	10.20313069705760	7.81889666759595
B	6.13775020428012	12.23297552363232	11.29795846270358
C	10.92319090718619	13.80334854155869	11.14278337647810
C	3.72722443861413	10.90526445430107	8.17779169348194
B	7.35905512704619	12.43387126672083	12.55644809451384
B	8.58575598635161	11.18489280143295	12.29860886102091
C	11.14274736562473	11.64035693470617	9.84371900377173
C	10.95699783465772	13.81792446752885	8.63256508989331
H	10.84269008563703	11.10167103728921	8.94065143227634
H	10.86759369626114	11.03772459298061	10.71132013041214
B	6.58382917730548	9.39621336106197	11.29759539407595
B	7.83174472828050	9.60129284410646	12.53191130970761
H	8.84404122039464	9.81687046809969	10.07405011920238
H	9.73123628053118	11.41453771598262	12.47157710911728
B	5.36554477612883	10.65806533354017	11.52148331552553
C	5.21295322860050	10.20028918076104	6.28560440071263
C	4.99913987417869	8.74848518609556	8.30641189018315

H	6.12731015334775	9.67248435903173	5.99123663583039
H	5.26610253421887	11.22099670412640	5.89442355389404
B	5.83003750021944	11.63088408249265	12.93569948474239
H	4.25400738472686	10.51056236461497	11.14544952652991
H	12.02146419425296	13.86887347754300	11.18346927351497
H	10.57790585119728	13.30661463639269	12.05259076468071
H	10.51217166112541	14.81681271526685	11.12811219683153
H	2.88272012017877	10.33307422001553	7.76260001761079
H	3.59096959730079	10.97551806384039	9.25917288477968
H	3.69481447447255	11.91742205189838	7.76382366887357
B	7.35737803879797	10.97831253558199	13.56249795635525
H	7.67967793797840	13.53436313189665	12.85137550675063
H	12.23760937175053	11.75377458942855	9.84154210401373
H	10.68141130343179	13.29114720365260	7.71404345149744
H	12.05168652535134	13.90972256455581	8.67008254311695
H	10.51327009873658	14.81480701094484	8.59254014773230
H	5.00987619505308	12.15719861497236	13.61511890957892
B	6.11308787616375	9.87399487757855	12.93370538404879
H	6.34165793182749	8.37620384835865	10.75305962800226
H	8.46089990122652	8.67600351518937	12.93206091414377
H	4.35376884300914	9.68834014586909	5.82841629078851
H	5.95904950315288	8.24232002610364	8.15354936191131
H	4.22867155214017	8.20286390620198	7.74196363456899
H	4.74533751729747	8.68766270331127	9.36655117651685
H	7.65376522131787	11.03304719782607	14.71243083568175
H	5.49613147010415	9.13345589004801	13.62974321771599
H	5.62567588611293	13.13083085703461	10.73381180290778

Cartesian coordinates of **F** (TPSS-D3BJ/def2-TZVP)

C	6.74299315804980	10.95492441091952	10.49223863838313
C	7.72691427615168	12.16125209340268	11.19629280074875
C	10.30220284770126	12.96338267611084	9.64319344528608

P	8.61648905932132	13.57111496998642	10.30403416176263
P	6.93122560267643	10.88609077757047	8.59532854873697
P	6.52823133656350	12.89877347891464	7.83324294414865
O	8.03628399016766	15.06280104334801	8.24603228096120
C	7.74055441673860	13.91565119513255	8.64443410353592
B	8.22942246934820	10.52983478962063	11.25711922699719
C	5.35473950621334	10.04171308197324	7.91149228487239
B	6.01172033628125	12.30402296466154	11.26336814364549
C	11.16549050858138	12.40475306789713	10.78433085693803
C	4.03934626567812	10.81011466851863	8.09222359581579
B	7.00697899298510	12.68503161073762	12.67607921868228
B	8.38992169428893	11.59092486689404	12.66939376514720
C	10.25352102803037	11.97355182040296	8.47339316132264
C	10.95433233956262	14.27866467592007	9.15747484859508
H	9.65689342663808	12.37023523884052	7.64677655760143
H	9.81952079622471	11.01508322704689	8.76462540201920
B	6.77725272449864	9.55436224336201	11.46815454189405
B	7.79784919373205	9.93868143689793	12.86629249873548
H	9.11893120171372	10.17510391304613	10.57176750223336
H	9.46156606428032	11.98249710505474	12.97580375138975
B	5.39150812406623	10.65583225393602	11.47699330136262
C	5.66333979656196	9.92237914034804	6.40272800488477
C	5.22711267321464	8.62577307759135	8.49165036087566
H	6.59369994070848	9.36823178495336	6.23385368407496
H	5.76156092704418	10.90905607274926	5.93948700336167
B	5.53906966353863	11.72728612331424	12.87536645454026
H	4.37131483665154	10.35448478722147	10.96447773394279
H	12.19324544410170	12.27461261202289	10.41505489987513
H	10.80852269646376	11.43527916923484	11.13683240814737
H	11.19276447184584	13.09334697112409	11.63547287694705
H	3.22636132680759	10.25668989780265	7.59841198464937
H	3.78013441653728	10.92672323824258	9.14622322488153

H	4.10383993177786	11.80718560500427	7.64679778230316
B	7.02068847459921	11.27489464070061	13.74920167187037
H	7.14899015465317	13.82247717569505	12.96646594100575
H	11.27766634918019	11.79560503513820	8.11176883952546
H	10.36208036668856	14.75646245183340	8.37317636095389
H	11.95282496742420	14.04344825278331	8.76246095178516
H	11.06534725996178	14.99080044195164	9.98266677617751
H	4.57832449390954	12.17861122832600	13.40833018795180
B	6.02084008609897	10.01354338868063	13.00359047213859
H	6.73796035635034	8.50253604362601	10.92940056928372
H	8.45903098733293	9.10154383579698	13.38912924855597
H	4.84205431020595	9.38159339319658	5.91133235932648
H	6.17503304990813	8.08104744778723	8.41869075998144
H	4.46553270910831	8.07204544634167	7.92363526558667
H	4.92143059802195	8.64226223590186	9.53989495528902
H	7.13273852221817	11.40783402646694	14.92486075574752
H	5.39773301574390	9.21961264327311	13.63187931262734
H	5.49274181384796	13.11880922269654	10.58906657289427

Cartesian coordinates of **G** (TPSS-D3BJ/def2-TZVP)

C	6.36268133628157	11.19810393977996	10.54796238276290
C	7.91747154036729	12.32931713527598	11.38991237978626
C	10.30517586974515	12.68044891528444	9.57696526395393
P	8.69153897209700	13.45903928619663	10.24316118241364
P	6.68132871896693	11.45966152183296	8.74109817342790
P	5.53225984168884	13.21431339175190	8.12213355202184
O	7.27875822254168	15.41117073228661	8.06806201517901
C	6.82450235552347	14.34195247008246	8.26092984759352
B	7.81410052960044	10.57927625446811	11.19729905653283
C	5.69665083014003	10.06713175053104	7.88858912841917
B	6.19434287260424	12.65661194639158	11.42196164466813
C	11.12885762248758	12.01273620790230	10.68514031491397

C	4.26325665939430	9.87843770148544	8.39537871005746
B	7.25757843903036	12.78555065067710	12.85670759851573
B	8.34977763608282	11.39271619429858	12.70829124523331
C	10.12701430798833	11.70706453244712	8.40342276403485
C	11.06624892009535	13.92211840743260	9.06316534807709
H	9.54732087029821	12.16612209233086	7.59684986621199
H	9.60031402270650	10.80198107326353	8.71274945084978
B	6.18092221366996	9.84059505099018	11.47349002257551
B	7.36866564254772	9.92379838914447	12.79175807349786
H	8.57679516888806	10.05226370277775	10.46039623563339
H	9.48997913185651	11.40030707289363	13.02534890862863
B	5.09735396490157	11.23956181956556	11.61831177725970
C	5.67994224988551	10.40215051797611	6.38638525965230
C	6.51917115691753	8.77712889206006	8.07751926107672
H	6.68998308783029	10.61213273957618	6.01633747333147
H	5.05535354692285	11.27444330299753	6.17238865233290
B	5.60676631371423	12.16791934013168	13.03864207162463
H	3.99523573846195	11.28282511049117	11.18110063282808
H	12.12602230101447	11.74884559183021	10.29826787713189
H	10.65051387485490	11.09653511658313	11.03952944163753
H	11.25681273759614	12.68223123154788	11.54218875900199
H	3.76977577208249	9.07637167965675	7.82553693281028
H	4.24450436765442	9.60725235525983	9.45311818248213
H	3.67848652006745	10.79588827299070	8.26817364430127
B	6.95964594861748	11.32236151140218	13.82083624988743
H	7.58431017458279	13.84732708594695	13.26654332971123
H	11.11538802445832	11.42126441946650	8.00805262888813
H	10.48767025223555	14.45080352678209	8.29637386498357
H	12.02443830757746	13.61448553453793	8.61986415394354
H	11.26758971795615	14.62624425341863	9.87795535721302
H	4.81042045937712	12.80952169139932	13.64484919690380
B	5.65852721113409	10.38573624067849	13.07551283513050

H	5.87748184795725	8.81277320024925	10.96706990489125
H	7.84891573604601	8.92545889230041	13.22437432971842
H	5.28132661969531	9.54005566105524	5.83291947103219
H	7.52546075053438	8.89755223503214	7.66207965898775
H	6.02295543829526	7.95041805195983	7.54922857825170
H	6.61307299044262	8.50209663380932	9.12936805132855
H	7.13360402261712	11.32936950048062	14.99783046467434
H	4.91241900932955	9.72244296813146	13.72277128784627
H	5.81718013263734	13.62665420315732	10.86809050614870

Cartesian coordinates of **H** (TPSS-D3BJ/def2-TZVP)

O	6.02917456230694	13.86086320902497	7.06265367051114
C	5.63904087595736	13.25672209989185	7.98402730748636
P	4.98834396196912	12.47147604108656	9.31304176269367
P	9.91236563340064	12.90838686147228	9.62987688049574
P	6.76994082820447	11.10787437224341	9.26467381914886
C	9.37950564610663	12.18495381180641	11.10720768683178
C	11.05457680276640	11.66770921795143	8.73167517653626
B	8.78383306074477	10.45847335525279	11.27416290278534
C	7.27180165641804	11.14010418938092	11.00720920044390
C	5.87870116141498	9.44991581307075	8.96744038479668
B	7.66714475927002	12.69945030118858	11.49822754292211
C	11.97049235306483	10.86052795211155	9.65786900836432
C	6.92844006762529	8.33434558705722	9.12158734875117
B	9.12442682479172	12.93311330205429	12.55203863822763
B	9.93144725846364	11.33070569929506	12.39243568587750
C	10.24436893018859	10.71904711572877	7.83095996034778
C	11.92047583149503	12.57289705199689	7.82983857643015
H	9.57954849707562	11.27976768050912	7.16610312141050
H	9.62508862464290	10.04736243043048	8.42980359904600
B	7.25542777322697	10.02070391564310	12.22144999351929
B	8.82032706528715	10.11543535209322	13.03459312194894

H	9.20901189956582	9.68503163520986	10.48255132200880
H	11.09884122436208	11.12824659818548	12.43340705171745
B	6.46469953136488	11.59884964939527	12.37285746435091
C	4.68163663401194	9.20530822452266	9.89196763721869
C	5.40421204024484	9.48927035325319	7.50501318598881
H	3.90725255512131	9.96432847040607	9.73233111100914
H	4.97399600779468	9.22191251113112	10.94367048897436
B	7.53640348461768	12.65466444783550	13.29283275206850
H	5.28938168771100	11.76937418406674	12.29458244589063
H	12.67783031336260	10.26766714992434	9.05628014191308
H	11.39943004710922	10.17326563544906	10.28551554239677
H	12.54660510234700	11.51864000678788	10.31650104022891
H	6.47170391913120	7.37478494925377	8.84104761920909
H	7.78691527552837	8.50885831067209	8.46436433205890
H	7.29030333019321	8.25619861021295	10.14810079418362
B	8.95084659192193	11.71276120675108	13.83308314041722
H	9.67103954378755	13.97572405708667	12.69679020754083
H	10.92633270970243	10.11034860062526	7.21545661100512
H	11.29576590672943	13.18998726313748	7.17269237690115
H	12.57702459319413	11.95569700177272	7.19973418651444
H	12.54621514779565	13.24480233500028	8.42835030471023
H	7.08039211712663	13.53719938578309	13.94770267278952
B	7.37705128951981	10.92631773862552	13.73276203019488
H	6.69306699352241	8.98569628208603	12.08170863546940
H	9.30226237262342	9.13410177073900	13.50525928900273
H	4.23913254684426	8.22279982374080	9.67108998559475
H	4.65597797017737	10.27486552670867	7.35560875147816
H	4.95033966062907	8.52354964447195	7.24334970831107
H	6.24069174397775	9.67459565913517	6.82167923937860
H	9.49172224311706	11.87380667968133	14.88166675302852
H	6.82356528938221	10.54164930685289	14.71392445415195
H	7.25893405306199	13.60813362220637	10.85545633571859

Cartesian coordinates of I (TPSS-D3BJ/def2-TZVP)

O	8.73476611744333	8.24068616452787	6.03492177408707
C	8.32339565827944	8.91993205193257	6.90637559751418
P	8.23309714437885	10.37093588971765	7.87726378569319
P	8.83542005500466	12.50252626162005	9.56167269547795
P	6.90313428816618	9.40323309863988	9.35139625265919
C	8.86826749457022	11.50038825736132	11.05887234363203
C	10.63700179846976	12.64213428800642	8.94067900872094
B	9.34411391411728	9.78056349095868	11.00156967831734
C	7.65414213054960	9.88660625173322	10.96478408004781
C	5.26047428216894	10.34657204147362	9.08305850109723
B	7.31660898052081	11.36134858107050	11.78127989545873
C	11.36529474290854	13.68520832122851	9.80739075727526
C	4.32120558082120	10.13011647082404	10.27759028890218
B	8.72414578498383	12.03028009300175	12.64701829481743
B	10.06994670240394	11.00882618310547	12.10101459509731
C	11.47380243425399	11.36130129108615	8.85819307841788
C	10.45177780725091	13.21181214641268	7.52032443411153
H	10.96898016413053	10.59820135892519	8.25877302214077
H	11.67422253466213	10.94538006272681	9.84763148021233
B	8.29784075912447	8.69638992860518	11.97039910607167
B	9.77358108699278	9.35772292572870	12.67489290804921
H	9.91074385833565	9.39039676551699	10.04541907810901
H	11.16598091818484	11.41224465951213	11.90928648394871
B	6.94925799868729	9.73182671400135	12.46011154288233
C	5.36748207792934	11.83683742027425	8.74275061336308
C	4.68221947667771	9.61268060220690	7.85425264062096
H	6.01599795005685	11.98924910092215	7.87415531977019
H	5.77016154809346	12.42350284981716	9.56897900015976
B	7.58489658748652	11.00359690388626	13.51923473018012
H	5.82893219965523	9.35728711064933	12.52033684299435

H	12.36357623426437	13.89313649566127	9.38971718890100
H	11.49208888127671	13.32744237363893	10.83323187310146
H	10.80146326655731	14.62387055035456	9.84290728534608
H	3.30866142508550	10.45591387440330	9.99967723959984
H	4.27314820808311	9.07354860787010	10.56418650364552
H	4.63691697399300	10.70725795161193	11.14865719087962
B	9.33319929346621	10.74798016687370	13.70651677261484
H	8.80760961473654	13.20126413433697	12.80502491572087
H	12.44177969353842	11.59225410705472	8.38668929938358
H	9.96444066489602	12.47873066561064	6.86739154319204
H	11.43012947050665	13.46802294240260	7.08927593199933
H	9.83554908645356	14.11955545454143	7.53614586605585
H	6.89163075819988	11.46982271536612	14.36477047190172
B	8.25210833315886	9.35444440473673	13.61406594035614
H	8.15607004052105	7.56983128978796	11.63146727637485
H	10.69607481956130	8.65003173697531	12.92190066024708
H	4.36476362525900	12.21925081463922	8.49819294524496
H	5.35453354361389	9.70608421786979	6.99409176639297
H	3.71478183548598	10.06100892565747	7.58973909349251
H	4.53019708029052	8.54713101945025	8.05961324518453
H	9.93078864122560	11.02403518056921	14.69719324729124
H	8.05524520622033	8.63670667720896	14.54157512061533
H	6.45140722729806	12.06316040790609	11.39255379262842

Cartesian coordinates of *rac-1* (TPSS-D3BJ/def2-TZVP)

C	-4.00887398347743	3.63794461883372	0.09883747919230
C	-3.04522883929376	3.18815791223410	-1.00665818488058
P	-4.73391815826649	1.94069262359652	0.39668841675851
H	-4.75098136972631	4.32222058373849	-0.30115430140012
H	-3.53941294852404	4.09581604926239	0.96406360810723
P	-4.20468347388343	1.91792210061381	-1.74173711570533

H	-2.16643242728402	2.71976358618313	-0.57374538822764
H	-2.72596340935596	3.96940729248613	-1.68944009339171
C	-6.60139484864877	2.10582853037121	0.44437886069566
C	-3.23932012236137	0.33111216273140	-2.00695535553212
C	-2.73536755948071	0.34637506647753	-3.44669805815617
H	-2.04343913248823	1.16913148824652	-3.61730604656641
H	-3.55747805353981	0.44680774054352	-4.15159421966083
H	-2.20816480998145	-0.58177158453677	-3.66885904254865
C	-4.24619718257001	-0.79921209777889	-1.82447341074943
H	-3.78308500172048	-1.75259611572301	-2.07763457253055
H	-5.11642633920639	-0.66848869312388	-2.46580577531102
H	-4.58723724894792	-0.85514440816500	-0.79261842583210
C	-2.07728348563966	0.13430027537283	-1.04841599702370
H	-2.39744746453852	0.22816800601612	-0.01290318462716
H	-1.28022696218278	0.85117227786596	-1.22895961557460
H	-1.65463884762340	-0.86180005952110	-1.18303580798323
C	-7.13581280087438	0.77343785009129	-0.06746203316522
H	-8.21961627601474	0.74055175619232	0.04147293642986
H	-6.71621374499698	-0.06609010768463	0.48459006073452
H	-6.89984268127989	0.64079759780988	-1.12167843677310
C	-7.15948101692942	3.23495346347742	-0.40483372183270
H	-6.80588554101178	3.17063276048209	-1.43158766645016
H	-6.88887127840814	4.21022639147015	-0.00772967105930
H	-8.24851594580836	3.18113426556565	-0.41839947312346
C	-6.99940080211622	2.30044152557415	1.90385169331221
H	-8.08523846087927	2.34084603035713	1.99310117721336
H	-6.59888814495880	3.23011380794241	2.30407005976338
H	-6.63786163798107	1.48383730299740	2.52442130589826

Cartesian coordinates of [Na(dme)₂]**A** (TPSS-D3BJ/def2-SVP)

P	9.56953805231964	10.92879101607239	10.75107841338460
P	7.29418877428851	11.08368341062667	7.88260860443112

P	6.43161734436182	13.05281805019725	7.15340698510195
C	7.36300027560533	16.40053544837721	9.00587011890332
H	7.66093252966587	17.45696216914732	8.85330052229161
H	6.98853084889974	15.98519655078267	8.06030244352180
H	8.23921859972571	15.81724081535292	9.33801934546224
C	3.73968008181100	15.67610256854331	13.15948262842623
H	3.47487292037142	14.61893942109233	13.29962449762775
H	2.86149970411764	16.23534258482554	12.77876073693295
H	4.05156987203445	16.10538651526054	14.13154085167534
O	4.81559369838122	15.71106053261719	12.22713164678438
C	5.37125036267844	17.00773007998322	12.04460537214908
H	5.63016665602576	17.45723833347889	13.02529115118162
H	4.63993573042744	17.67236615998664	11.53750398125841
C	6.63102938107025	16.87961074724007	11.21328420903723
H	7.37306192917930	16.23817291086524	11.72970751141327
H	7.07406459823394	17.88745389229797	11.07579604174478
O	6.29184300868506	16.31608893403238	9.94692422436286
Na	4.74852349753620	14.39887395220116	10.25572800691232
O	9.06386158478576	14.14437213859361	6.96427777196772
O	3.38205038126587	15.49131617668036	8.61613222323136
O	2.39118925276643	13.74182548186917	10.47370746293969
C	1.52097304812869	14.26099871204004	9.47835439585513
H	0.99918174323104	15.16523608548026	9.85773130424001
H	0.75324526861384	13.50876010965002	9.20338905821235
C	2.33157647844051	14.59934271455115	8.24178813228648
H	2.75613947485675	13.68023186596989	7.78860354172229
H	1.66636365145549	15.08098437215942	7.49663488819413
C	8.00382319599146	13.65239161968378	7.04881167000061
C	3.97713013617604	16.16138258840749	7.50641198687181
H	4.48171463789612	15.44470668453043	6.82877548030522
H	4.71525586536501	16.85941116426885	7.92551773402708
H	3.21209821644769	16.72630244987638	6.93773122143754

C	1.70095639133445	13.07121770589102	11.52644030884854
H	1.04008685789707	13.77176409071718	12.07616797169274
H	2.46423523748353	12.66006586201062	12.20015394129918
H	1.09472161578345	12.23758522226037	11.12390597584626
C	7.90456870860848	10.92200551793217	11.22604688912388
C	10.30492979091075	12.65023447382098	11.19296003511379
B	7.00189986025441	9.63546677344646	10.39988477903872
C	6.33355729506474	10.86709458947736	9.41685799759663
C	6.54446492811021	9.93631085512617	6.54322969250770
B	6.58188450941696	12.08534549589492	10.49537671481278
C	9.42044126201755	13.86570330467311	10.89445270959276
C	6.86101320900158	8.48821052224620	6.97651303878881
B	6.86931098243629	11.66986506613330	12.25555870914808
B	7.09511013580916	9.87296978004342	12.20755424237479
C	10.65684016949261	12.61231409977152	12.69633511761919
C	11.59766773818464	12.74551196230534	10.35366308493514
H	11.29944885765961	11.74661997067959	12.93570610751121
H	9.74590180300257	12.54114865366602	13.31469065083354
B	5.20989253965994	9.75044384016954	9.88718844331886
B	5.62469749833532	9.17728720304128	11.50783406439373
H	7.67435042980392	8.79777012235187	9.86616552527029
H	7.78012690757681	9.22893411034089	12.94930231290975
B	4.91083958018095	11.49582116283784	9.96813621258253
C	5.03722132363363	10.14016105610720	6.33266221604380
C	7.31350841874704	10.26036768692274	5.24701974022585
H	4.82314637334641	11.16649439431898	5.98075074505718
H	4.46856744815071	9.95778598432256	7.25767424695360
B	5.22506920719858	11.99203065425766	11.64555309934485
H	4.21276153205468	12.10528948757248	9.19884034612393
H	9.97948516557011	14.79657200955936	11.12132974250227
H	8.50297125120773	13.86080771061506	11.50384286854177
H	9.13251439975565	13.88933435996210	9.83110259910135

H	6.57148001058442	7.80009128435640	6.15994601674003
H	7.93914777703225	8.35587028337306	7.17181841448537
H	6.30658628375149	8.19940340230714	7.88163980910454
B	5.51404864856315	10.54740409581932	12.65284384250012
H	7.33164584183664	12.43914511174330	13.05280782680483
H	11.20360271046682	13.53355481154495	12.98395562136245
H	12.24421051274386	11.86281724121880	10.50974525404400
H	12.17498095844206	13.64629693869503	10.63930632620458
H	11.36549336131141	12.80984979484119	9.27558390453532
H	4.68491501077074	12.95464909083546	12.12711183361733
B	4.37764566987570	10.44998807260663	11.29377204389544
H	4.71873930403610	9.00972314183940	9.08573487322155
H	5.34465202332220	8.05017244360342	11.81349650208939
H	4.67014660544894	9.43978241313839	5.55785310594757
H	7.11756368571369	11.29432740230687	4.91162949920145
H	6.98765147277863	9.57103055453403	4.44569840796850
H	8.40264600400954	10.13930346760182	5.38433046566045
H	5.12407444838384	10.45350633427750	13.78634601908218
H	3.20556858060965	10.26276053668656	11.48572448812245
H	6.97389186178975	13.13598259345364	10.07127445246479

Cartesian coordinates of [Na(dme)₂]**A** (TPSS-D3BJ/def2-TZVP)

P	9.56825773823079	10.91249781679849	10.75092556130967
P	7.27771851465879	11.11759279039378	7.85896868824277
P	6.31759838652854	13.02080401039322	7.13667655356407
C	7.36924684216326	16.40986230207010	9.03382088602475
H	7.65508048898763	17.45629512873732	8.86088787932370
H	7.02119726562641	15.96153919748468	8.10385440007907
H	8.23096387293055	15.84865702339712	9.40947019851467
C	3.80462556865898	15.65046998790375	13.23341052949030
H	3.56036675556754	14.59837252704797	13.37936386627639

H	2.92224464025760	16.19465317765174	12.86822563434216
H	4.13587831300973	16.08680675839690	14.18482864672990
O	4.86369123029243	15.69337500641668	12.27253992788584
C	5.36752805159365	17.01490306156796	12.06725698523774
H	5.61833606683475	17.47550808876101	13.03449781818230
H	4.60770223288248	17.63473411687095	11.56672188536732
C	6.61769477100077	16.91842754226578	11.22425211728996
H	7.37247029533070	16.29311160609392	11.72163774380593
H	7.03349178155931	17.92640564657919	11.07578619990011
O	6.27246452323189	16.34487931455709	9.95728269389843
Na	4.75931192209282	14.38850865298538	10.24886500790270
O	8.90280715609504	14.12966251235893	6.73274623035991
O	3.33896973893009	15.54208168109704	8.62430977123428
O	2.37985450753951	13.74507622363643	10.48496167199954
C	1.48614703102186	14.33920498565217	9.54500184189124
H	1.03852292459912	15.24891326556961	9.97454890260983
H	0.67815686855005	13.63519383567489	9.29488662598955
C	2.25360293560816	14.66764260975891	8.28382158244387
H	2.64591820045920	13.75272954614169	7.81665367506049
H	1.58023636378973	15.16771726333311	7.57216440549985
C	7.85949952240869	13.63660386417885	6.90877245358251
C	3.91263898612427	16.16329501519835	7.46670879100879
H	4.35747111745511	15.41318979167704	6.79936795050059
H	4.68386728853362	16.84109676060050	7.83246212646618
H	3.14527580617003	16.73042984784879	6.92291497727844
C	1.68736901993647	13.08254666344590	11.55029427595832
H	1.09520452516652	13.80234186172357	12.13334388305128
H	2.44675355108964	12.61635675879126	12.17643290159933
H	1.02616015398617	12.30606786824693	11.14557700100885
C	7.91441731563787	10.91899818224904	11.21359843482956
C	10.30345720176533	12.61248924191748	11.19934850796005
B	7.00553730605216	9.64348691094668	10.37739887439972

C	6.34560202929170	10.88196789460808	9.39543928615129
C	6.59146681134724	9.92502882179736	6.54865422314365
B	6.57710456860432	12.10203749425747	10.46324289294958
C	9.45987849741997	13.82913348544177	10.81566982439687
C	6.94668985703913	8.49991292644597	7.01409444763467
B	6.86981558230343	11.67921060743296	12.21711274331616
B	7.08612997831324	9.88346421660897	12.18252370187602
C	10.56838753912888	12.62059975417224	12.71721190169751
C	11.64472298912961	12.66843026632922	10.44285314697020
H	11.17915509113091	11.76226851952451	13.01697021915453
H	9.63056261936505	12.58313322969167	13.27901846935541
B	5.22145400873284	9.76633650190112	9.85947903450541
B	5.62369020714457	9.19557917184409	11.47579928160302
H	7.66978190961001	8.81348002186704	9.85265599608445
H	7.75361094274213	9.24645107554715	12.92380964369211
B	4.91737147447024	11.50371251635576	9.93739315964361
C	5.08706145926807	10.06273625093937	6.29374491567587
C	7.37071614242905	10.24207890811721	5.26036743551362
H	4.84873195031502	11.05508591726809	5.89284598520775
H	4.50470935769618	9.90166179928680	7.20315377904270
B	5.22960960613514	12.00026404909450	11.60794637777722
H	4.22703434263962	12.10380774697228	9.17151027678832
H	10.02628260370167	14.74873203662527	11.02903255890551
H	8.52813281815074	13.86150130681516	11.38566184466234
H	9.21539981239743	13.81557529202053	9.74911507636109
H	6.70115642942182	7.79661977870165	6.20773248264719
H	8.01531169774212	8.40951177574250	7.23405723458778
H	6.38624509073934	8.21069818674539	7.90440961791699
B	5.51267060442415	10.56224919797660	12.61532937382104
H	7.32093005755384	12.44288349618302	13.00641791009108
H	11.10780745601016	13.53744508604568	12.99887807883813
H	12.26361280816522	11.79168559273162	10.66585123459713

H	12.20569526744799	13.56532712243703	10.73842899575832
H	11.48428302937710	12.70180637332457	9.35969313058419
H	4.69350667814684	12.95332575665028	12.08568250647230
B	4.38437345755439	10.46388482687474	11.25820307142724
H	4.74240561777202	9.03467994028117	9.06203858847849
H	5.34287520604977	8.08245456379030	11.77758420331885
H	4.77228824418047	9.31986935036873	5.54840999417280
H	7.14768866347871	11.25170543436110	4.89908392264544
H	7.08129496445369	9.52749174070852	4.47954209746049
H	8.45155069367378	10.16012215549718	5.41758043163898
H	5.12222885694186	10.47369472648161	13.73436104662875
H	3.22466740865271	10.28125824846391	11.44498285552521
H	6.97417178735024	13.13961738924951	10.04319189318059

Cartesian coordinates of [Na(dme)₂]**B** (TPSS-D3BJ/def2-SVP)

C	8.00361926883751	11.00193458114311	11.23791110447305
C	6.70684510556462	10.58468740043408	9.86151883835207
P	9.73206330414407	11.15138876601513	10.64516125770163
P	7.52718170168603	10.43621236751708	8.14935486618870
P	8.96041238911819	12.15361445745343	8.26638581709302
C	7.21341840200389	15.66691254404417	8.48669159026927
H	7.75421733102531	16.62652577886269	8.38087614995642
H	6.77045635930401	15.39275874662410	7.51997947691277
H	7.91176760295679	14.87027996643121	8.79704006353971
C	3.44308045925721	15.71374393967451	12.57149486288159
H	2.97019860009794	14.72940337142906	12.70338271622359
H	2.71164887896802	16.42406910389093	12.13585864374156
H	3.77298544212257	16.09235389839487	13.55839667726454
O	4.55545902308730	15.52629619284051	11.70423447899824
C	5.32181320627629	16.70930787092971	11.48644786214029
H	5.63975567254244	17.14259247165563	12.45651813995419
H	4.71084372975607	17.46302311869356	10.94708060016442

C	6.55136641682131	16.34713445732012	10.67830006111688
H	7.17270904768527	15.61270206425087	11.22626469238534
H	7.15710824121436	17.26150737465397	10.51542282674889
O	6.13387931640964	15.80555567678526	9.42435262448234
Na	4.58966307926688	14.01224140040274	9.93756372830726
O	8.74947742761086	14.01875106232208	6.12546501908269
O	3.24224746139866	15.01455938410066	8.23304829140507
O	2.36599510935477	13.11454206857885	9.98511012249721
C	1.42636693046937	13.75088903653840	9.12603282848794
H	0.97348841951885	14.62557425645067	9.63870032617133
H	0.61267353369590	13.04794423186936	8.85468963565156
C	2.14088092233557	14.18865794815678	7.86250694270239
H	2.49928281658419	13.30771744087839	7.29153165133859
H	1.43169135214145	14.75333773450913	7.22363422371565
C	8.54286098142439	13.07584891731065	6.82116841924225
C	3.80116239632483	15.74259806242534	7.13912978013586
H	4.22963991769282	15.05943523978952	6.38040230829219
H	4.59331414035413	16.37474535178913	7.56271955425109
H	3.02938908928088	16.37707541960387	6.66087016687382
C	1.75197842006944	12.39497485417693	11.05628205070698
H	1.15392348750681	13.07430753787293	11.69588039478741
H	2.55894632875880	11.93746723316685	11.64352395872943
H	1.09317640402008	11.59886512612312	10.65978902128592
C	10.41737972393748	12.81210780480645	11.32377299267333
B	7.41026606520338	9.41741988020424	10.93411964929599
C	6.13629439570125	10.87447890482660	6.88834616132709
B	6.67341287856260	12.04146340758538	10.71193169157291
C	9.52988229052274	14.04948727206910	11.15127694357945
C	5.04852394557028	9.78828636395870	7.02568003415515
B	7.10840728972569	11.78561904651792	12.43298716409725
B	7.56157766602289	10.07255962081314	12.58296490872769
C	10.77187882828156	12.60781714694403	12.81074021433115

C	11.71223474052753	12.99136920063137	10.50087876448949
H	11.43043323570862	11.73188825641013	12.94211811974477
H	9.86835494754779	12.44643000936057	13.42258664058171
B	5.68999576045695	9.40271727875869	10.47768790171156
B	6.14892801867128	9.08684509330750	12.17138779438569
H	8.17098898402539	8.62211267313019	10.47199684523095
H	8.46631448908822	9.70393982782570	13.27219499436612
B	5.19178356790267	11.09914772933611	10.36143978715928
C	5.50157521994315	12.26780143352866	6.99340790215440
C	6.82199839066033	10.69812662151893	5.51371970250972
H	6.26579247278313	13.06045972871308	6.98276359978035
H	4.90461967666132	12.35663681968173	7.91396785780718
B	5.40528491803484	11.85289647573662	11.94753820374367
H	4.40264742751248	11.48661085417240	9.55153097379367
H	10.07116355406092	14.95491704126605	11.49212014431703
H	8.60378067074884	13.96686977033705	11.74198683435669
H	9.25939605451425	14.18313293673724	10.09089675369686
H	4.34062327632258	9.87689266393738	6.17914618468202
H	5.48860952259690	8.77654105182361	6.99974380569439
H	4.47671761607040	9.88960160871503	7.96092474625229
B	5.94094208713145	10.59480411324394	13.09488251982595
H	7.62812577139904	12.66237693074654	13.05593315637556
H	11.29804813556719	13.50104774389098	13.20470852632399
H	12.36050052122296	12.09958662940293	10.57882403001671
H	12.28251756237486	13.86316690929323	10.87542448054920
H	11.48294311337405	13.15532476559279	9.43235033114863
H	4.72507053987845	12.78660630261660	12.28494338660435
B	4.78238869354638	10.17412200453914	11.81387352967170
H	5.31036744741857	8.54736898753799	9.73322831779683
H	6.00361655475165	7.99271342052109	12.63971020057520
H	4.82019491398728	12.42943842673807	6.13524893960339
H	7.59659415687149	11.46269784511831	5.34023440693618

H	6.06158039458514	10.78621218386887	4.71455953904190
H	7.29129504683380	9.70203438181199	5.43391850964869
H	5.63630011653365	10.62351052635504	14.25568205608111
H	3.63940678786087	9.88182438781944	12.04195374762678
H	6.92985781261012	13.05250046314039	10.12529823170263

Cartesian coordinates of [Na(dme)₂]**B** (TPSS-D3BJ/def2-TZVP)

C	7.95332912148464	10.99417511849096	11.21166869890638
C	6.70301096268585	10.61316143069081	9.76154617537973
P	9.68454763965731	11.14677258528899	10.68230654872409
P	7.61651808223836	10.46037960141260	8.11444505267935
P	9.06126978644251	12.12888286951699	8.32082197494714
C	7.12549463029487	15.62080764535766	8.37913588285768
H	7.65979070980107	16.55967709007699	8.18902331321119
H	6.64429857753793	15.28257576038440	7.46229179155617
H	7.82298774207636	14.85024766276192	8.72393498768118
C	3.71483403236647	15.78360250170046	12.76599645311892
H	3.31235117937022	14.79902177818815	13.00766653764479
H	2.91925876590628	16.42551103192275	12.36214505756901
H	4.12899661055285	16.24236763567851	13.67313554276510
O	4.74533457061460	15.57946998406142	11.79564917654968
C	5.41274259122031	16.79534673167954	11.43509076786279
H	5.78415446957368	17.29773674234502	12.34027719744418
H	4.70946883791059	17.46618595178606	10.91896502911592
C	6.58035281774778	16.45098567814646	10.54028098143262
H	7.27199788173764	15.76834603374336	11.05098115480378
H	7.12288946546086	17.37250435273700	10.28225708862907
O	6.07668653370975	15.83641077416327	9.34645679871060
Na	4.58208695381867	14.01770162243363	10.03506944374073
O	9.02805221469637	13.99756858473601	6.18227940581672
O	3.11566248145437	14.89490841615461	8.31925946009821
O	2.31058485348635	13.14698136192978	10.28753108379403

C	1.35168813627910	13.67285511748221	9.36770193845608
H	0.89817551542603	14.58562308636436	9.78356098675133
H	0.55601531717334	12.93401767970257	9.19014912216661
C	2.04723694896828	13.97500471240502	8.05955886851038
H	2.44743914189261	13.05638108234921	7.60637409673485
H	1.32470892792192	14.42559167567546	7.36375399186786
C	8.74929934661269	13.06553360520097	6.86127235842408
C	3.60126961880551	15.52134721541459	7.12269590932769
H	4.02062638757776	14.77772064415138	6.43338362480297
H	4.37659282839008	16.21959675618378	7.43648452686314
H	2.78658092962011	16.06308454238558	6.62472178927288
C	1.68662898993319	12.59165809127723	11.45392331750542
H	1.12029361488072	13.36481605182337	11.99217577916895
H	2.48483440925836	12.19858807729117	12.08170238131722
H	1.01025717321517	11.77644085744299	11.16785733729384
C	10.33602489082754	12.79259231913739	11.38852663264803
B	7.34539018552948	9.42780568834059	10.85308643637454
C	6.31691683259720	10.90077270742562	6.78730967759154
B	6.66012605759192	12.05301002538593	10.63268567574683
C	9.46781109481933	14.03667961024376	11.19015350631615
C	5.20292545903508	9.84174607253624	6.88002243788669
B	7.01297063409519	11.76941928572481	12.36679930601857
B	7.43076970558294	10.05176373474549	12.51316117674735
C	10.62950104193453	12.58704037386940	12.88506420893986
C	11.66503355140698	12.97736222276254	10.62971778835343
H	11.27652492340387	11.71767588665834	13.03934182482189
H	9.70928319731027	12.42906471101016	13.45502199216913
B	5.64952570079583	9.44357266405227	10.32047867731148
B	6.02871344449148	9.09962457447419	12.02248251517293
H	8.10507777760475	8.63709052614142	10.41643819513676
H	8.28748469697525	9.66245348367194	13.22851168703847
B	5.18043479758525	11.14393435640988	10.20482265750511

C	5.70068546560249	12.30093742139705	6.82619758058128
C	7.06342378319269	10.69042609775977	5.45372961199514
H	6.46668589088222	13.07312381270254	6.73870068102185
H	5.14268618181708	12.46000778179343	7.75187906801527
B	5.34285644702780	11.86457899560198	11.80614778378186
H	4.44608958305414	11.56060984538853	9.37289697674122
H	9.99955680567686	14.92164016849485	11.57004498444001
H	8.52191890945355	13.95414874398638	11.73129386589321
H	9.25425264889263	14.18969224054924	10.12833684865706
H	4.55955644724014	9.92713828231244	5.99379477107194
H	5.61879185272802	8.82943213775744	6.90378119658283
H	4.58100373141397	9.97664628846265	7.76761110125908
B	5.80188105201000	10.59054308652544	12.95498363282892
H	7.50713728733371	12.62323612582607	13.01726630386266
H	11.13723392055927	13.47405965305065	13.29250919814645
H	12.30405549863194	12.09256653059512	10.73147934219952
H	12.20854286158667	13.83994162002400	11.03766084538362
H	11.48803168065689	13.15036229565595	9.56230984015164
H	4.67230760429829	12.79354234169259	12.13585695010618
B	4.69751332923791	10.20760438268246	11.62111601464775
H	5.29622253609767	8.61133669402851	9.55842822439933
H	5.84797162667489	8.01398783753553	12.46199808078105
H	4.99994755958410	12.41012385734548	5.98579659121465
H	7.86840077989700	11.41749749559721	5.32034940515255
H	6.35229681919380	10.80353727979348	4.62488485416406
H	7.49210892857333	9.68419715146027	5.40314426309716
H	5.44700639417626	10.61189746443359	14.08728243917840
H	3.55415341992108	9.93597609243935	11.79378431764810
H	6.95042116519810	13.06106089198112	10.08093219771585

Cartesian coordinates of [Na(dme)₂] **meso-1** (TPSS-D3BJ/def2-SVP)

C	7.80643426700845	11.10838166463167	11.11010664259644
---	------------------	-------------------	-------------------

C	6.65934128440012	10.56793451896397	10.04268866946798
P	9.53347683861588	11.24570235220665	10.15377276081611
P	7.48441544901477	10.34461444764422	8.25871792061718
P	8.78222444264266	12.10503671029911	8.29188274811525
C	7.10887041371438	15.54907592783695	8.57717031680959
H	7.79282560676762	16.41668715663834	8.64670128164046
H	6.65985356485843	15.52227375548598	7.57301078941468
H	7.66391400949685	14.60410206117441	8.74512283002227
C	3.09561314023700	15.87797305466168	12.38879943250559
H	2.40461689607367	15.02405937968041	12.32552438817305
H	2.59896209528623	16.78502782629434	11.98939200012534
H	3.36683137767092	16.04949444126752	13.44886142083712
O	4.24152270741183	15.54067943887827	11.61875538391789
C	5.24469218575290	16.55389739909245	11.60063995878223
H	5.55549673385188	16.80564959207916	12.63517991153528
H	4.84472965036782	17.46991012030221	11.11824322074269
C	6.44319789572672	16.03308064763526	10.83136654405477
H	6.87269708701832	15.14400656336181	11.33342272644324
H	7.22237227991520	16.82069851308558	10.80166548472055
O	6.02141924821230	15.70445506635113	9.50684859860186
Na	4.39230114773442	13.96079965515755	9.91689811548232
O	3.05861005055873	14.95783604821828	8.23300777782673
O	2.21462473778901	12.98356330809090	9.91199577913380
C	1.27353033375879	13.59790368516252	9.03904995848761
H	0.76939677053454	14.44193722027376	9.55534774141072
H	0.49866870782135	12.86761982960669	8.72883522935967
C	2.00758411025105	14.09354212147890	7.80744182535110
H	2.42383405598575	13.24117640963872	7.23214446627559
H	1.29520446642496	14.64043873963003	7.15666912475296
C	3.64631464904894	15.71398884066973	7.17507690160298
H	4.12016075409655	15.05139919761577	6.42491003772430
H	4.40852032659923	16.35452137319632	7.64056760295341

H	2.88287818123776	16.34141777995993	6.67442952362601
C	1.60872985098960	12.23843608515947	10.97012221425199
H	0.98629036032464	12.89543224481347	11.60988575799885
H	2.42127077306038	11.79866911231316	11.56395186762207
H	0.97553277678300	11.42849843495244	10.55995934832250
C	10.48115878080683	12.70545754638427	10.95721688656577
B	7.36436253353525	9.44504439781339	11.13648521682412
C	6.13784208329423	10.86465234899465	6.98759604486074
B	6.51223540635733	12.12798254917303	10.70026592167334
C	9.77677371955745	14.06411165438284	10.87384452378424
C	5.01603317680110	9.80962306135364	7.01674483565572
B	7.08454074733882	12.01971905349805	12.36786318571991
B	7.62255014142525	10.35145407303435	12.63293063019774
C	10.78596784579266	12.33090715417224	12.42027810356420
C	11.79890643601250	12.75144165742052	10.15170303206637
H	11.24446667188237	11.32863647976908	12.48589070546464
H	9.87528470211641	12.33130508391555	13.04063467562647
B	5.63560342704032	9.40672451489463	10.78337558010436
B	6.20873415375632	9.27194780051881	12.46881551014459
H	8.14595629185974	8.66082283715371	10.69493360528917
H	8.61086501814706	10.12683830202679	13.26849916325633
B	5.10556555093538	11.07034561133824	10.52133823635603
C	5.56499520037867	12.27678129388376	7.16976768512455
C	6.88790290088404	10.78666641652143	5.63930293529057
H	6.37852187245866	13.01036767702110	7.30442280767419
H	4.90089091937770	12.31265239989192	8.04850538717867
B	5.34250296672585	11.99052944607599	12.02185454838737
H	4.27993365216800	11.32015898520362	9.69081866125728
H	10.41770100334942	14.85337563300385	11.31498300567302
H	8.82242949041407	14.05354547462982	11.42365229562039
H	9.56755096633168	14.32791312148555	9.82349996724690
H	4.30175660167660	9.99269292758535	6.18967818210786

H	5.42811531700398	8.79260113966150	6.89691878055921
H	4.45342491334030	9.83806674237275	7.96465803375404
B	6.02954735219290	10.87645409870951	13.23725278893767
H	7.67241291547431	12.94600766217989	12.84522526629878
H	11.49322706709902	13.06395692048369	12.85455363433610
H	12.32270945608724	11.77972000283573	10.18843769908229
H	12.46982943685989	13.52200870219418	10.57825378857853
H	11.60970293789487	12.99760172421109	9.09211946752695
H	4.63492215786899	12.92202447940141	12.30611063696279
B	4.79594302126589	10.29025158104142	12.08625257890772
H	5.20928578640280	8.52159318944382	10.09959224844200
H	6.12830073030707	8.24214155456950	13.07818660026940
H	4.96272744437566	12.56168127980798	6.28378425682233
H	7.69064725538163	11.54266946360269	5.58586607097843
H	6.17974114839746	10.96174227184327	4.80594567591677
H	7.34741630372450	9.79229716703577	5.49767919948094
H	5.81367639583800	11.00580717007391	14.41123412402730
H	3.67993453475877	9.99381215082262	12.42068127523755
H	6.74591433826031	13.04558447505434	9.96672023904444

Cartesian coordinates of [Na(dme)₂]C (TPSS-D3BJ/def2-SVP)

C	10.17058199050027	11.69779830372318	8.37666950102414
P	9.84006402457538	11.16357392374386	10.72327323738206
P	7.40305279784649	10.47091231514983	7.84001398259782
P	8.70929752298412	12.26510312295607	7.59340485199399
C	7.02325964936555	15.61121663704058	8.36568228393976
H	7.55346532336924	16.55948490216799	8.15225352191349
H	6.49921757510721	15.27502934458565	7.46005478305608
H	7.74797148641801	14.83314413786423	8.66602288371314
C	3.66594566650672	15.81157577646234	12.78248603277453
H	3.24390151175481	14.82084490394296	13.00618446626548
H	2.86772828753436	16.47875837042495	12.39933454601813

H	4.08754820189807	16.24508490837557	13.71015073759296
O	4.68449366567156	15.61650507998437	11.80753876190280
C	5.38335048861927	16.80759917609769	11.45554389125500
H	5.78050103675428	17.30258201470527	12.36513276390024
H	4.69758758673338	17.51407535832251	10.94227240021790
C	6.53998616679058	16.43707658225001	10.54953901682629
H	7.23321176824718	15.74893319959394	11.07064406367328
H	7.09818440885525	17.35735258571466	10.28186930518014
O	6.02132932866959	15.81801729753183	9.37128895808746
Na	4.52523560665736	14.03575412707037	10.10368171295693
O	11.35718998958541	11.71024111668264	8.27249912139982
O	3.02911636528863	14.86901612673362	8.46219808773061
O	2.30555192708742	13.14942827924106	10.44529516852971
C	1.31882679642655	13.57265122723982	9.51356425358902
H	0.77533890991852	14.45658476046565	9.90957052452250
H	0.58085899743539	12.76388402996101	9.33471774629913
C	1.99746689877723	13.91667189473564	8.20052698454859
H	2.42907308580512	13.00941507709366	7.73057453997810
H	1.24387611374703	14.34347762938607	7.50888983525221
C	3.43580440028497	15.61402934409787	7.31496889600076
H	3.84842015051038	14.95170909243689	6.52997173436939
H	4.21328711505865	16.31032432441548	7.65953907781368
H	2.58111309467125	16.18160721574527	6.89728837146660
C	1.75008767512306	12.54656251587192	11.61409874644233
H	1.09511946111651	13.26109292833776	12.15247084847216
H	2.59219583939474	12.24854838350828	12.25257027835195
H	1.16412130702556	11.64690365787872	11.34631818273356
C	8.10817292407618	11.02779341910364	11.14585551804617
C	10.41320995500983	12.87625661316170	11.39557662729588
B	7.40363283586566	9.55139934705596	10.59258518361811
C	6.60901463861740	10.65614657774858	9.50655086269697
C	6.07424704345614	11.01281179914821	6.55856902186469

B	6.73099495998800	12.02729218024558	10.46148249102511
C	9.52778804215122	14.06776817896861	11.01143860496193
C	4.87442809108916	10.05621661622017	6.69680052804843
B	7.10445788576697	11.76798241676712	12.22470519971005
B	7.52537346815495	10.02277154624524	12.33180049855386
C	10.48015116101560	12.70817407029974	12.93171601459151
C	11.85232390008155	13.11163912273772	10.88810213495218
H	11.16215566697305	11.88455631990582	13.20587112300957
H	9.49332304004503	12.49574190792836	13.37117668304132
B	5.64852624224144	9.47750624727815	10.13554691411218
B	6.10996015730165	9.10172412642665	11.80873182734029
H	8.14371506078573	8.74522337813361	10.10815709180727
H	8.35146881195865	9.54973673391735	13.05627448035839
B	5.16213821734157	11.19582772630186	10.07369893333543
C	5.61483119709092	12.47380035614335	6.66947891132589
C	6.75442976856896	10.78512965077939	5.19063573576681
H	6.45891363013919	13.16717154307955	6.51048493199703
H	5.17122814252338	12.68315480663616	7.65625397359112
B	5.42361607714193	11.86497411842883	11.68621017797520
H	4.36196473150469	11.65878211583617	9.30814893133621
H	9.98048183262505	15.00957541247829	11.38129094269726
H	8.52277960560642	13.97744692472889	11.45210563949743
H	9.42119924468080	14.13770785701806	9.91528140328671
H	4.17445998559281	10.22279405924866	5.85519091402318
H	5.20050781742840	9.00238866748391	6.66776174430725
H	4.32444304492714	10.21718078081165	7.63732006568911
B	5.89706407587482	10.56123264121529	12.80482776341964
H	7.53204057854521	12.65567180147245	12.90163325434688
H	10.86822620908309	13.64027523883866	13.38900006313053
H	12.47695398732098	12.20838809893951	11.00873377606055
H	12.31148058908002	13.92497750947837	11.48233546463761
H	11.88101824372601	13.40043378186681	9.82699336076868

H	4.78432627582782	12.80211403214373	12.09072665056728
B	4.75170663923293	10.21261126139791	11.49932784031534
H	5.26381578809265	8.62015469191741	9.39169956251860
H	5.95260874235941	7.98766728862991	12.22489571633159
H	4.84975280877839	12.68777727236215	5.89654299627860
H	7.65703044106602	11.41209005226686	5.08166654135003
H	6.04801320221355	11.04323398117459	4.37857041077354
H	7.05245839414725	9.72936602784985	5.06970780592041
H	5.56740540404990	10.55472029141343	13.96010667707176
H	3.60322409523846	9.93075678138525	11.71470199366413
H	7.00117812349863	13.07033395584156	9.93697591321065

Cartesian coordinates of [Na(dme)₂]C (TPSS-D3BJ/def2-TZVP)

C	10.19062080783950	11.63185786914463	8.43672823198374
P	9.82228952667272	11.17327078972525	10.76265957053320
P	7.43793944063089	10.45587000872419	7.85265271764831
P	8.75880963834469	12.21998870501292	7.63217043438037
C	7.03497507685384	15.62833127445657	8.31085830095552
H	7.55734850145871	16.57069604283636	8.10105997887197
H	6.52569452675335	15.28323297535836	7.41092190562684
H	7.75015519596676	14.86409399847235	8.63411562220851
C	3.78830359863774	15.74337299930602	12.81715779871783
H	3.43720715988406	14.74700358234190	13.08825361326810
H	2.95157639820291	16.34573321916202	12.43607340648675
H	4.21874171889337	16.23327892848406	13.70016647692975
O	4.78743900051022	15.56540884478695	11.80949535980117
C	5.39458930338798	16.79837866281934	11.40797434848860
H	5.78107345011780	17.32847009842885	12.29092897993244
H	4.64954671962377	17.43626671904384	10.90861031739484
C	6.54078939973134	16.48199377271384	10.47573665971023
H	7.26893903613024	15.82453303135227	10.96796692528292
H	7.04572843626046	17.41687709241234	10.19042965183393

O	6.01453555542303	15.84125579534227	9.30497264109273
Na	4.56546558016318	13.98604594069863	10.06642656873800
O	11.37522860179985	11.60197389401244	8.34306428537078
O	2.98719885708041	14.93180557584870	8.48013336301575
O	2.29683358611458	13.13748272698614	10.45278665595496
C	1.28333166873658	13.70335114002748	9.62159279002420
H	0.87449841704030	14.60981836606683	10.09437884752173
H	0.46475189811461	12.98187565561939	9.47961098201164
C	1.88759903292392	14.03389416310742	8.27536845928950
H	2.24014778972367	13.12288663206458	7.77010967071202
H	1.12419650737078	14.51415066267750	7.64614870074929
C	3.39305979584032	15.58043403945767	7.26702060733406
H	3.74224347539589	14.84746442341724	6.52840145407406
H	4.20528318972294	16.25457666820451	7.53758672490386
H	2.55485496829248	16.15112125015844	6.84595752558871
C	1.75091086431858	12.53881946184545	11.63674179920822
H	1.22689884308859	13.29200534903963	12.24223525635207
H	2.58833461787439	12.11909293690343	12.19191150218699
H	1.05192492061803	11.73762040379505	11.36585550119620
C	8.10190343499228	11.01819077823060	11.16109266610554
C	10.35482162930743	12.88865520657190	11.41188822531642
B	7.41428390310025	9.53926376694217	10.59129362875172
C	6.62681516148603	10.64005317190097	9.49569603684004
C	6.14209799159587	11.00276354389810	6.56670141733653
B	6.72348024861714	12.00708084574490	10.45315636430131
C	9.44182795438980	14.06055666203777	11.04703898449356
C	4.94376318177002	10.04623857983984	6.68094785132923
B	7.07502995255286	11.74549258523864	12.21940032314783
B	7.50467991599169	10.00722511737533	12.32931273745010
C	10.44718658866117	12.72804518423333	12.94454662390602
C	11.77578441181995	13.16942422683042	10.88773600555050
H	11.15163894321001	11.93249673865050	13.20870968152927

H	9.48031044201718	12.49012636948247	13.39295462994348
B	5.66963876042072	9.45489676698148	10.11124159578468
B	6.10969581987291	9.08145464559844	11.78326466646292
H	8.15960323396720	8.75037462098688	10.11899296719606
H	8.31428331760728	9.54533126305278	13.05702023872674
B	5.17115399266174	11.16328015617370	10.04542398633349
C	5.67632001987043	12.45790853756596	6.67323890203041
C	6.82803188038852	10.78460035174458	5.20400013966235
H	6.51271360882659	13.14750773626393	6.52165158132490
H	5.22860072259373	12.66012474334988	7.64988201373319
B	5.40747451064096	11.82925197203742	11.65613332852703
H	4.38549205933649	11.61898298566237	9.27728586975375
H	9.88576305997727	14.99937588992065	11.40975078668567
H	8.45507094953120	13.95278795179069	11.50267369273845
H	9.31983121530050	14.12920455971885	9.96146311286894
H	4.25561817136501	10.22994944932174	5.84443217751035
H	5.26909829316266	9.00227226477363	6.63249396943440
H	4.39412922918323	10.18771810148362	7.61431261058809
B	5.87216469000006	10.53174024414937	12.77648560522288
H	7.48250339728492	12.62239805072700	12.90057106598821
H	10.81123742165343	13.66711037534535	13.38602852031399
H	12.42424123256330	12.29219649302342	10.98763514276469
H	12.21272972075006	13.98468992776234	11.47976323578249
H	11.77544311424539	13.46914224131829	9.83830990181935
H	4.75916458933860	12.75156455593424	12.04728626142520
B	4.75211296221878	10.17804921053784	11.45917287486183
H	5.30530276157197	8.60823004769557	9.36627721880065
H	5.95620908599457	7.97861844608214	12.19061457927557
H	4.92168586923599	12.66411952188373	5.90027588329549
H	7.71112681637600	11.42199914266601	5.09346050175585
H	6.12018422459374	11.02671616062866	4.40012497711752
H	7.14035335131664	9.74197960742106	5.08710793621888

H	5.52849706560759	10.52215838383017	13.91322659934158
H	3.61578330882516	9.89115329902919	11.65678051052759
H	6.99165567866299	13.04421481870715	9.94023173474549

Cartesian coordinates of [Na(dme)₂]**D** (TPSS-D3BJ/def2-SVP)

C	7.99209729797715	13.27780591043618	8.61315323815742
P	9.03011013398604	11.93122900358439	9.47353898460275
P	6.47491608883247	10.59904016434508	8.53551193064256
P	6.45700602125037	12.69846671226819	7.87244545776134
C	7.07460458703857	16.17997326336145	10.90881617873765
H	7.24789422192567	17.21970346856500	11.24984874706388
H	7.47362125775027	16.02787472566830	9.89659949086591
H	7.58651322608515	15.48050758689141	11.59414365037517
C	2.34150268011116	13.49121001367282	11.58110251304449
H	2.32801527775692	12.63365571328214	10.89331433788169
H	1.39564054917208	14.06145310828810	11.48310707778476
H	2.43772225410630	13.11361646333161	12.61659998835221
O	3.46810746297460	14.28776409467366	11.23076448808917
C	3.63693695616904	15.44371660128853	12.05650871320240
H	3.24107861885690	15.25030867747900	13.07182828671062
H	3.07910409554215	16.29801044592816	11.61999329177871
C	5.11584363821356	15.75765355374961	12.17309522541512
H	5.63225492098176	14.94044367098588	12.71302794589693
H	5.24108595655308	16.69715807156706	12.75173463577032
O	5.67069473121000	15.89552821806052	10.86912169711602
Na	4.68645648724049	14.55090526589856	9.19405368567646
O	8.38960808182751	14.45762668860681	8.50552025055163
O	4.97163251757091	16.16715973193866	7.39760249292690
O	2.81601252461787	14.46676683808481	7.69740656800869
C	2.99434394643925	15.20341163055610	6.48645454273170
H	2.44831683297097	16.16715744028892	6.55449184786659
H	2.58836832671044	14.62870103642531	5.62870301932641

C	4.47348771533245	15.44957262650062	6.27093483088006
H	5.02035448598125	14.49091451486757	6.15356702186199
H	4.60264690706169	16.04748256292238	5.34477022383252
C	6.30245949967808	16.66483111364234	7.19812004304002
H	7.04393170535282	15.84391081436066	7.20289593342408
H	6.51015638189878	17.34380922656722	8.03862550548804
H	6.35785098807486	17.23480966858253	6.24966575323591
C	1.45992752074283	14.10987631581299	7.92915076477807
H	0.82119497972753	15.01058813639924	8.02991064220257
H	1.42807721252095	13.53239422401703	8.86342513733817
H	1.06944714928904	13.48274469980163	7.10337807292281
C	7.91116574919969	11.49144414001623	10.97823528723600
C	10.59701239651764	12.85020766780926	10.06171000404109
B	7.81032675626136	9.76972521056415	11.10358606067226
C	6.50731206899941	10.71727854581749	10.47364415010630
C	4.67936678818583	10.12581776824080	8.00548987148473
B	6.39105700931065	12.24829003946521	11.24101787262444
C	10.37768439538753	14.08512167304366	10.94619918667795
C	4.29159508177137	8.77702958330221	8.63611555485032
B	7.63586191122618	12.28017760059486	12.48646123494069
B	8.51998100700800	10.74446285108699	12.40193899630372
C	11.54818870212567	11.84697775030006	10.74356755921382
C	11.22834624556725	13.27048436916503	8.70862381627749
H	11.65753725174560	10.92447181291164	10.14656563429431
H	11.20147239054163	11.56795446772719	11.74949679252359
B	6.13656664518327	9.40972481786586	11.52988307952971
B	7.39154706498345	9.42544451801409	12.78582132551414
H	8.44902192930757	9.13175261890648	10.32500076401476
H	9.69847711427734	10.69758562953742	12.56886507534180
B	5.25287640815133	10.94636607644696	11.60708467318476
C	3.59274461991170	11.17367756136235	8.28719846390434
C	4.83279984210690	9.94595996008173	6.47695236058773

H	3.78826471081579	12.11460286318242	7.74760973871936
H	3.52158942550455	11.39696580367939	9.36360302875651
B	5.94831527199946	11.92113121744618	12.91980424733705
H	4.13106555393933	11.02492687476355	11.20709740060179
H	11.34464763680723	14.60486729765817	11.09175437907902
H	9.99420115696970	13.80583690710307	11.93939551168452
H	9.67634097099965	14.78131057762090	10.46341444048253
H	3.39643695804427	8.37963537580364	8.12041526902879
H	5.10299259153781	8.03526527706506	8.53799894373060
H	4.04734019495447	8.88183660827015	9.70410553206612
B	7.27721951503856	10.98417600494100	13.65127408446018
H	8.18770641136696	13.31468554107541	12.70737505067601
H	12.54688095787177	12.31291929330420	10.84479931366599
H	11.36553352278775	12.39874624846762	8.04341354511208
H	12.22570112848325	13.70563162719185	8.90790598256303
H	10.60820218637066	14.02208458327861	8.19692956270456
H	5.28163724676502	12.71237355523390	13.53003459586059
B	5.79161594367483	10.15454895314713	13.10767200407899
H	5.64643029303019	8.42493400928571	11.06959720969896
H	7.77325166911010	8.41023130899025	13.29660474295139
H	2.60960895383229	10.78580054659619	7.95366884407044
H	5.14915340783365	10.88667406918296	5.99221852514692
H	3.86059966326658	9.63952258786308	6.04570705060756
H	5.57879653893307	9.16811812160076	6.23849948268187
H	7.58072285064642	11.10035260539955	14.80637302136304
H	4.99812701635078	9.66371397647201	13.86287564384533
H	6.12325660576541	13.20242050041685	10.59481587036112

Cartesian coordinates of [Na(dme)₂]E (TPSS-D3BJ/def2-SVP)

C	6.49456686982452	10.85422939792117	10.52929232076239
C	7.75520412822758	11.79911060549742	11.13561280157111
P	8.77664388712482	12.73412052729104	9.90383100651078

C	10.65149465650577	12.68974772461691	10.16112322258218
C	7.97779176776211	13.61118220866066	8.45862033655217
P	6.64719648880107	10.86482570636116	8.58865694072639
P	6.38348642389290	12.93394974514523	7.93486222675008
C	7.10534945101947	16.13276124011865	10.70072444757711
H	7.43643642816867	17.06076242918274	11.20715211965521
H	7.39332317039243	16.15674321917783	9.64140296406524
H	7.58893757022726	15.25502121200419	11.16852851942957
C	2.32312084379476	13.72160398575246	11.73556604597802
H	2.29771970082115	12.81659192674065	11.11049451710508
H	1.36723496241839	14.27393422475310	11.63282819441566
H	2.46178398803363	13.41619713990013	12.78954115862122
O	3.42773030395366	14.49991286540684	11.28858294696471
C	3.70531958950353	15.65758370317087	12.08325578124048
H	3.36420905722280	15.49805654372792	13.12377132789166
H	3.16596753388188	16.53374603543136	11.66792091503504
C	5.20440638126854	15.89443965299751	12.10082586768485
H	5.71082232029043	15.04847940438315	12.60314865894315
H	5.41971389599499	16.82154165695962	12.67330047964533
O	5.67619113596592	16.01629138244093	10.76211965926958
Na	4.52200092671047	14.67524326384059	9.20108045155347
O	8.50035532619611	14.63490958637919	7.99788665145801
O	4.68527693076372	16.18425887866459	7.32737844587371
O	2.66719504043525	14.33080488312461	7.74177969097652
C	2.73936607674466	15.06838373717776	6.52002068071104
H	2.12894622784475	15.99137170084754	6.60556953453681
H	2.33866350435844	14.45829471819410	5.68473852238357
C	4.18672893455188	15.41396189605567	6.23586870648735
H	4.79343834902107	14.49323653893180	6.11122617504524
H	4.23397987891066	16.00219779355875	5.29568735981448
C	5.99335605085259	16.71645307799967	7.07591176996451
H	6.75430983590345	15.91503146649970	7.01445061933260

H	6.22765075815224	17.38035696226815	7.92121795968361
H	5.99081233440056	17.30897526686438	6.13961947943952
C	1.35972774314290	13.84703594947309	8.01968532296053
H	0.64135081886626	14.68233015049753	8.14490823472146
H	1.41633816299172	13.26966689112295	8.95331899333842
H	1.00335074270209	13.18382969980088	7.20700249277557
B	7.87832077346405	10.07404664281611	11.19401870565654
C	4.97662605313468	10.16281235152657	7.92034382247981
B	6.14803396969203	12.33683043774637	11.33457930483212
C	11.04412348984283	13.48768558052275	11.41993252733729
C	4.72632352515765	8.75927463421200	8.49949730120275
B	7.30834398811641	12.49217855405231	12.65571807377365
B	8.39569787324369	11.09581656135483	12.56098831285200
C	11.17409352898249	11.24269732637902	10.22757293404965
C	11.21663323545968	13.38257416920993	8.90069889234705
H	10.87860945923416	10.67731102121719	9.32904082879688
H	10.80103289507517	10.70819750143129	11.11431606147706
B	6.24926216736907	9.48040122429851	11.53604949298542
B	7.43917565335939	9.62570705869682	12.84603737361605
H	8.63096732972997	9.54835645729294	10.43526890218542
H	9.56028875013881	11.21335792389747	12.79040508329513
B	5.17209719411147	10.88995336629787	11.60174498780127
C	3.74775426619794	11.05638293654669	8.15747083130811
C	5.23878856628321	10.04052226712965	6.40129871401492
H	3.85500232192969	12.03226443502177	7.65549204628388
H	3.58123306918208	11.23607410643940	9.23209081046525
B	5.66694954883668	11.90379988396444	12.98282755270447
H	4.06660444644463	10.84546819096996	11.15001693688022
H	12.14548994125141	13.47754479716500	11.53556951394669
H	10.60235365063184	13.05514232103865	12.33178766630795
H	10.71127755762771	14.53569907329051	11.33661356573451
H	3.92338208768631	8.26519209520992	7.91945914840047

H	5.62994639741411	8.12797331928739	8.44067077124841
H	4.40393508557878	8.80264053382976	9.55075105922009
B	7.07058359589015	11.12301965966241	13.75497086752670
H	7.74478677006406	13.57913438192780	12.90085258680399
H	12.27956249725547	11.26440298154485	10.28592508589661
H	10.97353560383652	12.81041065639223	7.98965639891698
H	12.31712188171829	13.43308560609340	8.99894093233039
H	10.81697995987519	14.40115812240863	8.77812175362075
H	4.87148311064004	12.58325520128557	13.57374168094429
B	5.73802039913342	10.12487565732581	13.11129227661345
H	5.91469404553547	8.45191125041244	11.03402656531336
H	7.92973628390135	8.65440604389660	13.34955884649693
H	2.84301810349866	10.56030183180680	7.75216015509389
H	5.46001359544522	11.02488512114972	5.95298409058170
H	4.34145285816038	9.62041469158476	5.90763752676921
H	6.09173886502973	9.37016720419257	6.19644878489504
H	7.30365674327433	11.23217264792965	14.92693766681155
H	4.98618814372344	9.50530965160218	13.81216832321077
H	5.80318552019727	13.25905852099705	10.67715468693763

Cartesian coordinates of $[\text{Na}(\text{dme})_2]\text{F}$ (TPSS-D3BJ/def2-SVP)

C	6.66766797722115	10.87269405884482	10.80626873012325
C	7.77894336944760	11.99208740369443	11.43132842313022
P	8.76434148638437	13.30403405967486	10.48132415823692
C	10.33507526788158	12.55267158009560	9.67618921547176
C	7.76562968783978	13.72344548157849	8.91598324395924
P	6.75593314008998	10.67683476190628	8.90574957722704
P	6.56269171337423	12.71400236290302	8.06569595368417
C	6.78669974543090	16.34699897161924	11.22170950917955
H	6.86316411388748	17.40768391178127	11.53328660306728
H	7.41066257098481	16.15366077070846	10.33613399804818
H	7.12405756021194	15.69482431078603	12.04730204964822

C	2.62524273529930	13.54834260141061	11.57551454585950
H	2.62233864784117	12.63903912138235	10.95759128581913
H	1.61324464704637	13.71459942351745	11.99403920960814
H	3.34658338536601	13.41075048900228	12.39940236829754
O	2.99114738804088	14.63095497671102	10.71603133736741
C	3.12063504487987	15.88928629477734	11.38491296882887
H	2.36704853808217	15.98060026156615	12.19140945211358
H	2.91506919039723	16.66245837973445	10.62398145342156
C	4.52159322988453	16.09897262291783	11.94579302878900
H	4.77720265553080	15.32972646818588	12.70393907043508
H	4.56943902204343	17.09279065144601	12.43935882696307
O	5.43462615751706	16.03631200685219	10.85641573056363
Na	4.73315127284094	14.68619160993711	9.06758893447470
O	7.98341032856432	14.90519907932413	8.54391849940991
O	4.89591382190594	16.33480905474526	7.33063557012895
O	3.06478954561447	14.30483657715604	7.43177658318685
C	3.26902166513235	15.00750730364213	6.20863111159818
H	2.55576360001588	15.85577073273817	6.14528418333163
H	3.09479333167465	14.33690496157405	5.34169718012527
C	4.69569192184952	15.52211207249653	6.17421407479896
H	5.41853064813799	14.67961688552639	6.16657061034414
H	4.83789415193312	16.11925430202201	5.25007689150485
C	6.09826933503709	17.11493326676330	7.27217210579868
H	6.98705188676169	16.46003287536396	7.25193386118309
H	6.11633905443294	17.72283138344751	8.18948287232143
H	6.07663621262849	17.78332218656895	6.38837547496354
C	1.73410290018645	13.83336901637763	7.59459605499367
H	1.00948797097778	14.67161272547714	7.55535148930819
H	1.67876789879563	13.35351665166453	8.58160213562200
H	1.47564709172291	13.09508423531586	6.80961558495885
B	8.14626887177723	10.32277832438920	11.51674217589685
C	5.05435804983292	10.00340676510993	8.30440566903214

B	6.09535853875990	12.29432465649848	11.57521546362971
C	11.24469289453019	11.97378622126418	10.77614458545796
C	4.79576408135364	8.62632744494115	8.94246008822502
B	7.18684230775870	12.62035044898663	12.93116114332709
B	8.46756362537344	11.40318077184059	12.89137721537340
C	10.10498124270699	11.52516252367149	8.55865014578090
C	11.00964101388113	13.81604638471621	9.08485994612171
H	9.46427100282166	11.93499066339811	7.75980800919194
H	9.62923747791141	10.60554387230880	8.93203314138913
B	6.61351714906975	9.49047896902541	11.81527946951620
B	7.73297719118356	9.81132609959227	13.16342635454734
H	8.97603599884765	9.87406693030438	10.79217563871180
H	9.59486225617745	11.71255507862289	13.13242080542377
B	5.33141630684336	10.71838271988802	11.85604051084680
C	3.85132209299627	10.93546630231195	8.51438575373288
C	5.29604063594776	9.81350130877960	6.78729535990773
H	3.98992199266242	11.89097584152648	7.98147249034199
H	3.69011569939379	11.15140771167459	9.58215564251021
B	5.64420421299031	11.80638321485666	13.22294703550696
H	4.25491199158436	10.50453398885290	11.38786722601235
H	12.23577477315458	11.74969768534315	10.33794843370653
H	10.84324406112318	11.03875468192477	11.19555669415279
H	11.38869292204405	12.69289401522529	11.60096961987317
H	3.95156896887633	8.13752530666146	8.41980591310180
H	5.67999261845840	7.97160270399520	8.85486650765765
H	4.53160913167037	8.70864254077358	10.00764721172058
B	7.12160619967928	11.23880761012840	14.04547263841359
H	7.44801859455267	13.75861454883745	13.18513791934058
H	11.08182682592391	11.25179906111646	8.11449389801956
H	10.37040037727628	14.30937407380905	8.33434919717720
H	11.95661636819450	13.51542047178846	8.59873783913783
H	11.24354658180350	14.55253074632613	9.87348950988205

H	4.74832609368957	12.36639608818897	13.79396084937438
B	5.97190344942790	10.05416947460037	13.37602947198260
H	6.45007473649311	8.42767193034419	11.29687280987365
H	8.34411815404008	8.92012847558428	13.68235265377439
H	2.93552301641605	10.45020613103432	8.12344473315377
H	5.50808342445518	10.77568380943912	6.28826162413682
H	4.39016185322528	9.37478061506088	6.32749536475633
H	6.14423618450283	9.13218173144548	6.59943873875441
H	7.29873857703505	11.39602838215141	15.22137693075025
H	5.29780249095930	9.33158675874544	14.05645585432654
H	5.61513304969998	13.15190002367927	10.90598075855403

Cartesian coordinates of [Na(dme)₂]**G** (TPSS-D3BJ/def2-SVP)

C	6.46580229495576	11.37590582133896	10.29767909145129
C	8.20565188812301	12.14899045208401	11.38303273024653
P	9.39463497371307	12.89236098444296	10.28862960057181
C	10.81564691323699	11.65160810605981	9.93500089937626
C	7.89828719522895	14.23959553073631	8.12799603603102
P	7.14350124106652	11.38131181360911	8.57232833984206
P	6.52891156326463	13.29379040311257	7.64998479738829
C	6.73018601558443	16.50088275013395	11.33110772160730
H	6.92234614871887	17.57905832977171	11.49808104848113
H	7.39198778383636	16.12654200475107	10.53777859667498
H	6.92546006605528	15.93905475472438	12.26201210535051
C	2.28575846732163	14.45571973094746	12.28596980827965
H	2.24376442352326	13.37738766580275	12.07550803016625
H	1.26927032960132	14.83408135305149	12.51204673677237
H	2.94303841179571	14.61415866483564	13.15968774034076
O	2.79952185842930	15.08794741605443	11.11184564784600
C	3.03255192418364	16.49336780448256	11.24968140732975
H	2.25303035053123	16.95605799919373	11.88615368609813
H	2.95779638351497	16.91210767425911	10.23180124855735

C	4.41528732175860	16.79125885667254	11.81427053726876
H	4.55760808786841	16.31061154562538	12.80395141617998
H	4.52994859520691	17.88822227635376	11.94751100179480
O	5.38222802824181	16.30106512974460	10.88977242239834
Na	4.54602708057437	14.37448051480295	9.67181763252576
O	8.49931372205477	15.25272484979423	8.12821151560857
O	4.03917140334709	15.94838841688660	7.95996201732091
O	2.77203521286017	13.47591645216177	8.28010062917678
C	2.26552450042937	14.45951477908756	7.38355965562191
H	1.53584333777334	15.11021017799974	7.90982628617311
H	1.74681774309277	13.97354040965605	6.53111966809488
C	3.41930552072769	15.28872634603737	6.85818518964133
H	4.15871725409915	14.64176246479657	6.34282797037580
H	3.03057540155919	16.03232285422918	6.13179875533260
C	5.10116642602466	16.81969519734687	7.56796761273274
H	5.89252903172852	16.26270946041684	7.03050801775187
H	5.51248309077813	17.24163102016582	8.49594291503370
H	4.71937698383866	17.63157298099355	6.91767833126501
C	1.74700991143746	12.64938759370585	8.82449130918497
H	1.01866218884119	13.25403535235832	9.39990976650346
H	2.23691308869874	11.92661471264480	9.49274360812337
H	1.21505859720504	12.10308922235434	8.02082910227914
B	7.56992089993368	10.47909562828244	11.22631273632503
C	6.02366855350038	10.17224472850369	7.59519203382586
B	6.65593206321693	12.88150156007282	11.06458994317337
C	11.22403743458129	10.88720110663473	11.20528353804101
C	6.43870010295876	8.75213201992746	8.03858868897076
B	7.45987626455846	12.90511513074903	12.66786825261400
B	8.10275749346751	11.24320331845904	12.78014970873563
C	10.52642940614346	10.66698656406346	8.78858846237624
C	11.96550400400016	12.59339755586617	9.50391847510353
H	10.22342645888061	11.19906948144554	7.87078641609286

H	9.71709642779728	9.96819117155617	9.05251786269173
B	5.75710626073052	10.23083278140429	11.26127945732610
B	6.71594089868482	10.12684586893139	12.75965257108013
H	8.25566615411731	9.67628642592880	10.66311801526332
H	9.12791612431812	10.93958001732560	13.31465044316493
B	5.14080951990185	11.89086796889400	11.13859499045345
C	4.52113984044299	10.40354564175792	7.81149032046472
C	6.38834376535817	10.35566983339985	6.10780366370670
H	4.22873286707636	11.43303881728291	7.53928989564604
H	4.23904672023373	10.23107135402405	8.86232760918257
B	5.68741553325151	12.79425874363464	12.56643111155473
H	4.15971045910509	12.19469216447613	10.51319970061607
H	12.15644879356812	10.32006888950059	11.01359896417129
H	10.44820836741426	10.16766497616373	11.51016996111587
H	11.40615122358994	11.57413848916619	12.04958059496718
H	5.86941943304513	8.00655382395848	7.45170794677230
H	7.51459176368790	8.58125052661647	7.86165028434915
H	6.23058726883090	8.57717255456881	9.10509282114768
B	6.58835058698270	11.68693921214877	13.63287845047635
H	7.99895574761681	13.88800323464472	13.08880347013632
H	11.43928947320048	10.07806301995510	8.56727003126918
H	11.68391178136696	13.18943696721381	8.61648938704778
H	12.86188202977728	11.99798784998182	9.24510324854415
H	12.23583844268059	13.29503731674850	10.31271155720026
H	5.04149526304286	13.72072341611736	12.97715854061535
B	5.18909800442555	11.08345755698346	12.72145470917541
H	5.22948052110219	9.27398091871953	10.77190232919016
H	6.81263678789514	9.07843703637893	13.33577373696128
H	3.93812588340339	9.70181070154015	7.18298212738827
H	6.06973633206514	11.34119342724294	5.72540366836991
H	5.88312341505581	9.57281548132650	5.51110186500194
H	7.47695307625581	10.26286690374873	5.94603335786762

H	6.56666128698261	11.77079578053367	14.83076562637802
H	4.17721997701942	10.73905115383542	13.27117091513955
H	6.67950952790111	13.87136200705932	10.40160487750624

Cartesian coordinates of [Na(dme)₂]H (TPSS-D3BJ/def2-SVP)

C	6.43974561644013	11.19974950146956	9.73326332986004
C	7.88757506156180	12.07219135863273	11.40646139812255
P	9.25646867629122	12.95278303424972	10.79732488428414
C	10.76335295951405	11.77020526658709	10.72575082355138
C	7.07835987224441	14.12234132465039	7.13114531550352
P	7.26252760428176	11.47650923025692	8.12633597407841
P	5.84325981927515	12.97362024144108	7.17025304272774
C	7.25812097305457	16.25897364822568	10.47425407417595
H	7.69365937486605	17.26413473278359	10.31084795166143
H	7.59085625105666	15.57970739885752	9.67951555050092
H	7.59551362703093	15.85892598819582	11.44797849874212
C	3.16471140910730	15.65176886756458	13.00089664864604
H	2.64997697034989	14.68742487137881	13.11607718194093
H	2.58623774784993	16.44613110260349	13.51286237254884
H	4.16745858965545	15.57130703258852	13.46061137438762
O	3.23785143789970	15.91719698068202	11.59864894791981
C	3.76934572807189	17.20283613725438	11.26983956820068
H	3.33314565759426	17.98069198631867	11.92881662290133
H	3.45345042428752	17.39185192146212	10.23099158330410
C	5.28894550388120	17.25264738128850	11.35502533724650
H	5.64395139831019	17.00785689177650	12.37782853225684
H	5.63289812361878	18.28291176425781	11.12064001547817
O	5.82624909653212	16.32524125921434	10.41789345938930
Na	4.32639126100408	14.44968000983912	10.00511374854314
O	7.86243838116233	14.99071171459325	7.07757322673750
O	3.43644375063417	15.79620845583855	8.25431525426008
O	2.15463188637957	13.64239859840906	9.45136890504874

C	1.40752780205260	14.64719325832944	8.77913993591445
H	1.11184311113753	15.44488400052998	9.49252334234756
H	0.48662537376331	14.21588501561295	8.33423419891541
C	2.26763941178802	15.22271294544884	7.67062382642664
H	2.55764127592156	14.42568928561581	6.95588313398182
H	1.69095718050839	15.99660888347951	7.12297873023138
C	4.28430138566693	16.44376317107125	7.30816337037370
H	4.59459214554057	15.74255588471681	6.50905837126878
H	5.16853049760032	16.78668764283381	7.86523452597478
H	3.76808489286984	17.30986258805236	6.84793847665767
C	1.40231968475708	12.93537229786682	10.43611640632295
H	1.03096636675382	13.62557401309751	11.21935885052940
H	2.07755523097490	12.19292777494251	10.88469350530835
H	0.54015382172881	12.41882447264706	9.97029710357650
B	7.38779376645175	10.38986945131921	10.86337171620848
C	6.84676730551632	9.97552374970846	7.01040224142797
B	6.38186652608260	12.62521117203319	10.59939649558614
C	10.83300487552456	10.78159670605900	11.90007852473071
C	7.55234898184707	8.75380286686680	7.63723512203159
B	6.69213587403209	12.65083619380674	12.38685027778605
B	7.43609932349272	11.01841560431308	12.58681197531187
C	10.79446960132593	11.01709437835168	9.37977920055851
C	11.97336910752620	12.73263255343021	10.78711660367877
H	10.73396853386260	11.71594444132738	8.52766095734744
H	9.94925703549228	10.31516268349960	9.29872903295553
B	5.63292019677060	9.93731463437187	10.44050083515758
B	6.21440689557000	9.81893569867916	12.11211146788915
H	8.26816974382569	9.68048634303831	10.47136096605430
H	8.27017184987089	10.71969629565089	13.39114974951928
B	4.90899716402448	11.54003830349748	10.23629171927955
C	5.33930558685801	9.72491579975881	6.85848844797342
C	7.48051805978125	10.29082258039183	5.64126835778595

H	4.84074261061891	10.58151070618918	6.36829328136028
H	4.85568917309690	9.54644766410163	7.83138903795068
B	5.04109865673305	12.39293641276405	11.78156316493201
H	4.09152796974870	11.82619302685761	9.40193481019753
H	11.78733369930333	10.21995666323451	11.85810666441666
H	10.00950704198500	10.05219895669227	11.86585970925506
H	10.78507724288518	11.30522634969980	12.87011829865135
H	7.44347920449864	7.88933594617611	6.95557457142068
H	8.63035502843580	8.94279392867019	7.77969823778104
H	7.11421449056682	8.48071744177909	8.60891139722185
B	5.71742172908184	11.29365429725485	13.00971271387973
H	6.94328403410432	13.64405732183958	13.01239214893462
H	11.73664014111804	10.43935980218239	9.29317977983856
H	11.93581735079020	13.47837364442403	9.97186540135461
H	12.91489501164099	12.16007502358220	10.68366151581435
H	12.00599521259944	13.27817364442276	11.74720436255731
H	4.22865560065293	13.23344739262061	12.07133339104203
B	4.65612797645157	10.64585103840102	11.74354675705982
H	5.34254926210107	8.96584765230979	9.80416980276682
H	6.26915098486966	8.74435476013805	12.64521327783436
H	5.17164003985743	8.83556169281974	6.22098210837562
H	7.01202260350300	11.17723421517648	5.17754712016498
H	7.33632657593540	9.42986505365123	4.96195528234738
H	8.56454818591139	10.48013662993463	5.73448167199395
H	5.37392502960085	11.29302768848584	14.16158083404829
H	3.57388730018232	10.20041815284651	12.02075140609966
H	6.50581503285354	13.64144650297770	9.97384516157072

Cartesian coordinates of [Na(dme)₂]I (TPSS-D3BJ/def2-SVP)

C	6.73623120711476	10.96481464417930	10.19868571665545
C	7.74970291558770	12.10620526567137	11.19927939913036
C	10.74032086228815	12.17218411088118	10.40001569315551

P	9.06901497129075	13.11814569578700	10.38439710520381
P	7.53573018905408	10.75507164322227	8.46648365721623
P	8.04319397234120	12.88435713709305	7.98688811848603
C	7.24085682610632	16.19890594833240	10.25168800587586
H	7.66912952568548	17.20901386720338	10.09971794640482
H	7.30799900667322	15.61528783169115	9.32065283795292
H	7.80418309686411	15.66237863273008	11.03507189439225
C	2.04263075725462	15.99391977804583	12.14199597714081
H	1.64304971670401	14.97083245778749	12.07121382342425
H	1.53781047238385	16.64140115769016	11.39688632662112
H	1.84699711521821	16.39000814178740	13.15758066084555
O	3.44114116805516	15.91188614530496	11.88946268764738
C	4.11389843058010	17.16850538281741	11.98084268880391
H	3.91118044948125	17.64027175553599	12.96373534316605
H	3.74841679565868	17.84839923673961	11.18302167692467
C	5.60657094985973	16.93666276868518	11.83602863013274
H	5.98523668140161	16.30574848025154	12.66529749365421
H	6.12464097861413	17.91680136355988	11.87867063025785
O	5.84674310112035	16.29863997394401	10.58602751380420
Na	4.33220824312352	14.54850572972688	10.21948178540267
O	6.72391809972866	14.07133137340193	5.75100393177367
O	3.76746724206981	15.46523103582285	8.13892381634831
O	2.61956516156418	13.25982747720185	9.28193850942806
C	2.09335850958734	13.75831390030921	8.05181671739909
H	1.25158048848077	14.45128707721971	8.26127034913285
H	1.71122668735094	12.92185455331464	7.43264881247104
C	3.19561876519562	14.47028656308270	7.29028919870430
H	3.97671384755091	13.75727173425243	6.96632629683350
H	2.75649089854465	14.93695871427575	6.38499610950157
C	7.06122204132007	13.20365548502324	6.49355384799067
C	4.67016617083212	16.33843494673980	7.44545813741026
H	5.46366755990072	15.76338160807233	6.93426310945303

H	5.10826205293324	16.99664810799559	8.20905305147292
H	4.11841730723090	16.94263516636557	6.69864865574749
C	1.71233053280591	12.40507478070780	9.97646824010076
H	0.76575610351502	12.93570064068955	10.20382978625379
H	2.20495718171444	12.10170231092361	10.91095214556679
H	1.48678920899212	11.50446971980669	9.37409842082745
B	7.79942654697729	10.40959949639400	11.43875128857409
C	6.12595091841671	10.13321292455866	7.31311322264761
B	6.16403675032603	12.49015088671455	10.64062589348817
C	11.13091449714557	11.72931148991790	11.82065161187691
C	5.65228899853950	8.77850098605574	7.88022578323343
B	6.68496500461818	12.88049537673073	12.29440077204815
B	7.72531111000039	11.54894930463293	12.81367253062014
C	10.85184135186581	11.00124168245910	9.41027326303240
C	11.69536352323838	13.29867185702322	9.93510382738031
H	10.58317437934535	11.32289545766499	8.38933708212075
H	10.19071226978097	10.16469015363752	9.68170947722705
B	6.17825746713270	9.71616674695363	11.19462388296145
B	6.75545502666384	10.06834812132396	12.84576824327043
H	8.77209706615698	9.80171409275482	11.12326042866604
H	8.70145660417081	11.74473183958514	13.47175666990699
B	5.12213945011577	11.04424757495314	10.69318532942061
C	4.91821710531812	11.05147890032974	7.08261200299328
C	6.86045626775663	9.87843506732209	5.97627822208636
H	5.22024672244733	11.95986079828613	6.53873708160611
H	4.43597369633419	11.35047556303932	8.02482508133942
B	5.06001132389224	12.23724685102855	12.00786869186776
H	4.26284639926322	10.90738065289636	9.87913662198443
H	12.18404014633696	11.38446070681609	11.82462479320112
H	10.50533022141793	10.89495466264162	12.17460335148152
H	11.03754768605674	12.56050162088490	12.54105954899727
H	5.05253647044982	8.25760476245387	7.10974496192587

H	6.50530220609144	8.13062291857758	8.14759679020964
H	5.02133583320701	8.90493380102031	8.77318049554511
B	6.03141352386850	11.61507141807494	13.36449718705963
H	6.92519447385943	14.01849934719608	12.57567143189433
H	11.89539582784222	10.62734570244854	9.39666987952457
H	11.41533245311199	13.66673732125370	8.93122520601113
H	12.72945859296884	12.90850658790370	9.88044342899880
H	11.68234158916647	14.15424607614942	10.63361026888071
H	4.09260821869486	12.93846800528763	12.16736092544717
B	5.07750687533144	10.48394121947915	12.37277690868916
H	6.09776046333288	8.61408117613674	10.74224324888458
H	7.01468656746752	9.17367053584992	13.60080520176358
H	4.16829469035469	10.51832554919766	6.46526504907052
H	7.24974226007263	10.81739995234360	5.54837786610171
H	6.15413265079612	9.42873877775364	5.25281456764882
H	7.70402955708130	9.17958013264860	6.11425401302475
H	5.76521322032802	11.86127402347674	14.50865640560447
H	4.11631921511531	9.90038318690850	12.79426746395800
H	6.09453648576344	13.30188234736216	9.76702624901141

Cartesian coordinates of [Na(dme)₂] **rac-1** (TPSS-D3BJ/def2-SVP)

C	6.57778152298806	10.14641740176129	10.17606600683122
C	6.87713891983734	11.71428920923093	10.67983100890661
C	9.24161748574036	13.19382585001210	9.20543965505211
P	7.32356407105479	12.95819023158723	9.30388569731339
P	7.16680584905924	9.88281221119229	8.36142757624873
P	6.64393511559405	11.89252825010361	7.56065697729293
C	6.95859545085193	15.44932826327061	13.05316427505685
H	7.60766031645954	16.14779677568821	13.61664635672343
H	7.56440249487015	14.64050930033644	12.62499655116965
H	6.20715771701949	15.01232332180041	13.73793423719447

C	4.15351518565507	18.01321453354494	9.03838926378973
H	3.78235934742738	17.27771330468072	8.31090117772514
H	4.98111538654811	18.59771211848060	8.58756684202544
H	3.34357244002609	18.70985782422370	9.33333873127065
O	4.61218044424015	17.26715457867680	10.16410851446415
C	5.19382861217236	18.07702769406846	11.17805182212451
H	4.49577996147060	18.88467368052868	11.48257356225859
H	6.12569695953364	18.54873817395124	10.80082195372080
C	5.49745721024949	17.20291250999646	12.37910393748972
H	4.55876196814255	16.80927891539131	12.82349860498506
H	6.01083414824218	17.81584163027092	13.14783578945237
O	6.33132629313960	16.12716886378647	11.96103161528259
Na	5.43780021434014	15.01769130581778	10.00561949749242
O	4.48243119706793	15.08637019937550	7.79113498931776
O	3.31192911909219	14.07768026237440	10.09131707096526
C	2.61258537021481	14.01885192677997	8.84930163723156
H	1.95670596760780	14.91028645858640	8.75066495373884
H	1.97499274943346	13.11224780071307	8.81341780305632
C	3.61282201092934	13.94707582136768	7.71366228157517
H	4.22528252872849	13.02083459852830	7.76754415533097
H	3.06096147890811	13.95557873146269	6.75101305115647
C	5.38347696044178	15.16912671496240	6.68246652319159
H	6.00646217517683	14.25663460826804	6.60699239216251
H	6.02646253081240	16.04600897334943	6.85896727610657
H	4.82259183294702	15.30883172645119	5.73682640234635
C	2.46671759363949	13.91865254937735	11.22442003694017
H	1.69031611959091	14.70982242773122	11.25591116306331
H	3.10504550549197	13.99084610033784	12.11740114188205
H	1.97907849722984	12.92524052355579	11.21409026560436
B	7.94487593796582	10.46701529798656	11.17476590140844
C	5.81501271140527	8.82389664055720	7.49913270062438
B	5.24788413926599	11.17342219390176	10.52868266199335

C	9.85513802979392	13.54156140980201	10.56843121653516
C	5.92016275837879	7.39073105178870	8.05530450660085
B	5.76181615267582	12.16436452399605	11.90165178857413
B	7.42617740523453	11.73389171778507	12.30228968103821
C	9.98268857459144	12.03590300632512	8.52501545227659
C	9.31078446384409	14.43116628856026	8.27933443355646
H	9.47549490767991	11.76651209141408	7.58150699468599
H	10.02172985938574	11.13766831438959	9.15891787659399
B	6.93312524758454	9.03914022346632	11.43456435213871
B	7.45866142544201	10.03574796898518	12.82208105066873
H	9.02625239213979	10.40685780799144	10.68537283186029
H	8.20811747727325	12.57224734758323	12.63155820038487
B	5.26272074360838	9.47772941908900	11.04472072378410
C	4.37867657532339	9.35747772930348	7.59194604139220
C	6.27417330689926	8.83636705787871	6.02291306912605
H	4.34002314268886	10.41659387386778	7.28112665882367
H	3.97966867341707	9.28200238187591	8.61461875499017
B	4.73088001508246	10.74847368654494	12.16947316978369
H	4.53791045128958	8.70205786996433	10.50062045680510
H	10.88245712239858	13.92838682691703	10.42532888298627
H	9.91634912680495	12.66169281062739	11.22650931647394
H	9.27163787161317	14.32525222450521	11.08566823637593
H	5.26424624193932	6.71408989386369	7.47408065715778
H	6.95579873152434	7.01401573639385	7.98351887163772
H	5.60930578905672	7.33791826607478	9.11143766561237
B	6.08698032008640	11.08975847486753	13.27900666942448
H	5.41257292200731	13.30820462965157	11.95092424737715
H	11.02151845112063	12.34430734419116	8.29710332733211
H	8.81091616052182	14.22218925390831	7.31574252746365
H	10.36852972311019	14.68179241736228	8.07399434909433
H	8.82778376436756	15.31254616805839	8.74134632711867
H	3.57583102654398	10.86689476558367	12.47723944593436

B	5.78350401103712	9.41786315350942	12.74379258953065
H	7.37466783555047	7.97198843237876	11.12289018711956
H	8.27595143280795	9.64047531512706	13.60577810506400
H	3.72004795005987	8.76686547966296	6.92554763317010
H	6.19236400221632	9.84863765036393	5.58779086043362
H	5.63682705618248	8.15192741513385	5.43111470931445
H	7.32293151329786	8.50229502641677	5.92368382792167
H	5.91696637888873	11.46781836444358	14.40649124105169
H	5.38576242834211	8.55843529715427	13.48061870694620
H	4.59804699757735	11.59531177912531	9.62821229427432

Cartesian coordinates of **TS-*rac-meso*-1** (TPSS-D3BJ/def2-TZVP)

C	6.00821579488036	10.59161570657541	1.14243240011904
P	5.58573927375457	9.04346410528771	2.12088385561653
P	3.80908046674836	6.99433143164357	3.55161855924652
P	4.96282948371503	7.03037237544862	1.71383046935424
C	4.91497972986968	8.06055323592240	4.70280291037498
C	1.28297597235976	6.78936980110087	2.70256094281111
H	1.72741898273274	6.45071563331332	1.75943686912363
H	0.27076295590214	7.16632733092866	2.49779840216039
H	1.20746903043805	5.92848226875602	3.37643518605380
C	6.01855291764568	9.11856515451683	3.89161298033462
C	5.11032147837248	11.76891727075821	1.56298074259443
H	5.36471196440339	12.66695010834962	0.97717767383532
H	5.24104412655570	12.00614273381739	2.62190630355804
H	4.05772473605600	11.52542966330391	1.39421665360628
C	7.48992133276659	10.96702241156307	1.29861234497277
H	8.13020517205467	10.14378068185450	0.96945905736709
H	7.73299867739764	11.19188480129864	2.34087918309751
H	7.71602673162680	11.86061477806570	0.69498562470649
C	2.13359023280103	7.91785418282191	3.32614910652990
C	1.50853522221495	8.31555395292583	4.66845242459763

H	0.45255551639809	8.58597229288720	4.51484288324773
H	2.01425349752475	9.17526904550326	5.11259132852966
H	1.54635450161431	7.48768325142272	5.38579061570028
C	2.13393970293735	9.09487541027415	2.34827318944200
H	2.62296730915992	8.80278106149795	1.41272800370877
H	2.66330345410876	9.96125512021719	2.74755725668302
H	1.09382147956500	9.38752312010288	2.13278282701033
C	5.71193603285368	10.21192696078940	-0.31770818322879
H	5.87114219551541	11.09059017226185	-0.95846641965802
H	4.67631674475247	9.87607030637911	-0.43414083586364
H	6.37006867500365	9.40495189785649	-0.65418427195118
B	4.54967109913103	8.67351557045335	6.27119524752805
H	3.47475229176903	8.46503966105685	6.71591232426073
B	5.69936492921727	7.35600826989669	6.04703222729679
H	5.40589080600283	6.24330973102305	6.32551736784565
B	6.35163108625988	10.44756088258268	4.88721964213160
H	6.54000838217881	11.50530592532349	4.38750434523967
B	7.19142338436974	9.79903052429720	6.31606169305121
H	8.00372475723745	10.45401781096580	6.88707737189510
B	5.44795422523826	10.18837333795263	6.40432829785411
H	5.02467673266670	11.10973631941680	7.02526578484363
B	7.33871113633249	8.04111779115265	6.10384191586839
H	8.25384114513403	7.39807947914928	6.50673138116779
B	7.52184687184112	9.12450996424163	4.71569667166374
H	8.49497123607014	9.25849250273211	4.05349968259278
B	6.07750187568295	8.69834009697602	7.16041645277682
H	6.09642049284476	8.54213823302997	8.33915732263287
B	4.72015629128769	9.74423501755833	4.86908282372889
H	3.83276707962710	10.28366479140955	4.31535403544891
B	6.59224131628476	7.63529130755507	4.54997317387016
H	6.87795146909495	6.76647651578233	3.81036415462263

Cartesian coordinates of **rac1-1-H** (TPSS-D3BJ/def2-TZVP)

C	8.32379087003199	2.72909801193657	3.20269401719928
C	7.85266961179363	1.11496254397327	2.99428019708058
C	6.91005337025156	5.41001563013286	3.46639610652520
C	6.05911837517315	0.02867552547667	5.31001914235958
B	9.21095611104343	0.08399066755294	3.04073857850846
H	9.06793578803132	-0.99616069455929	3.49279271485366
B	8.45628055826465	0.51279506597209	1.49985869714960
H	7.77606029940115	-0.26762594017136	0.93061212481072
B	10.22040091194308	0.55493853242803	1.65882448332880
H	10.89448936069507	-0.24741108082318	1.10613210041700
B	10.60666198322927	1.14795346246496	3.29664333969955
H	11.54627843307050	0.78611003477900	3.92051549628454
B	9.09133418098306	1.48779120720598	4.12256578291008
H	8.85160539398223	1.42486926463337	5.27104376968186
B	10.01275992401172	2.82268004094949	3.41757141769626
H	10.41612924594775	3.66255312702391	4.14623066125599
B	10.71317715033090	2.24327381946833	1.89303309532819
H	11.74483976226942	2.67795556405728	1.50491570542429
B	9.36722192492536	1.85058877217318	0.78424863523856
H	9.41896724014882	2.00105993048861	-0.38942799753946
B	7.85768771233895	2.17473157638023	1.64110028189251
H	6.81621858692620	2.52971776448720	1.21340531709597
B	9.25601153149177	3.24432198502749	1.87364496572948
H	9.17967847630597	4.36865803548028	1.52945877788352
P	7.12462525710716	3.70499168607171	4.26875628002164
P	6.12441020127141	0.60650536714230	3.49457380663081
P	5.30150962946706	2.67934833730911	3.46568924284556
C	7.00331458278127	-1.17730231791191	5.45349982397547
C	4.59739706419348	-0.46697981992086	5.40213342052714
C	6.30822280223143	1.03590337504656	6.43613744382496
C	6.52026356205532	5.45475874949055	1.98519577474686

C	8.19963081948344	6.20691895120982	3.73233570883575
C	5.76013032201051	6.00969375381903	4.30445510293811
H	6.88657325434975	-1.88391282530979	4.62462974490890
H	6.76444850705926	-1.70413952307136	6.38584743079455
H	8.04873872035567	-0.86566863860190	5.49779122116034
H	4.38248982434232	-1.23169405740636	4.64895908894078
H	3.88283437192988	0.35421581622503	5.27362614891589
H	4.43297897462452	-0.90140196023726	6.39546278884829
H	7.32531314047860	1.42678078314147	6.43177778254290
H	6.14201858720620	0.52933914491340	7.39602100650901
H	5.61849107854555	1.88280579357570	6.38581213870332
H	7.30724124377931	5.06740701709310	1.33785004714919
H	6.33389663325670	6.49875571001677	1.70114437931623
H	5.60417294107309	4.88612563971018	1.79844169036772
H	4.81833421513074	5.47633131948230	4.12637963951323
H	5.61174916634848	7.05635043531537	4.01318181007675
H	5.98115350986690	5.97964166594911	5.37724655683660
H	9.04515742230912	5.81219382273029	3.16407645673427
H	8.46141233264690	6.19034564364086	4.79582919941413
H	8.04688074264706	7.25153573078699	3.43337002221236
H	4.64754429085792	2.54881755325192	4.72022883189504

Cartesian coordinates of **rac2-1-H** (TPSS-D3BJ/def2-TZVP)

C	8.33487193008807	2.73431220761130	3.17132809941489
C	7.87043701915830	1.12916037311944	2.99674422789662
C	6.90089930792909	5.41746105817985	3.46962125073959
C	6.04773592702163	0.00576019526154	5.27534550071465
B	9.23071144987949	0.09547158311248	3.06973946229088
H	9.08819186373300	-0.97680584528128	3.53925525691895
B	8.48280950335725	0.49270526553055	1.51831451235275
H	7.80566926067243	-0.30048607070099	0.96250541787330
B	10.24666782379072	0.54003525560518	1.68481708042983

H	10.92501845733329	-0.27191414630452	1.15162825087560
B	10.62479586584365	1.16644753235760	3.31158794852179
H	11.56296205052988	0.81993752499571	3.94627119565895
B	9.10504893763921	1.51676173581007	4.12395587558207
H	8.85309592416352	1.47877342121075	5.27195549926182
B	10.02397918387062	2.84061274743900	3.39569462385456
H	10.41829658597332	3.69710730223765	4.11008147279766
B	10.73582189620745	2.23480099692033	1.88733000262578
H	11.76987907448891	2.66255191115440	1.49780954540083
B	9.39814764699219	1.81621352238905	0.77931494423500
H	9.45497213573803	1.94233564349767	-0.39712278806488
B	7.88364069840978	2.15488889899933	1.61801013829323
H	6.85045596636989	2.49529222952849	1.16534693194722
B	9.27421535845145	3.23172514911823	1.83875810352974
H	9.18895983061858	4.34976443177831	1.47277449046669
P	7.14904001156938	3.71267783163172	4.25793048711043
P	6.11944659014701	0.65010438229586	3.48614883856334
P	5.25998768378703	2.65892699279167	3.76755062270215
C	7.01965501422740	-1.17095681523377	5.44502466077815
C	4.59592962009208	-0.52291175346094	5.33546495102213
C	6.24192537667278	1.02822235665426	6.40201846199451
C	6.47447193759237	5.45732861081867	1.99925248825926
C	8.21686950376429	6.19084738202775	3.68222787337516
C	5.80078949670667	6.05329445665034	4.34541210335641
H	6.94203721072829	-1.88476551728140	4.61811140288563
H	6.77310443482637	-1.69887799955333	6.37465625669726
H	8.05516360798788	-0.83189166159485	5.51294523177491
H	4.42304422553803	-1.30805496473640	4.59283140043969
H	3.86986798613397	0.28070085200296	5.16760036441060
H	4.41339252463728	-0.94020803246923	6.33314578389280
H	7.23865314073265	1.47048364333810	6.39859119820602
H	6.09603368655461	0.52264612104931	7.36578994420581

H	5.50576431514957	1.83648508841966	6.33772585767537
H	7.20724708962110	4.98489259647369	1.34377550148731
H	6.37112821824405	6.50535778027495	1.68949465722212
H	5.50627677610773	4.97190436437511	1.84660543350147
H	4.83766648396860	5.54883325042891	4.21193731466853
H	5.67848128509208	7.10400399953798	4.05611962926986
H	6.06357335249632	6.01997402733987	5.40830179540438
H	9.03474317905766	5.77610457584839	3.08894359364534
H	8.51364678329338	6.17880224016727	4.73618181035483
H	8.07062982290702	7.23479863021468	3.37782384099424
H	5.18407694410464	2.91790463841861	2.37627145248480

Cartesian coordinates of **meso1-1-H** (TPSS-D3BJ/def2-TZVP)

C	1.42830620656746	6.73701895988835	2.51234704218544
H	1.63706586350742	7.24299848240688	1.56192555416747
H	0.34098813782419	6.72329277406298	2.65312135015145
H	1.77724321635252	5.70057971467849	2.44087611149356
C	6.17064477522334	9.10817019271866	3.83275205734387
C	5.65747910995837	11.54245143708745	1.42549157542117
H	5.86508329018832	12.39107550009066	0.76063513278403
H	5.73330367558525	11.89622295006276	2.45434160722383
H	4.62908873725457	11.21451610731576	1.24295031035697
C	6.65617870376480	10.42171999406324	1.12493660974938
C	8.10275031086253	10.86282437053066	1.41503217543746
H	8.81367283681256	10.06559499784423	1.17302638611638
H	8.24098102683965	11.14013780439630	2.46263546136155
H	8.34409235062653	11.73645549368969	0.79676546928391
C	2.08129782738571	7.47986936533197	3.69787040414561
C	1.71603275827006	6.75634994237227	5.00717451976735
H	0.62679859914699	6.77480294990249	5.13744943541901
H	2.16979940464749	7.23632505205121	5.87735080484156
H	2.03993544913967	5.71038698868300	4.98271503104141

C	1.59968332922961	8.93307083138255	3.70710987346450
H	1.88524585712292	9.44954876429934	2.78506425870743
H	1.99418358682142	9.49205343029158	4.55643616021931
H	0.50401101916042	8.94382346341733	3.77557648700047
C	6.53914090889795	10.02362262623331	-0.36218861416991
H	6.81075142975200	10.88355818434411	-0.98588145156014
H	5.51222210572849	9.73520490737542	-0.61742817733683
H	7.20851236513110	9.19320999082405	-0.61403247404108
C	4.89428868653249	8.28725896781629	4.55061897646066
B	4.34623296892561	9.13055562895894	5.92668773780706
H	3.19922895923449	9.09235673642416	6.19667212508486
B	5.35956710018184	7.68399364484525	6.07929676246075
H	4.88270894645130	6.65219264847347	6.40753496562180
B	6.52387159208949	10.53117081589118	4.70192784392470
H	6.90675424591596	11.47700567396713	4.11136687210853
B	7.05603444458527	9.98927170992560	6.30071352408238
H	7.84846582165144	10.62204896343992	6.91347620050083
B	5.38037862504703	10.56001117852518	6.05093285353952
H	4.96604275559076	11.58213153170922	6.48312629085086
B	7.04164232101803	8.20709307750889	6.31392260985824
H	7.81062002794731	7.54839776491482	6.92798239825426
B	7.54054361428039	9.08676380004170	4.85264653786139
H	8.59556487753121	9.04027272510042	4.31922070058053
B	5.70562687248673	9.12072946627578	7.06020207975824
H	5.50984694586970	9.11791924993530	8.22874778612085
B	4.84659437770577	9.99998281440398	4.46143313647873
H	4.09877970381247	10.49167513279927	3.69408746413081
B	6.49736885043115	7.66724150809596	4.72884691900807
H	6.76523735574854	6.70349307256451	4.10302110945675
P	6.39715110613921	8.76082686340536	1.99978018789572
P	3.92546281254781	7.17120960582454	3.38990844789134
P	4.22852737708195	8.44124195597376	1.57988474607766

H 4.46902672939274 7.32644018783462 0.73285862361027

Cartesian coordinates of **meso2-1-H** (TPSS-D3BJ/def2-TZVP)

C	1.36924786350380	6.65131708492223	2.54853137028202
H	1.50077636412834	7.14408944608561	1.57937870845667
H	0.29427689446372	6.58183782576964	2.75398610036121
H	1.76938141738194	5.63428975567447	2.47581749006156
C	6.11025731987461	9.17221944761215	3.81172495760399
C	5.74543499653060	11.61172842117773	1.33470002088928
H	6.11044083255266	12.48015936205724	0.77113312603075
H	5.70868528055379	11.88778164507413	2.38977705529159
H	4.72739404022665	11.40017744184405	0.99392484845133
C	6.67874175680852	10.42493530004395	1.07965594397373
C	8.13117633895767	10.77161158339252	1.46058681230115
H	8.80020210376767	9.92592874667872	1.27018389996950
H	8.22234130483685	11.05327758647197	2.51174598997237
H	8.46671332003660	11.61926357967961	0.85023705155194
C	2.04536489538328	7.44516086019449	3.68590595708884
C	1.80886156334425	6.70616523416966	5.01739560900887
H	0.72940306825917	6.64352953860081	5.20302706817999
H	2.26861647335782	7.22546767346598	5.86092755374081
H	2.20967145212541	5.68789918558179	4.97848325297835
C	1.47481881928815	8.86520156641570	3.73627484308016
H	1.56942631384660	9.36851458968490	2.76931194869444
H	1.96171004050823	9.47820589831256	4.49649110390043
H	0.40572370411011	8.81181282823170	3.97957690746964
C	6.63398665066405	10.03764068787386	-0.41332525101397
H	6.98700276449814	10.88637682103253	-1.01134631362046
H	5.61659021702715	9.79205920259042	-0.73579739906811
H	7.27994019957001	9.17875098112667	-0.62490583800881
C	4.84202906399596	8.35632397173665	4.52511310205915
B	4.32230450204940	9.17157615641684	5.93329535975986

H	3.17692242020972	9.14458208941126	6.21557297902389
B	5.31848116622469	7.70865492817997	6.03542450459008
H	4.83432315397944	6.67562872531308	6.34873810144954
B	6.50056318862622	10.57303124787120	4.70788809004779
H	6.88254391406728	11.52872552632219	4.13078553535157
B	7.05135263934678	9.98608284332198	6.28595906424443
H	7.86159856112561	10.59209415309783	6.90257042668165
B	5.38097325734019	10.58293773008062	6.07917012810020
H	4.98546239217665	11.60026959501683	6.53962740397206
B	7.01192666876291	8.20576008606202	6.25968703354376
H	7.78133633201627	7.52303533941553	6.84655656828742
B	7.49958544614451	9.11193412075303	4.80844340591594
H	8.54688567952682	9.06420963886507	4.26019614904404
B	5.69899438925771	9.11600848659925	7.04673147769741
H	5.52302145972097	9.08751385355788	8.21813062430152
B	4.81541563248205	10.07200922953966	4.48951394031786
H	4.05942645493585	10.61508357002855	3.76678334170426
B	6.44044547533269	7.70828480232643	4.67492584026378
H	6.68794234825022	6.75578576679626	4.02540899025582
P	6.26305192729438	8.80377755857611	1.96344728806790
P	3.89021124007796	7.27772670530170	3.29796745989058
P	4.12152713955269	8.53214631986451	1.49431773925309
H	3.62630955189722	9.75830526178043	2.01539262854915

Cartesian coordinates of **TS-*rac1-rac2-1-H*** (TPSS-D3BJ/def2-TZVP)

C	8.36149346150686	2.86566999908595	3.26628297030031
C	7.91238637929165	1.23032491599963	3.17687912109546
P	6.14526275506627	0.75228891714595	3.57682629908295
P	5.35972539128548	2.80987951473722	3.98981898528544
C	6.85868737399829	5.50896819930024	3.31702407963203
C	6.03004729789242	-0.17014305809329	5.22990750152055
B	9.29000910560559	0.24084512362388	3.31975787461413

H	9.18066736280695	-0.79713996177292	3.86992357196752
B	8.53550426127441	0.52540088931539	1.74243411903199
H	7.86753720058289	-0.30898663804181	1.23844387637110
B	10.29381070418068	0.61196197800402	1.89906591656766
H	10.98202964504123	-0.22013251656007	1.41162621782374
B	10.66823410533729	1.34495474344406	3.48190550657437
H	11.61427821072522	1.04987946850801	4.13057493249596
B	9.14284848995929	1.72555699078050	4.28114905285559
H	8.89399225058973	1.77746565403452	5.42852827183229
B	10.04855831787557	3.00859192650207	3.46154273783265
H	10.42911909846607	3.91389885671870	4.12099940354950
B	10.75533720444412	2.32270933943041	1.99031150608866
H	11.78005671681253	2.74159572035548	1.56809795413893
B	9.41704628233227	1.81874604204621	0.92026509326751
H	9.46854300735267	1.87332360331711	-0.26169774136853
B	7.89807932740485	2.18187393819578	1.75353297977965
H	6.83988158000431	2.47028045529603	1.31548118041172
B	9.27510310646460	3.29227898275441	1.89357381337901
H	9.16779841361687	4.38158797834903	1.45633704532879
P	7.25035052290155	3.94687327910712	4.31536976641568
C	6.50524423236961	-1.61035157388016	4.94933275512292
C	4.50669837473235	-0.21184427056917	5.48507347025733
C	6.75247109021497	0.40658102948806	6.44800727182150
C	6.36455117777020	5.31782300296536	1.88052048802017
C	8.11024979359334	6.40525402684439	3.36927458143305
C	5.74189707139081	6.16625127279608	4.15620833711309
H	5.98914546209830	-2.03680550817098	4.08277594107440
H	6.28160381746048	-2.23485076310957	5.82329928433990
H	7.58072085335609	-1.65341091819046	4.76680105520817
H	3.95852296877058	-0.55061260305957	4.59821404075452
H	4.11263048778350	0.76375193582014	5.78499627740402
H	4.30692830443024	-0.91976289719385	6.29812169349604

H	7.83212958936252	0.26828182570913	6.37358174682747
H	6.40747167403628	-0.11583431999142	7.34964197685289
H	6.54924166821797	1.47452718651292	6.57903983690558
H	7.13576883649209	4.89901730668700	1.23265571153001
H	6.07397181188792	6.29402344955552	1.47074771972848
H	5.48628599190446	4.66493317465438	1.84817989083640
H	4.81785488251768	5.57737147654724	4.12194662459559
H	5.52464680023214	7.15923600493056	3.74482381963940
H	6.04151409078694	6.28837832429538	5.20341917274843
H	8.94226508101579	5.97999900900646	2.80382930855460
H	8.43944745875750	6.56028206926274	4.40227688536732
H	7.86948478475035	7.38414208103068	2.93610990123041
H	5.13412412324821	2.59827733647554	5.37490817326364

Cartesian coordinates of **TS-*rac1-meso2-1-H*** (TPSS-D3BJ/def2-TZVP)

C	8.33487193008807	2.73431220761130	3.17132809941489
C	7.87043701915830	1.12916037311944	2.99674422789662
C	6.90089930792909	5.41746105817985	3.46962125073959
C	6.04773592702163	0.00576019526154	5.27534550071465
B	9.23071144987949	0.09547158311248	3.06973946229088
H	9.08819186373300	-0.97680584528128	3.53925525691895
B	8.48280950335725	0.49270526553055	1.51831451235275
H	7.80566926067243	-0.30048607070099	0.96250541787330
B	10.24666782379072	0.54003525560518	1.68481708042983
H	10.92501845733329	-0.27191414630452	1.15162825087560
B	10.62479586584365	1.16644753235760	3.31158794852179
H	11.56296205052988	0.81993752499571	3.94627119565895
B	9.10504893763921	1.51676173581007	4.12395587558207
H	8.85309592416352	1.47877342121075	5.27195549926182
B	10.02397918387062	2.84061274743900	3.39569462385456
H	10.41829658597332	3.69710730223765	4.11008147279766

B	10.73582189620745	2.23480099692033	1.88733000262578
H	11.76987907448891	2.66255191115440	1.49780954540083
B	9.39814764699219	1.81621352238905	0.77931494423500
H	9.45497213573803	1.94233564349767	-0.39712278806488
B	7.88364069840978	2.15488889899933	1.61801013829323
H	6.85045596636989	2.49529222952849	1.16534693194722
B	9.27421535845145	3.23172514911823	1.83875810352974
H	9.18895983061858	4.34976443177831	1.47277449046669
P	7.14904001156938	3.71267783163172	4.25793048711043
P	6.11944659014701	0.65010438229586	3.48614883856334
P	5.25998768378703	2.65892699279167	3.76755062270215
C	7.01965501422740	-1.17095681523377	5.44502466077815
C	4.59592962009208	-0.52291175346094	5.33546495102213
C	6.24192537667278	1.02822235665426	6.40201846199451
C	6.47447193759237	5.45732861081867	1.99925248825926
C	8.21686950376429	6.19084738202775	3.68222787337516
C	5.80078949670667	6.05329445665034	4.34541210335641
H	6.94203721072829	-1.88476551728140	4.61811140288563
H	6.77310443482637	-1.69887799955333	6.37465625669726
H	8.05516360798788	-0.83189166159485	5.51294523177491
H	4.42304422553803	-1.30805496473640	4.59283140043969
H	3.86986798613397	0.28070085200296	5.16760036441060
H	4.41339252463728	-0.94020803246923	6.33314578389280
H	7.23865314073265	1.47048364333810	6.39859119820602
H	6.09603368655461	0.52264612104931	7.36578994420581
H	5.50576431514957	1.83648508841966	6.33772585767537
H	7.20724708962110	4.98489259647369	1.34377550148731
H	6.37112821824405	6.50535778027495	1.68949465722212
H	5.50627677610773	4.97190436437511	1.84660543350147
H	4.83766648396860	5.54883325042891	4.21193731466853
H	5.67848128509208	7.10400399953798	4.05611962926986
H	6.06357335249632	6.01997402733987	5.40830179540438

H	9.03474317905766	5.77610457584839	3.08894359364534
H	8.51364678329338	6.17880224016727	4.73618181035483
H	8.07062982290702	7.23479863021468	3.37782384099424
H	5.18407694410464	2.91790463841861	2.37627145248480

Cartesian coordinates of **TS-*rac2-meso1-1-H*** (TPSS-D3BJ/def2-TZVP)

C	8.32379087003199	2.72909801193657	3.20269401719928
C	7.85266961179363	1.11496254397327	2.99428019708058
C	6.91005337025156	5.41001563013286	3.46639610652520
C	6.05911837517315	0.02867552547667	5.31001914235958
B	9.21095611104343	0.08399066755294	3.04073857850846
H	9.06793578803132	-0.99616069455929	3.49279271485366
B	8.45628055826465	0.51279506597209	1.49985869714960
H	7.77606029940115	-0.26762594017136	0.93061212481072
B	10.22040091194308	0.55493853242803	1.65882448332880
H	10.89448936069507	-0.24741108082318	1.10613210041700
B	10.60666198322927	1.14795346246496	3.29664333969955
H	11.54627843307050	0.78611003477900	3.92051549628454
B	9.09133418098306	1.48779120720598	4.12256578291008
H	8.85160539398223	1.42486926463337	5.27104376968186
B	10.01275992401172	2.82268004094949	3.41757141769626
H	10.41612924594775	3.66255312702391	4.14623066125599
B	10.71317715033090	2.24327381946833	1.89303309532819
H	11.74483976226942	2.67795556405728	1.50491570542429
B	9.36722192492536	1.85058877217318	0.78424863523856
H	9.41896724014882	2.00105993048861	-0.38942799753946
B	7.85768771233895	2.17473157638023	1.64110028189251
H	6.81621858692620	2.52971776448720	1.21340531709597
B	9.25601153149177	3.24432198502749	1.87364496572948
H	9.17967847630597	4.36865803548028	1.52945877788352
P	7.12462525710716	3.70499168607171	4.26875628002164

P	6.12441020127141	0.60650536714230	3.49457380663081
P	5.30150962946706	2.67934833730911	3.46568924284556
C	7.00331458278127	-1.17730231791191	5.45349982397547
C	4.59739706419348	-0.46697981992086	5.40213342052714
C	6.30822280223143	1.03590337504656	6.43613744382496
C	6.52026356205532	5.45475874949055	1.98519577474686
C	8.19963081948344	6.20691895120982	3.73233570883575
C	5.76013032201051	6.00969375381903	4.30445510293811
H	6.88657325434975	-1.88391282530979	4.62462974490890
H	6.76444850705926	-1.70413952307136	6.38584743079455
H	8.04873872035567	-0.86566863860190	5.49779122116034
H	4.38248982434232	-1.23169405740636	4.64895908894078
H	3.88283437192988	0.35421581622503	5.27362614891589
H	4.43297897462452	-0.90140196023726	6.39546278884829
H	7.32531314047860	1.42678078314147	6.43177778254290
H	6.14201858720620	0.52933914491340	7.39602100650901
H	5.61849107854555	1.88280579357570	6.38581213870332
H	7.30724124377931	5.06740701709310	1.33785004714919
H	6.33389663325670	6.49875571001677	1.70114437931623
H	5.60417294107309	4.88612563971018	1.79844169036772
H	4.81833421513074	5.47633131948230	4.12637963951323
H	5.61174916634848	7.05635043531537	4.01318181007675
H	5.98115350986690	5.97964166594911	5.37724655683660
H	9.04515742230912	5.81219382273029	3.16407645673427
H	8.46141233264690	6.19034564364086	4.79582919941413
H	8.04688074264706	7.25153573078699	3.43337002221236
H	4.64754429085792	2.54881755325192	4.72022883189504

Cartesian coordinates of **TS-meso2-meso1-1-H** (TPSS-D3BJ/def2-TZVP)

C	5.01329492940395	8.13517400912457	4.67673938958790
P	3.87268517666822	7.04102476177945	3.66735627762242
P	5.08307970985687	7.42700880909654	1.93998891540921

H	4.81419979436458	6.78624031869602	0.72879112891261
C	1.59742949810723	7.04176143540066	2.27660274828552
H	2.07749388656474	7.40256505876247	1.36056454520939
H	0.51746400731239	7.21159445472390	2.19332135762795
H	1.76306936654384	5.95996224570022	2.35491320584014
C	6.34572293219859	8.99243399864878	3.92743935753059
C	5.07215374809540	11.30521421086762	1.56056094985835
H	4.92425435241388	12.09139130728331	0.80833635340900
H	5.19846745509176	11.78824610168818	2.53107981176050
H	4.16873608632055	10.68882068746003	1.58576308661627
C	6.29023157451410	10.47358986534004	1.17443202127748
C	7.58465341005066	11.30626944816209	1.26374820393247
H	8.45963280170676	10.71391419364289	0.97429752233237
H	7.74897184319962	11.69135635169611	2.27314312733839
H	7.51024171527437	12.16087825730343	0.57979464666359
C	2.13131241671326	7.79542345243393	3.51337585725063
C	1.36911036071061	7.30896215827307	4.76199245365975
H	0.29929656958752	7.51529615700282	4.63313596338672
H	1.70786856051654	7.81933051249614	5.66687908640161
H	1.49228250475624	6.23018148027957	4.90829846956449
C	1.95399092164623	9.29571871697491	3.30838727191640
H	2.56870342387612	9.65270886079323	2.47679540274754
H	2.20775258613142	9.86321981922040	4.20544462502258
H	0.90315012979138	9.50083039637334	3.06459192561518
C	6.12409477185295	9.96063896182406	-0.27176303462960
H	6.11215393026327	10.81743200904555	-0.95577849289627
H	5.18363117485390	9.41103244369040	-0.38668235410029
H	6.95105990836744	9.30379889350736	-0.56941321053292
B	4.49560296163900	8.98620519915131	6.04505532421228
H	3.34301123660368	8.96608643311328	6.30089112548634
B	5.51244371232165	7.54112013114989	6.19423532212849
H	5.05150368697380	6.50445098906071	6.52554672516213

B	6.68314040705763	10.39364584674612	4.81467179684850
H	7.04394622718629	11.34731637655554	4.21907453441001
B	7.21192325799400	9.84315919716532	6.41764148300079
H	8.00629844652979	10.47113808505182	7.03289822211339
B	5.53814828727192	10.41264530569913	6.16551295827622
H	5.12178424971809	11.43531211558538	6.59491484979605
B	7.18942877110664	8.06220416645911	6.41260329419379
H	7.95874990808197	7.39335223701265	7.01536017472277
B	7.69637852440283	8.94627849259216	4.96598539493679
H	8.75456747783479	8.88705590360394	4.44287724266136
B	5.86467771941269	8.97632145901195	7.17534685141236
H	5.67388017249953	8.97034821373136	8.34474282151786
B	5.00892352302322	9.84758951232678	4.57834797456556
H	4.26355846774072	10.36208221561714	3.84123384300816
B	6.62818491940513	7.53398640481605	4.81043384040862
H	6.91462827044506	6.56278177799457	4.20865392865767
P	6.68093022599719	8.84938956026464	2.08800467986087

Cartesian coordinates of **rac1-1-Me** (TPSS-D3BJ/def2-TZVP)

C	8.28572689846971	2.73382635125749	3.18743835545598
C	7.82054201436283	1.11023518978419	2.97908298780982
C	6.91416634938952	5.42757718294560	3.45805639340121
C	6.09505244993191	0.00171229813225	5.32750076771557
B	9.18876915620780	0.08878668986512	3.04828721950497
H	9.05073565970810	-0.99152112285264	3.49936160937013
B	8.45360467068473	0.50573184983048	1.49711096511312
H	7.78921211215081	-0.28132697126745	0.91810666951663
B	10.21783993189806	0.55564865759157	1.68254211429938
H	10.90256095012433	-0.24863070959048	1.14557230584193
B	10.57514623176863	1.15965639935995	3.32174106121466
H	11.50364305906913	0.80410637747107	3.96594409505002
B	9.04549251202289	1.49855237321891	4.11809871123857

H	8.79844309933981	1.44181389916454	5.26369237502138
B	9.97329672023255	2.83244852159161	3.42485373786638
H	10.36433379087959	3.67498496174050	4.15721348446730
B	10.70120210030140	2.24719989236604	1.91579386847223
H	11.73684393549012	2.68509656628897	1.54160930059953
B	9.37544105261387	1.84195255072199	0.78977114430861
H	9.44394440399107	1.98663785749581	-0.38395220529069
B	7.85157602853885	2.16640264283169	1.61450048651856
H	6.82927440800304	2.51783988266925	1.14786662715174
B	9.23885299654586	3.24163640507693	1.86851935400292
H	9.16585588384875	4.36209192024702	1.51120900264266
P	7.05635454086436	3.70012957907245	4.23639296707483
P	6.09977630099354	0.59124933415297	3.50876999220096
P	5.30013822250286	2.66329885482840	3.31002212130619
C	7.06253666406222	-1.18913125295518	5.44395970851807
C	4.65270769741630	-0.54341384537701	5.45581061391805
C	6.36286408387562	0.99611715774700	6.46290280034639
C	6.53840539407600	5.49983514296149	1.97433052790477
C	8.23436008600605	6.16601177718974	3.74187617061064
C	5.79066470961598	6.08043724197882	4.29112454578674
H	6.94512854265800	-1.89132795595703	4.61164386842115
H	6.84292530684007	-1.72640654119917	6.37562328632942
H	8.10290297041818	-0.86189002495546	5.47792270797731
H	4.44056271116043	-1.29397405908313	4.68764985979012
H	3.90317357887360	0.24881643197361	5.37860940123224
H	4.54259236864531	-1.01541506460551	6.43966235379188
H	7.39509310876547	1.34311130703953	6.47463642033270
H	6.16540821643113	0.49071213935950	7.41788489348597
H	5.72098574470104	1.87542349625137	6.41024249898753
H	7.31600326328149	5.08836190988977	1.33064905707417
H	6.39124721013686	6.55174365912345	1.69619134185473
H	5.60694035704131	4.96074391106248	1.77498647365480

H	4.81677046037525	5.63159106033560	4.06885584527670
H	5.73097341273520	7.14587176779941	4.03866358461440
H	5.97815581828854	5.99367062117089	5.36725161771709
H	9.06729753247907	5.74386694209282	3.17570948850513
H	8.48690564868178	6.12693448719800	4.80710166043415
H	8.12597058959286	7.21947103121077	3.45405804314919
C	3.93286969334490	2.81490890534115	4.56532903392299
H	3.51245024965443	3.81820077522142	4.45240681273184
H	4.21625877468848	2.66500341957119	5.60681731941636
H	3.15236032622027	2.09911812562023	4.28982455234087

Cartesian coordinates of **rac2-1-Me** (TPSS-D3BJ/def2-TZVP)

C	8.37190738384367	2.73572173261076	3.15303784057832
C	7.92703318154261	1.12629391380931	3.01848816117497
C	6.97946476734910	5.43937255201285	3.46772114669408
C	6.09760858640101	-0.00746576284632	5.28637298329255
B	9.29758753320612	0.10673310847470	3.13254780987899
H	9.16237851719676	-0.95722227412547	3.62130299373366
B	8.56633422893113	0.45794252845709	1.56252457992958
H	7.90434587626903	-0.35615333264111	1.01847662304023
B	10.32779514161235	0.52608453042489	1.75095970266837
H	11.02059409191383	-0.29358268537071	1.24886279962079
B	10.67758782284971	1.19635187972169	3.36633425738501
H	11.61091453024458	0.87600183900925	4.02176058598091
B	9.14531163965258	1.55014735666223	4.15000639245543
H	8.87789703392051	1.54013544759900	5.29436004907035
B	10.05760356739056	2.86544084601075	3.40149687020402
H	10.43683076926737	3.74162789126020	4.09956009737073
B	10.79828699569094	2.23047830779235	1.91843107393515
H	11.83368097192131	2.65896244291650	1.53306688524742
B	9.48275086654668	1.76976576837181	0.80165239605236
H	9.55484439541502	1.86616685931484	-0.37691383968742

B	7.95589544886843	2.11473393672457	1.61048143778979
H	6.93093744246140	2.43694026629045	1.13598879080588
B	9.32896319349667	3.21126613065231	1.82376313963277
H	9.24031000674462	4.32037307854751	1.43166720837673
P	7.13149698455363	3.69931095195777	4.19056507990936
P	6.16934960657610	0.65325398100897	3.50019332321191
P	5.23897441474898	2.62930587927489	3.79010535599086
C	7.05719377685062	-1.19604625376013	5.44267635901831
C	4.64114550793283	-0.52237598956475	5.34437029334931
C	6.30296877487511	0.99880884982985	6.42573969445018
C	6.62075249150042	5.56452015998750	1.98273176003083
C	8.31690646268879	6.14740239957330	3.76112319573648
C	5.87155734785134	6.08507252775609	4.32541837010711
H	6.98087353532010	-1.89531917180008	4.60318442076483
H	6.79841257172651	-1.73725349315308	6.36138672902859
H	8.09471680875873	-0.86714829986061	5.52591872759920
H	4.45624404349163	-1.29433924068947	4.59059748735571
H	3.92500539103205	0.29351256274306	5.19415637161396
H	4.45953066519257	-0.95333027185258	6.33647024336503
H	7.30843456085541	1.42024578743319	6.43327232696808
H	6.14231063124027	0.48259878563108	7.38164368075619
H	5.58379068382106	1.82098933464350	6.36182396481106
H	7.31197460468074	5.01596810613637	1.34149748457600
H	6.66648830853484	6.62363083609489	1.69694859886312
H	5.60756636360785	5.21145842467928	1.78622108727614
H	4.89956432952292	5.61027269022082	4.15246385038075
H	5.78528506983822	7.14517869036964	4.05785807140750
H	6.10130126882627	6.01869036606252	5.39405063058608
H	9.13317300872114	5.73689893712789	3.16244000099972
H	8.58699861474906	6.06303602536957	4.81873472554691
H	8.21600198792013	7.21179283557784	3.51431697432848
C	4.45962392589299	2.92891328761764	2.11965071253139

H	3.79207320164719	2.07505248479105	1.96030470756427
H	5.14177115522199	3.01081796849757	1.27596148540498
H	3.84652990908453	3.83171448661696	2.19357430123698

Cartesian coordinates of **meso1-1-Me** (TPSS-D3BJ/def2-TZVP)

C	1.43610730318620	6.77594298874761	2.50271648426761
H	1.65141668045625	7.28583917531061	1.55619645872117
H	0.34832509283845	6.77033758017139	2.64054610351902
H	1.77580385638387	5.73624046915494	2.42919519085917
C	6.18486305336756	9.10196065097668	3.84668772056716
C	5.59952011654802	11.51827238750124	1.45463669796842
H	5.76922654714867	12.37130290077489	0.78444047783539
H	5.68197972557015	11.87761607267672	2.48106481697766
H	4.58035779223125	11.15403444930477	1.29078860605999
C	6.62788122364876	10.42845636870133	1.14004616092349
C	8.06439071031900	10.91190853137539	1.41132888018861
H	8.79525767921288	10.13901294469284	1.15073339072866
H	8.21137476640660	11.18361756775549	2.45916091244591
H	8.26847931333703	11.79848324554194	0.79788120688996
C	2.09103349837793	7.51066887095449	3.69152487208215
C	1.68383742962667	6.80841922352355	5.00010753855559
H	0.59406827881577	6.86385631618061	5.11538691071896
H	2.14142580633889	7.27865597377160	5.87358576613695
H	1.97378442006121	5.75238761865285	4.98663715939136
C	1.64556279722728	8.97545520796102	3.67898281873261
H	1.96649035012034	9.47468772111604	2.75919652866389
H	2.03492663825310	9.53101432627997	4.53295938088933
H	0.54915798021332	9.01394525695327	3.72361791072361
C	6.50368996599487	10.03403845256347	-0.34685316557098
H	6.76471504830380	10.89838550662627	-0.96902437234360
H	5.47631630504363	9.74127958318133	-0.59390287383650
H	7.17815028343234	9.21007410382731	-0.60741242467588

C	4.90510696484048	8.27950997269486	4.56627409230485
B	4.35853806302909	9.12478114327438	5.94073382001204
H	3.21151577158999	9.08704567216997	6.21137044692033
B	5.37145649738964	7.67864109028212	6.09504779215492
H	4.89542134001247	6.64692297424807	6.42467684194105
B	6.53613063011490	10.52426958919240	4.71636952573569
H	6.91975239982309	11.47027995985516	4.12634685851190
B	7.06825283291269	9.98343745501642	6.31623416147364
H	7.86094363323469	10.61651431501780	6.92846312792104
B	5.39264603878425	10.55364473769638	6.06454319034345
H	4.97772047389945	11.57621978251064	6.49529140588124
B	7.05342576474289	8.20131194600441	6.32950215108952
H	7.82233528975829	7.54206898757445	6.94324953968079
B	7.55276675237049	9.08063643766707	4.86850435210833
H	8.60862356476296	9.03363247563549	4.33679482096644
B	5.71763871637462	9.11542678088107	7.07558900866228
H	5.52094987865392	9.11265811917501	8.24404228109389
B	4.85897421820352	9.99253170784947	4.47400412767145
H	4.11242625262364	10.48385626314674	3.70744591779216
B	6.50842874294584	7.66168426995941	4.74355069269243
H	6.77616798497721	6.69756100710934	4.11746155537054
P	6.42575971954498	8.76120747920400	2.01977194831094
P	3.93375616545612	7.15793803005834	3.42116218729215
P	4.29656737759373	8.30772534348509	1.54870435987812
C	4.59656782533521	6.85075112079694	0.41358178950639
H	5.30246627858402	6.13479557575823	0.83964746117470
H	4.98452574468183	7.22562309437225	-0.53808113898241
H	3.64084241529612	6.35411117508691	0.22259852507245

Cartesian coordinates of **meso2-1-Me** (TPSS-D3BJ/def2-TZVP)

C	1.31943610095504	6.65765992902915	2.58794428832850
---	------------------	------------------	------------------

H	1.35800281375416	7.22451203452906	1.65166975695919
H	0.26586652628105	6.49970801969311	2.84856223174696
H	1.77977690591742	5.67928961882793	2.41423651265353
C	6.05452069713339	9.24259809184680	3.79992043743720
C	5.97407267842142	11.74946820222747	1.34254085699621
H	6.50387540278234	12.57689890174987	0.85242747591679
H	5.90989914804931	11.97906223763499	2.40675295099556
H	4.96423563044822	11.71462194594425	0.93371568647784
C	6.74145754609764	10.44957989716044	1.07532764659600
C	8.22207937962974	10.62062437024592	1.47196213264767
H	8.79039747423636	9.70190280221750	1.29535401230322
H	8.32974250548369	10.89671762123117	2.52348895151221
H	8.66053288041434	11.42152575475066	0.86349128917897
C	2.01334043147588	7.41094370131049	3.74051786796668
C	1.91344814671292	6.56307742313340	5.02511053708835
H	0.85395765117315	6.40298653479178	5.26128508288248
H	2.37836893317629	7.06390774189303	5.87752442124081
H	2.39003139919078	5.58621548708143	4.89539186158624
C	1.34173769542225	8.77162342323168	3.95791076820945
H	1.26378898693101	9.33794797769102	3.02992366992128
H	1.87119445413119	9.37988935742137	4.69211803769111
H	0.32345437891154	8.60416667623480	4.33293598294121
C	6.66203251478964	10.08766659486468	-0.42135628063362
H	7.11102558548111	10.89800525337625	-1.00841485973217
H	5.62617424211029	9.95951461480654	-0.75308363268091
H	7.20758399168635	9.16353554137253	-0.63955609572240
C	4.79207884446933	8.43079121624789	4.51222892102327
B	4.29580383956865	9.22713983566121	5.94255631630059
H	3.15633821873487	9.19672278160413	6.24708083536504
B	5.28003345234355	7.75347285147369	6.00913845072350
H	4.79289404852938	6.72066775067339	6.31669249606109
B	6.47241095201487	10.62653262335853	4.71395089984582

H	6.86926322053805	11.58409845077847	4.15033886351312
B	7.03556703106488	10.01026127285886	6.27539571136337
H	7.85957142746283	10.59935545289266	6.89037282692373
B	5.36969352656906	10.62698982827683	6.10013892312043
H	4.99075264753656	11.64041020818497	6.58311373419262
B	6.97930303834402	8.23141056664122	6.22376474826541
H	7.74900910396058	7.53259463512814	6.79136747056825
B	7.45735522872257	9.15312630209450	4.78028220492221
H	8.49994143205178	9.10345438216477	4.22432696297146
B	5.68373088638570	9.14127488669243	7.03832700611361
H	5.51925317243508	9.09523795209960	8.21095002956439
B	4.77901948416557	10.14874237293177	4.50903431124253
H	4.02251838351204	10.70122304665475	3.79935646704939
B	6.38734504537682	7.76188150768881	4.64046843279711
H	6.61813732428791	6.81791825054912	3.97381817555788
P	6.15545119044552	8.87694716290002	1.94742902529785
P	3.84065791618772	7.38921296430037	3.25282020084581
P	4.05021058103397	8.53912004507478	1.38165352516135
C	3.00235341731032	10.08515159364514	1.28472209028187
H	3.30826136014981	10.60467264739669	0.37159448109555
H	3.04751015271142	10.76596014969125	2.13225237425833
H	1.97288097329059	9.74790950803867	1.13058292506605

Cartesian coordinates of **TS-*rac1-rac2*-1-Me** (TPSS-D3BJ/def2-TZVP)

C	6.69148608077662	5.51275915589582	2.85704433466044
P	7.43724325359783	4.35331643642306	4.16632734862275
P	5.94415448222705	2.90846781349512	5.03126818660637
C	4.22751468721540	3.47854350303416	4.56886124758964
C	8.51317650775649	3.04432054805562	3.35996657612026
C	7.97429391770445	1.42424807851086	3.31656701232633
C	5.93310451144361	-0.24908010647790	4.80680520354455

B	9.25579124298079	0.37672497681769	3.71366768388803
H	9.02005911712889	-0.61479529872783	4.30470076754573
B	8.72346695835137	0.58204203842621	2.03855874904064
H	8.07537621040757	-0.24879124488299	1.50086329318925
B	10.45206135013198	0.57467866324822	2.42338687630851
H	11.13430260384675	-0.33496566709429	2.08988040246660
B	10.66945847965479	1.40705344237615	3.98874019371164
H	11.49716376468517	1.10496096815075	4.78031140408573
B	9.07327373800228	1.93628083681544	4.54404980776441
H	8.66095959492831	2.06375075794286	5.64279451118953
B	10.17806787841691	3.09187905081434	3.77274433328510
H	10.53101035729245	4.01985855121952	4.41343812334631
B	11.01915663212593	2.25432704848432	2.46046226761705
H	12.11585740804914	2.57694369600358	2.14881721757858
B	9.79909293598257	1.75714762042760	1.25717590422218
H	10.00879167413990	1.71907420796314	0.09191167653604
B	8.21643957525992	2.26685396718507	1.84446467006837
H	7.25577287807856	2.55480293994181	1.23310776826739
B	9.63238564912862	3.30503296857403	2.10169852954697
H	9.66014833206302	4.36077859620203	1.57856816153430
P	6.14002248986936	1.20935442857325	3.60467193541813
C	6.17813163052710	-1.53569169510756	3.99797865792618
C	4.43859104319079	-0.16968405338240	5.18260472411293
C	6.76373751241704	-0.22667839141985	6.09404994819854
C	6.02079253182393	4.91692318239910	1.61623959631410
C	7.83927851662828	6.45799382076789	2.44140512562098
C	5.68588293434461	6.36246988718504	3.66579640482289
H	5.55156159114728	-1.56167039483056	3.09995407111867
H	5.92505379638345	-2.40488809943074	4.61831173811005
H	7.22202243929109	-1.63112722100339	3.69067918445799
H	3.79657154925041	-0.09384895664864	4.29712752844597
H	4.24257552582935	0.68651425680948	5.83818213781038

H	4.15865018107984	-1.07784982852327	5.72971204942226
H	7.83035136524101	-0.34106193762006	5.90062312575126
H	6.44648547474883	-1.06137071354438	6.73307383561201
H	6.60658621220454	0.70444586746654	6.64683630607664
H	6.76174245852254	4.53909064330730	0.91011946180591
H	5.44459828612142	5.70155442492607	1.10833513358378
H	5.34038227773897	4.09749773461153	1.86217767143805
H	4.75969767681424	5.82702423211013	3.87344853470833
H	5.43494235020688	7.25371217512056	3.07824356926325
H	6.11805913365089	6.69840440855010	4.61583234922892
H	8.60026778836983	5.94606189233512	1.85154304356477
H	8.32103791719956	6.90556721760441	3.31690990492541
H	7.41936605031548	7.26717032274646	1.83014622304658
H	3.55582600643214	2.66009500695324	4.84461255444228
H	4.09000689616268	3.70303084378350	3.51073737620825
H	3.96288354311202	4.34584439743673	5.17862755790277

Cartesian coordinates of **TS-*rac1-meso2-1-Me*** (TPSS-D3BJ/def2-TZVP)

C	6.71065746661943	10.44470926980211	0.81078766211853
P	5.33968191520523	9.89528294830021	1.96082793058854
P	3.45479731027071	7.91268622647820	2.97027190070305
P	3.31753394944118	9.56973912474994	1.51202453410184
C	4.60722565414608	8.55832200502361	4.34552128859166
C	0.86121788920591	7.26859325345379	2.57520445921497
H	-0.14015125506280	7.02012899888211	2.94753490603942
H	1.27278981781315	6.38302956570447	2.07943023497799
H	0.75674904567105	8.06192044201596	1.82651258606948
C	5.72943086975060	9.59873131090007	3.72368584492490
C	6.00537643220525	10.79232009603381	-0.51052197419760
H	6.76897320719540	11.07629772997524	-1.24455880259521
H	5.31609148194370	11.63299453545059	-0.38643272719042
H	5.44930791741587	9.93715504199518	-0.90608559251344

C	7.42200499791269	11.68055632154376	1.38419323366735
H	7.88798945849644	11.46320274444945	2.34866744799401
H	6.72298042420947	12.51064391114289	1.51573765443233
H	8.21301222586257	11.99000403412561	0.68848667865200
C	1.74314691914338	7.71524362405546	3.75928211727171
C	1.85787294966104	6.54852919140798	4.76016143940284
H	0.85138017270566	6.26630063174350	5.09427031835386
H	2.44190218963015	6.82426587298798	5.64067912287949
H	2.32343833818894	5.67184649893175	4.29746212823277
C	1.11428486588228	8.94094873084388	4.43163899274394
H	0.87825004358336	9.71793863892594	3.70257655132612
H	1.75887506985649	9.36956215067696	5.19989164211811
H	0.17404667716955	8.63965042419407	4.91239307421875
C	7.70654071778375	9.29213468133424	0.59431248664582
H	8.50076679043675	9.62620362798543	-0.08647609424518
H	7.20718483195281	8.42401033083843	0.15673196510121
H	8.17218856163896	8.98572021504819	1.53411809809974
B	4.33029850429133	8.90387797249891	5.99704550443473
H	3.25344517276856	8.72861614304669	6.44516556802077
B	5.33370685293789	7.52245634468177	5.51424734486279
H	4.91344153013783	6.42007143734594	5.59654343006126
B	6.26034914151614	10.71950030574528	4.91043821610160
H	6.52589429657223	11.81092517355159	4.54140286513120
B	7.07469033170543	9.72839866236475	6.13022003310934
H	7.98301767426417	10.16391029576782	6.75445078108685
B	5.39892015441040	10.26494796964977	6.39451588399265
H	5.08339207195494	11.07835194717573	7.19618764509258
B	7.03588398722663	8.02468093500259	5.59301001748604
H	7.90136582859061	7.24924531879705	5.82363463681842
B	7.26398163697787	9.33584603783955	4.40799984839253
H	8.21664177108675	9.50818128195063	3.72979840471073
B	5.87595311047928	8.60127871326109	6.81437191511159

H	5.90193211138254	8.22612259095182	7.93810958896859
B	4.57160048696076	10.21436754043825	4.84186864534296
H	3.70987831535861	10.89325241491276	4.42072281888294
B	6.21009906483329	7.96000957663773	4.05303191135606
H	6.34863298378212	7.25759421602510	3.11743329573907
C	2.29740605535667	11.06231994005434	1.99824355713356
H	2.64329037455576	11.87307361055132	1.34782470054992
H	2.39327226965025	11.36789948708791	3.03864609225743
H	1.24824933726490	10.85451990566074	1.76003818762782

Cartesian coordinates of **TS-*rac2-meso1-1-Me*** (TPSS-D3BJ/def2-TZVP)

C	6.11878128735896	10.62460467746251	1.08606196506866
P	5.60039150006722	9.16035976901129	2.13363375644167
P	3.79239551981507	7.04486503046121	3.60089366406851
P	4.61134934169482	7.39278180749441	1.56452435103687
C	4.88919461546832	8.13665966183711	4.69195849596853
C	1.30175851013561	6.69327253989431	2.69217084810192
H	1.73643823538527	6.44703736099839	1.71671563396257
H	0.26589881155104	7.01508178207607	2.52970989811419
H	1.29121145434802	5.78862363756891	3.30859859948241
C	5.96225481031380	9.16974395764120	3.91908027498206
C	5.26756694009210	11.85321605793413	1.44975628829515
H	5.57607226388901	12.70390972863412	0.82757772828893
H	5.40080751358222	12.13386304996521	2.49748516103702
H	4.20655828098142	11.65560553054899	1.27612145220934
C	7.61393448615056	10.91902987432037	1.28011716574040
H	8.22311701667877	10.05481172906195	1.00303208061833
H	7.83787803836718	11.18283960394669	2.31705871830787
H	7.89555614041255	11.77009163397819	0.64584939887387
C	2.07794530070118	7.83962641511295	3.37898836582460
C	1.45965473055385	8.10528727296324	4.75992398213651

H	0.38535804262252	8.28992382775216	4.63427847935401
H	1.89997361110423	8.98347249483238	5.23562864085139
H	1.58099741610830	7.24899884087049	5.43213049530795
C	1.98045599303371	9.09305145570963	2.50120283067201
H	2.34084037839539	8.89424067143087	1.48772778982765
H	2.54915736308223	9.92924056103462	2.90891790770816
H	0.92528700795893	9.39099049423967	2.43614577683709
C	5.83462298069755	10.18971754776052	-0.36118093736854
H	6.06576136045519	11.02962845895557	-1.02727312824670
H	4.78266341105586	9.92145701000213	-0.50010548564235
H	6.45580470740093	9.33696905630495	-0.65062751107374
B	4.52580461710606	8.71753289548863	6.27124435558364
H	3.45358080041825	8.50516430131089	6.71296520711405
B	5.66600348836054	7.38772437539954	6.03213649322632
H	5.34514866795554	6.27608888439324	6.27436691287918
B	6.33500879881805	10.49533959225603	4.90681793019276
H	6.52380498699375	11.54381091568186	4.39402908489598
B	7.18451076729487	9.80993755209971	6.31018765341478
H	8.01331529363651	10.44185047129798	6.87425662190279
B	5.44745536556755	10.22139603618565	6.43085273511710
H	5.03947841095355	11.13281589304208	7.06861594808207
B	7.31389940145936	8.04975223724900	6.07538180394060
H	8.22713983857128	7.39407547515527	6.44890434978545
B	7.48861281515538	9.15583451139583	4.69594782025074
H	8.43836622223797	9.28563485324696	4.00415375995369
B	6.06598109279674	8.71001719997529	7.14953993870985
H	6.08361033257510	8.53228399547980	8.32089529452502
B	4.68874623815491	9.82883841996590	4.90104054586196
H	3.80186478084442	10.36681144528278	4.34757506478306
B	6.54754516999182	7.67351246704768	4.53458604460748
H	6.80568527771213	6.82369356906258	3.76592346193038
C	5.80880274497134	5.97846850669707	1.34520915016010

H	6.56318759946683	5.88815809342903	2.12518380171828
H	6.29776065029133	6.12370093050826	0.37677750994153
H	5.21284956920484	5.05923583854464	1.30041582463678

Cartesian coordinates of **TS-meso2-meso1-1-Me** (TPSS-D3BJ/def2-TZVP)

C	5.02065526724546	8.10785061795331	4.65478248606630
P	3.86866396041890	7.05601832747509	3.62072456093310
P	5.07544800964849	7.42811749477694	1.89933810410467
C	4.77944604383164	6.51961679201945	0.33258018132071
C	1.57004832945469	7.13516332844351	2.26234349043047
H	2.03518469694746	7.54189188869336	1.35819857910448
H	0.48871419198054	7.30764183171798	2.20413283116564
H	1.73702285937369	6.05079636514966	2.28269976429166
C	6.35608627786999	8.98777853318638	3.89633579811387
C	5.03846296870767	11.36323308686139	1.62361145627935
H	4.88063985615733	12.17139613355939	0.89679942851652
H	5.19240788216783	11.81839954863536	2.60351657613844
H	4.12915927187019	10.75560582419032	1.65466626465235
C	6.23826112939292	10.53002213213202	1.18597485626230
C	7.53986036985567	11.35210583305460	1.25836650913362
H	7.73606803081689	11.70827130739969	2.27276369723646
H	7.45279330258250	12.22587966168657	0.60026580352774
H	8.40166350707893	10.76141443810607	0.92878646861045
C	2.12523408539687	7.82530375096054	3.52564955442896
C	1.37718487981325	7.28560695922338	4.76059730475121
H	0.30782773801942	7.51169132371745	4.66300991011745
H	1.73927099437961	7.74494466702333	5.68381639214637
H	1.48958462288713	6.19953070659072	4.85008138978274
C	1.94655063767937	9.33401653760246	3.39443279533561
H	2.54007560803023	9.72959090667495	2.56492053695358
H	2.22452448727327	9.85987515479495	4.30944140767210

H	0.88989544942145	9.55117461497256	3.18786466652969
C	6.02533077831445	10.05565135526900	-0.26687632572900
H	6.00905566573204	10.92802274881006	-0.93103125917471
H	5.07310730035498	9.52453191262232	-0.36907190164810
H	6.83236089232799	9.39220051492783	-0.60248702361754
B	4.52904775750248	8.93541147211819	6.04477539734039
H	3.38000803295687	8.91522290954250	6.31734463383634
B	5.54588973419839	7.48701194971964	6.14915870133254
H	5.09446876908696	6.44252594741455	6.46919782527754
B	6.70190611467546	10.36718802176007	4.81086187296377
H	7.05165888142794	11.33572138682939	4.23240993501544
B	7.25184849970524	9.78359700747933	6.39545235376333
H	8.05566290160594	10.39751918869580	7.01294607708148
B	5.57551607262321	10.35807128757379	6.17764388110263
H	5.16575883073931	11.37248140476111	6.63265683636883
B	7.22611987803181	8.00372722372659	6.35238571963503
H	8.00350778245986	7.32100998237911	6.92910050471128
B	7.71511827720903	8.91643819760464	4.91735265897746
H	8.76825722464403	8.86309251205398	4.38330951957988
B	5.91509391634071	8.90278626766089	7.15455064737163
H	5.74242372977773	8.87334463544368	8.32657155284284
B	5.02610830801108	9.82133259936401	4.58686121556420
H	4.27058068872988	10.35524989001625	3.87491382054495
B	6.63922284863222	7.51096704913717	4.74711237108165
H	6.92349024440122	6.54887313300165	4.13086348714966
P	6.63703050643803	8.87638260489083	2.04916799583819
H	5.74419807369460	6.39102156582760	-0.16624682295853
H	4.08263291881613	7.02369607539394	-0.34029857418966
H	4.38730091326106	5.53253338937462	0.59392408633263

Cartesian coordinates of **rac1-1-Cl** (TPSS-D3BJ/def2-TZVP)

C	8.30318556143279	2.72417068320279	3.18832721217537
C	7.84385855381465	1.09179490042511	2.99176914063727
C	6.92471605439837	5.42028950972969	3.46978964762790
C	6.07090256224360	0.01330908486955	5.31570745650524
B	9.21678475924585	0.08037241102718	3.05192902122912
H	9.08732036656805	-0.99787283326673	3.51082107040676
B	8.46286690638729	0.48775663972455	1.50493439030502
H	7.79303920382503	-0.30316515649702	0.93789040855386
B	10.22676484935617	0.54984247595731	1.67109208364190
H	10.91002109253416	-0.25180288004128	1.12907788903637
B	10.59775470071561	1.16200714527091	3.30586984584742
H	11.53638679016331	0.81517458694955	3.93943160456573
B	9.07341734233982	1.49451147015968	4.12026986950218
H	8.83146153912845	1.44121166292490	5.26835750492974
B	9.98890891133213	2.83166218050857	3.40855765418861
H	10.38294897649463	3.67988402947484	4.13227321201899
B	10.70174010377937	2.24524966237158	1.89242376461411
H	11.72967704824670	2.68876803646784	1.50487283864482
B	9.36641558529814	1.82794935214525	0.78098287477012
H	9.42121658620314	1.96821588567484	-0.39361787119278
B	7.85278786913664	2.14449676532843	1.62822935573392
H	6.81325081502319	2.48919723398515	1.18317501529451
B	9.23414634705994	3.23172085934939	1.85663431330547
H	9.14791327298263	4.35018405842154	1.49684926703405
P	7.07159537771019	3.68673252474349	4.23047137705240
P	6.11964305936039	0.55905296528236	3.49029350503658
P	5.33125525879242	2.66207102505125	3.24644546574197
C	7.07609865649334	-1.14262280362127	5.46897425580527
C	4.64266265497931	-0.57297274582019	5.41655848612874
C	6.28440586175530	1.04672581164207	6.42641630294091
C	6.53432381731869	5.50939981102710	1.99072552837137
C	8.24998215154417	6.15197853640264	3.74775545822380

C	5.80882988754072	6.05974280382143	4.32489919862973
H	6.99656364854462	-1.86559591400975	4.64991798819309
H	6.85304930814472	-1.66754049865289	6.40652067449192
H	8.10518522034480	-0.78285263535339	5.51797037266613
H	4.48546983205767	-1.36484596382315	4.67683905876295
H	3.87494475009032	0.19224713984617	5.27689157524019
H	4.51571164440350	-1.00509420974742	6.41658273087569
H	7.28567867957547	1.47661555343913	6.40500974487879
H	6.15608441465149	0.53889451819368	7.39183565012054
H	5.55959505071940	1.85922452783564	6.37394338767684
H	7.28676339823225	5.07148465699493	1.33435393051726
H	6.42371511074435	6.56704782801872	1.71854895335447
H	5.57769726684608	5.01252697363438	1.80101795220703
H	4.84016224958686	5.58073088171120	4.14942924753899
H	5.71825050805574	7.11794309834993	4.05175222899301
H	6.03425835838199	5.99964927698960	5.39509518270398
H	9.07349838918133	5.74614952427407	3.15639056137400
H	8.52130881852829	6.08941409308619	4.80722639669941
H	8.13350010277609	7.21164839057778	3.48790143598549
Cl	3.85354072593083	2.85052706594272	4.72233578041376

Cartesian coordinates of **rac2-1-Cl** (TPSS-D3BJ/def2-TZVP)

C	8.32540857919062	2.73056933491824	3.12244795584389
C	7.88818519519429	1.12618615774161	3.00751018564992
C	6.91500052255858	5.43943036674171	3.46754820532755
C	6.07033339291408	-0.00526256884453	5.30279615229643
B	9.26097843205626	0.11138081837697	3.10874208819864
H	9.13349403541772	-0.94964397793718	3.60641217731199
B	8.50335919689666	0.45199014416185	1.54633123807998
H	7.83634900291045	-0.36986120514029	1.02078180667052
B	10.26718211850514	0.52772990839693	1.70914885207537

H	10.95641992111559	-0.29174691612454	1.20237447158416
B	10.63946985177866	1.20857789431129	3.31608874784795
H	11.58362131679895	0.89643168604369	3.95959373678308
B	9.11937242427281	1.55907705114240	4.12197329762882
H	8.86191344460669	1.55660768054158	5.26931302710381
B	10.01260224343973	2.87531136820043	3.35042473625348
H	10.39457945719032	3.75863604872303	4.03782185410313
B	10.73246342167920	2.23459025550797	1.85973762423730
H	11.75965694108159	2.66602240986431	1.45676436017258
B	9.40273241770062	1.76240578047084	0.76352603910794
H	9.46147545658473	1.85073474627503	-0.41594305277200
B	7.88076485688006	2.10761308633349	1.58558670286760
H	6.83788501480845	2.42868251285481	1.14663478108486
B	9.25831166743566	3.20843838179029	1.77981904647442
H	9.16151925591936	4.31712431125375	1.39014402667194
P	7.07877596381894	3.68284033845059	4.14111504228752
P	6.14261502299030	0.63847322392751	3.50780770761590
P	5.19557205334540	2.61497415047284	3.82846524924928
C	7.03905586639439	-1.18638594587062	5.45987250492261
C	4.61668713723892	-0.52773465834213	5.36140473686767
C	6.27690547413305	1.00880804193078	6.43511476333783
C	6.57311516124714	5.58452029982671	1.98020334466460
C	8.24265170972348	6.15048830311805	3.79313484633431
C	5.78364328050501	6.04576609148397	4.32281153142190
H	6.96048880644630	-1.89240430192548	4.62645293071305
H	6.78846176506309	-1.72161436185877	6.38434178462929
H	8.07518540742964	-0.85081625430290	5.53333351985893
H	4.43915060774787	-1.30784676094971	4.61472484149771
H	3.89298776439357	0.27933120806451	5.20041431742358
H	4.43497498179271	-0.95007132414989	6.35707652415854
H	7.26872763253906	1.46143598607748	6.41452942062287
H	6.15637266958389	0.49071284126684	7.39573578166233

H	5.53214194857971	1.81030102910776	6.39250318796930
H	7.31152503085787	5.10357933799562	1.33799678121077
H	6.55851398716459	6.65440629841623	1.73402551720675
H	5.59182957954517	5.16720312971012	1.75316363787851
H	4.82021796215580	5.57251204716421	4.10611338098174
H	5.69779468613403	7.11283547120428	4.08570602487290
H	5.98846033618278	5.94848304379000	5.39424693563035
H	9.07020623304788	5.75349190658037	3.20029385282777
H	8.49806488887093	6.05693973667666	4.85379235454980
H	8.13643134482575	7.21636981420101	3.55651139392380
Cl	4.30632453130650	2.90188603233026	1.93249002507702

Cartesian coordinates of **meso1-1-Cl** (TPSS-D3BJ/def2-TZVP)

C	1.41440062263861	6.72061696623398	2.54118859911114
H	1.59208249753238	7.23277788157605	1.58917666753394
H	0.33130004812935	6.68485299158329	2.70861345363916
H	1.78286201296832	5.69280494643223	2.45296384438852
C	6.16458454723298	9.12583832252457	3.83476628497395
C	5.70299386137946	11.57184622616923	1.41981808242594
H	5.95375164640771	12.42412676890328	0.77502949745051
H	5.75501566534177	11.90863002812009	2.45569303027218
H	4.67233023515122	11.27553101245524	1.19923281761423
C	6.68016978071844	10.42888351395807	1.12969017155523
C	8.13246370671615	10.83528241587471	1.44132933392593
H	8.82792953558751	10.02162310522715	1.20946990450344
H	8.26319406051116	11.11179845319120	2.49005481518405
H	8.40177543104306	11.70142723103376	0.82416483364916
C	2.07517912187925	7.46807686162720	3.71971693047515
C	1.74849364504147	6.73015683195171	5.03121766861036
H	0.66113646346781	6.72406821344366	5.17696072855222
H	2.20451636480445	7.21516973883556	5.89736896714100

H	2.09381270927220	5.69142356589859	4.99553727538982
C	1.56736361898308	8.91264264229324	3.74677221741356
H	1.80579916610606	9.43231459894622	2.81305299153487
H	1.98245270830690	9.48235624625781	4.57882839586054
H	0.47521662005431	8.90190138857038	3.85683549776801
C	6.57367146357322	10.03698204083241	-0.36005042331926
H	6.87771786664839	10.89379751087709	-0.97310994679583
H	5.54642043890086	9.77309190004864	-0.63455278133386
H	7.22382922290994	9.19033545290637	-0.60583232006521
C	4.88344013225549	8.30169253661789	4.55562160281343
B	4.33730814956708	9.14734046303789	5.93053123428182
H	3.19099496830793	9.10885316212139	6.20228367122347
B	5.35067817141903	7.69940679272054	6.08223249772351
H	4.87493592024117	6.66797684263102	6.41264716179319
B	6.51488073955260	10.54829885487158	4.70532983636340
H	6.89866698784904	11.49429610425564	4.11614489361077
B	7.04749980599114	10.00536681333224	6.30359021879382
H	7.84056358959763	10.63775293500024	6.91559141336873
B	5.37208012727668	10.57647132094736	6.05511601101992
H	4.95794452899977	11.59836534129817	6.48754466081530
B	7.03284835267972	8.22289396656299	6.31568564206248
H	7.80189960005438	7.56388486945817	6.92901045529402
B	7.53229248416468	9.10295903000086	4.85478136100303
H	8.58820800467888	9.05691075540824	4.32349135414396
B	5.69730724333700	9.13672838994501	7.06324823855853
H	5.50150666788212	9.13294099889998	8.23160469294624
B	4.83794653000010	10.01707335164885	4.46611686026560
H	4.08928697309622	10.50725302943949	3.69609117979431
B	6.48925335554582	7.68228399399511	4.73137826494317
H	6.75658964304623	6.71913722384342	4.10518083471894
P	6.37153102615106	8.77625444519694	2.00265231388435
P	3.91963814098138	7.19951830273353	3.38203206131635

P	4.18620523398214	8.53482497779219	1.61235901639555
Cl	4.29607056203667	7.05931864246951	0.12477798540737

Cartesian coordinates of **meso2-1-Cl** (TPSS-D3BJ/def2-TZVP)

C	1.36125508828835	6.63396796229012	2.55258817943015
H	1.38973497849585	7.23345650454645	1.63692689150874
H	0.31040162092660	6.44304444010484	2.80073317799166
H	1.84649444657150	5.67186070120479	2.35656518855601
C	6.05901718670948	9.24874199529823	3.81475706363518
C	6.02087052302919	11.74320629432042	1.31474890870311
H	6.55031624037305	12.54301227055893	0.78040169556326
H	5.99700964895582	12.00710660388887	2.37258956644656
H	4.99722098766617	11.70262062450941	0.94374430873120
C	6.76552841301805	10.42745824203492	1.06313210870315
C	8.25204986262555	10.57169412979611	1.44636383987753
H	8.80361744532647	9.64135500770981	1.27645740910741
H	8.37223875095845	10.86046360708654	2.49342923740407
H	8.69832342793999	11.35731409453699	0.82433458629316
C	2.01904690124734	7.37521647012328	3.73344650085631
C	1.92825209537771	6.50409132288243	5.00247846114725
H	0.86986731649288	6.32296793908809	5.22674956923344
H	2.37642386362762	7.00166633333618	5.86605683236994
H	2.42231937149107	5.53709666808758	4.86296670423019
C	1.32151392833715	8.72094105035366	3.96035360425392
H	1.27169773472717	9.30712394766623	3.04327909645062
H	1.81640052026931	9.31721647486050	4.72761794165748
H	0.29619902506387	8.52145211293790	4.29872194268137
C	6.65327070124393	10.03483707613656	-0.42342350283343
H	7.11982641212201	10.82064704317352	-1.02934312406386
H	5.60811619191109	9.94163126058933	-0.73583782015299
H	7.16708189618334	9.09070215197311	-0.63348130514663

C	4.79530125719728	8.43531728505989	4.52614438686715
B	4.28720636115789	9.23603097749805	5.94583399108261
H	3.14613637138693	9.20090576121713	6.24181341438240
B	5.27871272844007	7.76564460485380	6.02675663865644
H	4.79470943040905	6.73156159538170	6.33451879513995
B	6.46559028738287	10.63835713785410	4.71926510734746
H	6.86106767616938	11.59242586788534	4.14980913466398
B	7.02269012536969	10.03202865532019	6.28692757957423
H	7.84141493086642	10.62735442116802	6.90245699953086
B	5.35474657952461	10.64086424747738	6.09860888330409
H	4.96947212180032	11.65498606778406	6.57379736947175
B	6.97525199244183	8.25146553872970	6.24502101057386
H	7.74481562174153	7.55824797257953	6.81920670299521
B	7.45780932541816	9.16836481706598	4.79999194382483
H	8.50203408823703	9.11797369256419	4.24743093924995
B	5.67116944982684	9.16199505094381	7.04786419762986
H	5.50178735876517	9.12124447262263	8.21971925438085
B	4.76966184182701	10.15534433931403	4.50441626111078
H	4.01583186276243	10.68971564930638	3.77683241731221
B	6.39324223013169	7.77128850842694	4.66228486790683
H	6.62829895815139	6.82557586002981	3.99837034237691
P	6.15719418822622	8.88767071709396	1.97494804111433
P	3.85178206321148	7.40463876749536	3.27219307601317
P	4.08014961021885	8.50950091208504	1.39609658032128
Cl	2.88863896035686	10.27753475114815	1.29843500253423

Cartesian coordinates of **TS-rac1-rac2-1-Cl** (TPSS-D3BJ/def2-TZVP)

C	6.71763263530742	5.56522804739964	3.09029449204750
P	7.51879482974160	4.33055662401712	4.28288481425197
P	5.98345815543322	2.91324696014796	5.17319457650686
Cl	4.05413084432002	3.50747250239035	4.56939171906930

C	8.51637966403174	3.03037165142650	3.36716105688575
C	7.97425876897189	1.42001089702515	3.36698135777829
C	5.99587919754530	-0.23403544906357	4.98019716069989
B	9.26925455233867	0.36462971052947	3.69463201331672
H	9.05733455469160	-0.62129698899707	4.30405715546718
B	8.63975067856990	0.56911069293736	2.05018450026605
H	7.95721675144846	-0.26150786476283	1.55681669135418
B	10.38831761670820	0.55335491398308	2.33569202779378
H	11.04526047367704	-0.36058871567126	1.96613327600854
B	10.70114450642007	1.38971028143094	3.88293301723461
H	11.57222122553674	1.08866289538412	4.62648895590133
B	9.14174972509078	1.92617481072115	4.52495425170428
H	8.78164181478910	2.06588533356110	5.64284621724790
B	10.20125695904979	3.07591926634426	3.68806416107043
H	10.58828116313850	4.00610482125813	4.30600988485243
B	10.96406924349532	2.23150728771951	2.33385859665796
H	12.04226373036966	2.54825378571234	1.95913252899099
B	9.67495186904420	1.73463053959498	1.20255127596789
H	9.81953339489567	1.68842713589630	0.02807203190336
B	8.12962599226642	2.25749326835590	1.87350846460570
H	7.13383337261453	2.55394337461238	1.32325854296373
B	9.56371918395206	3.28727871685691	2.04796837973062
H	9.56481678878320	4.34285394974554	1.52415208286718
P	6.16137074398095	1.20329713245247	3.75305059083470
C	6.20328299520770	-1.53351345182073	4.18060751893195
C	4.51515438040053	-0.13701703991579	5.40663884359353
C	6.88138393589844	-0.19459028680400	6.22963250723951
C	5.91168122945004	5.01761471461538	1.91012582401833
C	7.86561011763863	6.46525287065475	2.58593169180834
C	5.83884199707064	6.42737136603094	4.02468780557277
H	5.54505076264620	-1.56679729570291	3.30597220093328
H	5.96259426357020	-2.39008191143018	4.82260844290422

H	7.23504684197909	-1.64440838908914	3.83963115421221
H	3.84308882219978	-0.10782399555676	4.54203517319323
H	4.33028779053817	0.75300153996054	6.01817685476742
H	4.26342318904962	-1.01820405100350	6.00880420085034
H	7.94152136120123	-0.28259986117070	5.98990001821538
H	6.61219088007492	-1.03689170351707	6.88014905848840
H	6.72537898335824	0.72984614800262	6.79481740535389
H	6.56640113739503	4.55971427079964	1.16653188143728
H	5.38649214523288	5.85082881829703	1.42498389348809
H	5.16767456782820	4.28290295865207	2.22364865166697
H	4.96804679338434	5.88648033131697	4.39692033829978
H	5.48573783164260	7.29608211364665	3.45606607214917
H	6.41751737091147	6.79680312968314	4.87909833678362
H	8.51788626769938	5.94502577521272	1.88361292327767
H	8.47371668203377	6.84201092978469	3.41503540863697
H	7.42352321737684	7.32602743834572	2.06849897019855

Cartesian coordinates of **TS-*rac1-meso2-1-Cl*** (TPSS-D3BJ/def2-TZVP)

C	6.72221973977967	10.45377123593091	0.84135483168918
P	5.36304780360681	9.87333948314794	1.98626025318908
P	3.48148612450264	7.83946711389647	3.04531113532386
P	3.44285016817450	9.34742565020652	1.43315951460849
C	4.64760685849019	8.51433361847695	4.36967389434790
C	0.86325079766013	7.39209312183094	2.57384633317896
H	-0.14105659746037	7.13635152758079	2.93212486941484
H	1.25732959577246	6.53098383910886	2.02237334331641
H	0.77006407352087	8.23916126421566	1.88659665692939
C	5.75516332049019	9.55622412377682	3.74172942148045
C	5.99976512283386	10.81969753511002	-0.46702239247872
H	6.75263909722918	11.15276115628988	-1.19105307559713
H	5.28094220900846	11.63005159543755	-0.31557800743964

H	5.47531185197494	9.95827704569560	-0.89133153161528
C	7.41250950619103	11.68964421855785	1.44076268870383
H	7.90018218831495	11.45743763085148	2.39071068986872
H	6.69834210849533	12.50095917685852	1.60357352106400
H	8.18321289061571	12.03369119201188	0.73960402671641
C	1.74537776842402	7.74639865240751	3.78898758676239
C	1.78008212331149	6.54711063674093	4.75850423659310
H	0.75951529783889	6.34857961134864	5.10855029506835
H	2.40328998432042	6.75026456224869	5.63300110439235
H	2.15632196763629	5.64402020398244	4.26626396638279
C	1.18452844636616	8.98993709557290	4.48762493793870
H	1.13581138671337	9.84300603164004	3.81064568583604
H	1.77123846697496	9.26971009460262	5.36252778089306
H	0.16572770890963	8.76087385139148	4.82751520371341
C	7.73146074899352	9.31828848869502	0.60074013639642
H	8.51404926985858	9.67790021075911	-0.07984285762292
H	7.24320469097789	8.45114905961623	0.14869901478189
H	8.20971416407004	9.00286857120649	1.53115070854780
B	4.36855749473999	8.86542791879414	6.01766071668961
H	3.29928864848979	8.66750528270080	6.47105296983475
B	5.38806920597529	7.49250122265980	5.53949355239285
H	4.97538559320414	6.38742833011905	5.62620438526014
B	6.27113304907977	10.69660394237548	4.90871250290353
H	6.52307583221931	11.78656325969027	4.52744326910738
B	7.10175030600391	9.72551495294748	6.13484203812130
H	8.00514011162495	10.17843940971474	6.75307145629723
B	5.41735238646380	10.24490923280716	6.39659172000238
H	5.09737248380837	11.06060760481727	7.19317129901482
B	7.08525430621561	8.01582714594224	5.61101316794723
H	7.96012609321088	7.25275105268279	5.84543520209142
B	7.29549205777297	9.32020694313186	4.41847107263657
H	8.24032323594665	9.49956036355934	3.73155646437556

B	5.91996779887009	8.58896828931382	6.82900706387021
H	5.95293013270479	8.22227072734687	7.95495756483316
B	4.57945632045009	10.17602654464462	4.84678841726086
H	3.70936672191919	10.82869832266494	4.39524380213621
B	6.25659214657160	7.92912123136006	4.07166673902348
H	6.39509012596137	7.22330602158009	3.13740830873354
Cl	2.08918706517159	11.03140460195038	1.76156431508365

Cartesian coordinates of **TS-*rac2-meso1-1-Cl*** (TPSS-D3BJ/def2-TZVP)

C	6.12641417057398	10.61653092009259	1.09057528394968
P	5.65940863187975	9.13491181982554	2.13365491096595
P	3.78999798809047	7.07082977043678	3.60727575349716
P	4.55079192909369	7.48558864969765	1.54560914951111
C	4.88435756726869	8.16186101997440	4.69200365187539
C	1.30971035696998	6.70778810687090	2.67409243656031
H	1.75190269907607	6.47526207534931	1.69865920167560
H	0.27147350183261	7.02003260920590	2.50851100743976
H	1.30533716699153	5.79541228173685	3.27856445786623
C	5.96266823506833	9.17678785630345	3.92804716234427
C	5.23552253392311	11.81484815585386	1.45767125835536
H	5.51973995519761	12.67395960420210	0.83623618167068
H	5.35952224354642	12.09942546837628	2.50554532490012
H	4.18138715041399	11.58622991582183	1.28030799032619
C	7.61251599686817	10.94832921783547	1.29919954841235
H	8.24720663120367	10.10319054141575	1.02078881201955
H	7.82251951691376	11.21423519023275	2.33838898448247
H	7.87304146230801	11.80874301235060	0.66967564015775
C	2.06760450466204	7.85350138576576	3.38228154123988
C	1.44820054164537	8.08496014933715	4.76911993061349
H	0.37026758239907	8.25037177150822	4.64818970120561
H	1.87317759097000	8.96357980041187	5.25801079029279

H	1.58722665368309	7.22024747113014	5.42700412580848
C	1.95695869263100	9.12451865931035	2.53089031897349
H	2.27179928809234	8.94052318856909	1.49894407563497
H	2.55446690879948	9.94469376295757	2.93035920292787
H	0.90595446296913	9.44195917646542	2.51104334627926
C	5.86710415708830	10.17167212605030	-0.35873912001283
H	6.11727045606172	11.00628152851439	-1.02420265579459
H	4.81622485061182	9.91064715011906	-0.51662682056615
H	6.48732781814582	9.31300570234925	-0.63146093828847
B	4.52977951949459	8.74585094909396	6.26824726943281
H	3.45526704511288	8.54937993057235	6.71144738851492
B	5.65133462187356	7.39756953626004	6.02781854368742
H	5.30931634782529	6.29289108623291	6.27094905029008
B	6.36309352297220	10.50016767057905	4.90736887931430
H	6.56493991662552	11.54315648888445	4.38864790926946
B	7.20560614832161	9.79689144171127	6.30422675188509
H	8.04597231181698	10.41398673371830	6.86690868858932
B	5.47522055732261	10.23693642133002	6.42975778184606
H	5.08202278721583	11.15229045172946	7.07066169016920
B	7.30890927769886	8.03398176086202	6.06426274252839
H	8.21465487868142	7.36881002027107	6.43731909634273
B	7.49325426865628	9.14031268757710	4.68708634018130
H	8.43821502815851	9.26063095350391	3.98735541879214
B	6.07198457177881	8.71365901587806	7.14313369818790
H	6.08876583540567	8.53568719264665	8.31416589617880
B	4.70466441078267	9.86012440978167	4.90051753128531
H	3.82328555618076	10.40756954691983	4.34661977962413
B	6.53579997926553	7.66100324942359	4.52456828854054
H	6.75853567768959	6.81962122830920	3.73143238656153
Cl	5.82633649214179	5.77912113664453	1.26864461445490

Cartesian coordinates of ***rac1-1-tBu*** (TPSS-D3BJ/def2-TZVP)

C	8.27933050199083	2.69666113047257	3.17698201807362
C	7.81152586906705	1.07879086773586	2.98972418396328
C	7.05713225685451	5.41417078948720	3.72062429695075
C	6.33385175933998	-0.02538486749962	5.49103808570142
B	9.19190469639072	0.06084410122185	2.96237449076161
H	9.09153999149705	-1.02456171029958	3.40928620953948
B	8.35753156346171	0.48064726094686	1.46616477099971
H	7.66484162153616	-0.30867616314852	0.92419878453344
B	10.13215989712170	0.53981296455665	1.54050420296417
H	10.78570360715273	-0.25896265071208	0.95802397994942
B	10.58674067537858	1.13858717870467	3.15500302311133
H	11.55401178956873	0.78728809646056	3.74228306577623
B	9.10992683028003	1.46218495616538	4.04591261255013
H	8.93897007179444	1.40293241574617	5.20446821018447
B	9.98061087407592	2.80656561265446	3.30514769500841
H	10.41652582263674	3.64156394216758	4.01973972126372
B	10.61929697788621	2.23561013342378	1.75226820071472
H	11.62771330687693	2.68233114947668	1.31833735506288
B	9.23309721803458	1.82340484435085	0.70925253669869
H	9.22482573210640	1.97529982190208	-0.46575079996427
B	7.76150824199911	2.13688556220946	1.61670088984768
H	6.72836759201291	2.48529395063502	1.18296067812950
B	9.14588739727502	3.21918735691086	1.79933096368720
H	9.02987375474631	4.33650530141614	1.44076706803406
P	7.11718302839921	3.62470374521524	4.35202960981812
P	6.13546890918687	0.55109223922430	3.66606823352641
P	5.35353527124319	2.61605903906152	3.38452625106587
C	7.37651259713020	-1.15639617104167	5.53011288621134
C	4.95739468996870	-0.66829408909479	5.77724466435332
C	6.63282528760018	1.00530045322220	6.58497165477678
C	6.46941188007702	5.61181746622148	2.32056284656147

C	8.47613055522789	6.00401853425109	3.82230602270894
C	6.18813913751842	6.12771479989312	4.77729309671280
H	7.21835296038413	-1.88460040596719	4.72760052377671
H	7.27518252824985	-1.68168710522268	6.48864183522551
H	8.39569062087932	-0.77650436723943	5.45949798859564
H	4.67608428568648	-1.38692203676834	5.00033539702592
H	4.16449033241115	0.07802662689549	5.86323548268156
H	5.01546662280369	-1.20062940173782	6.73424027668284
H	7.65667423750037	1.37392268620650	6.53987006005572
H	6.48815600718938	0.52571008098011	7.56285186159225
H	5.96936400679578	1.86783777673177	6.52770015884923
H	7.05694459977679	5.09680828598099	1.55828016746259
H	6.45893134564080	6.68251116185088	2.07748764991547
H	5.44243331443570	5.23927428975481	2.26231964944628
H	5.17272515957761	5.72485771016785	4.82120659284463
H	6.11585830217243	7.19212047652556	4.52310814184666
H	6.63176675327523	6.04183013743174	5.77474499828489
H	9.15037326285525	5.59560838993239	3.06925634117965
H	8.90938148460874	5.82041984911500	4.81150256177677
H	8.41616123409906	7.08986862075060	3.67414513948952
C	3.69980660278717	2.86146218957365	4.28863399477272
C	3.09221328639164	4.12982673196389	3.64954066779493
C	3.71196386707329	3.01344120887298	5.81145708511793
C	2.82271117032154	1.67414455343330	3.84285305884453
H	3.97755866687999	2.08097359608740	6.31131690065563
H	2.70990516274130	3.30283773899522	6.15488517608785
H	4.41586666380642	3.78734698797523	6.13328662706658
H	3.07836917047183	4.05241575209163	2.55795563563937
H	3.63745579959112	5.03648953949312	3.92158775525218
H	2.05955857304938	4.24241316325931	4.00270798619877
H	2.80019547520306	1.59524881493534	2.75072167215600
H	1.79593481292168	1.83787450513920	4.19364494745231

H 3.17422428498372 0.72107438085406 4.24167615695260

Cartesian coordinates of **rac2-1-tBu** (TPSS-D3BJ/def2-TZVP)

C 8.50950784474761 2.77539211291564 3.18563433875627
C 8.05002371544821 1.18117461590799 3.00742395025180
C 7.15371089308868 5.48641382120490 3.48587022280374
C 6.12145207934149 0.01070443954915 5.17494809636254
B 9.39644856111327 0.13665717924840 3.17377943965636
H 9.22002428835677 -0.93346950581712 3.63395075302320
B 8.75197875707733 0.52479833997419 1.57429063952202
H 8.10656944293004 -0.27081109939579 0.98432677382717
B 10.50282363711809 0.55937023179191 1.85492011977531
H 11.20868208311867 -0.26419406901530 1.37779423643694
B 10.77801075958517 1.19933274264662 3.49762879102729
H 11.67040925220613 0.85325915173706 4.19572475058233
B 9.21384700803643 1.56624075613963 4.20651406351884
H 8.88685832998424 1.54431831006442 5.33483968622891
B 10.18303729244778 2.87798836260899 3.52823669820732
H 10.54030005990149 3.73576584360935 4.25969042176899
B 10.99183551580970 2.25301914316336 2.07514607265585
H 12.05271586818716 2.66988250219127 1.75090648504144
B 9.72928440589475 1.83103167895379 0.88293528135978
H 9.86426743281191 1.94451368016938 -0.28869709041660
B 8.16961102712126 2.19106963150827 1.61943982451427
H 7.17435727912375 2.55565650438211 1.12150417430937
B 9.54740447988890 3.25783731793534 1.91923944805810
H 9.49811232337681 4.37380893830023 1.54064177851648
P 7.19269769350459 3.71977466851494 4.14212479034167
P 6.26950497413049 0.71361433263112 3.40573443803182
P 5.30055651065742 2.66930920612493 3.67869409309048
C 7.06672007473799 -1.18732446160033 5.34467379810950

C	4.66267531418347	-0.49860733235301	5.16438469226247
C	6.28183464928489	0.98971130667945	6.34403404156828
C	6.89475287392190	5.65472568256869	1.98628037042858
C	8.49474378963526	6.13763829742388	3.87878809767673
C	6.02379047999002	6.15115814452927	4.29919980056671
H	7.02290904644202	-1.86657810955757	4.48665192073252
H	6.76502460162127	-1.74752716824154	6.23863885571156
H	8.10126796716049	-0.86765941161913	5.48104138041579
H	4.49774109020783	-1.23848975634688	4.37442362125765
H	3.95665325813015	0.32704743055991	5.02583227811328
H	4.44854370841071	-0.96860646337218	6.13196522325973
H	7.29111898769160	1.39615660414081	6.41177748450902
H	6.06559278171180	0.45507200393275	7.27870621742599
H	5.57868043056450	1.82322402696500	6.25772689038242
H	7.66266213893441	5.17158798785936	1.38121967148293
H	6.89109979386533	6.72453044649662	1.73888404612416
H	5.92586429963654	5.23989411921776	1.70509516300278
H	5.04821455717227	5.70883315248556	4.07672121992096
H	5.98174410394775	7.21742474650023	4.04566378611494
H	6.20400607852198	6.06095466498098	5.37535381244605
H	9.33154313375325	5.71683599013947	3.31724722294486
H	8.69755019116711	6.01524951169841	4.94760504602006
H	8.44304428370724	7.21137513254051	3.65904587811759
C	4.17333445277891	2.83935119716375	2.11907857540547
C	3.19581724069552	1.66463173173909	2.33855789867367
C	4.76060345874299	2.73019368141557	0.71340211267094
C	3.39249170118424	4.15381053027470	2.28724957849512
H	3.93981569538070	2.78490871934152	-0.01507947441911
H	5.27276450344452	1.77484369076055	0.57128327383226
H	5.45882329222271	3.53944418979750	0.48909617567722
H	2.56563989791705	4.17251721050114	1.56601154872621
H	4.01419021996563	5.03271518053560	2.10003414973145

H	2.96871072284159	4.23764637746558	3.29387293673582
H	2.40670954723972	1.72279444784117	1.57789299445329
H	2.72307346028118	1.70965399154190	3.32520985252628
H	3.70124665789734	0.69958366894916	2.23303758164509

Cartesian coordinates of **meso1-1-tBu** (TPSS-D3BJ/def2-TZVP)

C	1.23025611987815	7.26204783814492	2.43068906574325
H	1.55719382716296	7.69380750875624	1.47898059071822
H	0.16037267714404	7.47021708304371	2.55202826550792
H	1.35989007747014	6.17554266013978	2.38826878114786
C	6.17988073311861	9.08068833977549	3.79215798706621
C	5.23605939501434	11.63138048746171	1.66970855603823
H	5.25563370313471	12.53285266843758	1.04312785191451
H	5.39415020184105	11.93970864221991	2.70400554656335
H	4.24232025464494	11.18013601056212	1.58239278220792
C	6.32305625594640	10.67018748459269	1.18431128560071
C	7.72954425658024	11.26840756649509	1.38802471187475
H	8.50028247993391	10.59771050866637	0.99419775863152
H	7.94697317123776	11.46110573491839	2.44031764280405
H	7.79429244572464	12.22088265720389	0.84706163226294
C	1.98750218393589	7.88081804233731	3.62193334107912
C	1.45473432663140	7.23278988587245	4.91565488368837
H	0.38438389078163	7.45468721717811	5.01136017778372
H	1.96023303972795	7.61255930057761	5.80557225923952
H	1.57783375190384	6.14511722115576	4.88718944311027
C	1.75766699437448	9.39345456334441	3.62415710898861
H	2.19215094959049	9.86017083291098	2.73410029886994
H	2.17548896128929	9.86967271754787	4.51208825630920
H	0.67687247651933	9.58700865673719	3.61554066661248
C	6.12627939381561	10.41300076860641	-0.32245526494244
H	6.21702492727246	11.36808218702830	-0.85375478645377

H	5.13538153868572	9.99711486014220	-0.53273305594130
H	6.88627828050841	9.73222040780393	-0.71999546632538
C	4.88786084057434	8.24952324385855	4.51895553633283
B	4.46070024798796	9.00268701024796	5.98456967942260
H	3.32605063114406	9.00854777003280	6.30532959568830
B	5.41016350000402	7.50824089914265	5.96807332917557
H	4.90908743748633	6.47092986084234	6.23570391976778
B	6.63943210081588	10.40425436466315	4.75887246383138
H	7.02036461697455	11.38516418067581	4.22683155507480
B	7.22521952305392	9.70947844322881	6.28034836066406
H	8.07684722590893	10.25401250463701	6.89855015516438
B	5.56850948615319	10.36860945349370	6.16504735538090
H	5.22345822949197	11.36966514522346	6.69639118694849
B	7.12330049803595	7.93562734475499	6.14659779075604
H	7.88969883123986	7.19160377599273	6.65823664533660
B	7.59194877189344	8.91185673293984	4.74059562340021
H	8.61525276680191	8.85545248891635	4.15031550874180
B	5.87540816975874	8.84114202497516	7.03972849617483
H	5.73974516057627	8.75058567787135	8.21333757758449
B	4.93142587601157	9.96152308102647	4.56701610761742
H	4.17359454595399	10.55770766865519	3.90116884704602
B	6.46607167245020	7.56116730685629	4.55019596879387
H	6.66203031554126	6.63841040969564	3.84331205053677
P	6.36684928689687	8.92535265246568	1.93657878051482
P	3.76762948010213	7.25323072242221	3.39850713698193
P	4.36141152066092	8.11714017794210	1.44438332640892
C	4.87921337599594	6.51093971715688	0.52847490430102
C	5.87434735926318	5.63510510712930	1.29373150166382
C	5.49524198567539	6.95465141066354	-0.80659082420290
C	3.58509542770557	5.72524840293510	0.27012935212643
H	3.81724185648953	4.82707088807010	-0.31570650422494
H	2.85452058418530	6.32143073277588	-0.28680243555671

H	3.12860880922960	5.40147528313448	1.21093322656519
H	5.74502272738473	6.06817350081625	-1.40289278727390
H	6.41919925014936	7.51865947558378	-0.64369814798001
H	4.80292540553784	7.57578318820057	-1.38473128132018
H	6.10883898786911	4.74538029008060	0.69436062193975
H	5.45617725718945	5.30342596102181	2.24887792782038
H	6.80743992393834	6.17296125021107	1.48680712869746

Cartesian coordinates of **meso2-1-tBu** (TPSS-D3BJ/def2-TZVP)

C	1.29479726633984	6.60989178591020	2.80146086504951
H	1.23219018239177	7.18842036381609	1.87690360271876
H	0.27468957263045	6.38804902082987	3.13806118975036
H	1.79573460323643	5.66281421165986	2.57680535927895
C	6.06173344289551	9.27873200079499	3.84883123664536
C	6.31943623322668	11.84635344136209	1.43239291500061
H	6.91304341449402	12.58474330357412	0.87706773021268
H	6.38174694527285	12.09397643094817	2.49245564746553
H	5.28081841401950	11.94820649008257	1.12140317020039
C	6.87237755327565	10.44684774302775	1.14840545985949
C	8.34973634294898	10.38811773024410	1.58865204620529
H	8.77074570236617	9.38667754422331	1.45487600678477
H	8.47253505947658	10.68090136402289	2.63312051061424
H	8.92353383377424	11.08873765500635	0.96904285853680
C	2.03440220946163	7.37077913932356	3.92054719118040
C	2.14014622852563	6.44066772571435	5.14672471528475
H	1.12730805745821	6.13317791754722	5.43593252811742
H	2.59710300655543	6.94608681376184	5.99966932315507
H	2.72144489195779	5.54096220069794	4.92170242393993
C	1.28095733237298	8.64291269856481	4.31950505983773
H	1.15571559546040	9.32547485494098	3.48040587720148
H	1.79416462502992	9.17854614208436	5.11865392628151

H	0.28224688398157	8.36747342240669	4.68376495534069
C	6.80505632386617	10.11269123596729	-0.35572432540602
H	7.34912697273955	10.88362241350973	-0.91499186455213
H	5.77878134889475	10.07936425475168	-0.72850395321226
H	7.27326426730256	9.14477038987282	-0.56144151039974
C	4.80254629524671	8.47820931009488	4.56972199535387
B	4.38902941952764	9.21973913961697	6.05580853403868
H	3.26216878245145	9.21293072352081	6.40485451137222
B	5.32440475948933	7.71253706408462	6.01506435463356
H	4.82798206977442	6.68013097129032	6.30294288545501
B	6.56369349778470	10.60248722979206	4.81042862388950
H	6.97386015694412	11.57284813121420	4.27953880358757
B	7.16377228309954	9.89552530000045	6.31764811036801
H	8.03198557985107	10.42531599865083	6.92602458254746
B	5.51582550810069	10.57394385570034	6.23816133314126
H	5.19046366400374	11.57538884947309	6.78178347060468
B	7.04314951034093	8.12384355561938	6.18455392431171
H	7.80880946160833	7.37354104770677	6.68874412708530
B	7.49878251160574	9.09506377398107	4.77002946046002
H	8.52372978758308	9.03024764595397	4.18659918847268
B	5.81170121347598	9.03568220310157	7.09184041058615
H	5.69096357362011	8.93644357125359	8.26664761639935
B	4.85035491812730	10.18999305057427	4.64955800925451
H	4.08989137824437	10.78440870505323	3.98193937012125
B	6.37818518901368	7.74897937970516	4.60683724806747
H	6.55308071378419	6.82956341673893	3.89114227124270
P	6.01504012512366	8.97951878702441	1.97685345214060
P	3.79146887004746	7.56619873703351	3.25092543568972
P	3.87009459417481	8.84484576234623	1.44583603833762
C	2.70289949311375	10.35331371703356	1.07959349234296
C	3.20102662742140	10.88654817334922	-0.28029859840246
C	2.55139623212953	11.49438670306825	2.08278663363208

C	1.33614542746539	9.70123305098237	0.78709977636920
H	1.43905548967137	8.87178120433565	0.07889005756383
H	0.68368427563947	10.45642857685613	0.33012906774715
H	0.83883722178731	9.33033831992661	1.68283780434082
H	4.14337778931512	11.42889570151615	-0.20824733465424
H	2.44595676786495	11.57719645803204	-0.67731516267260
H	3.32447449308637	10.07093102025905	-1.00116658593683
H	3.50011066879207	12.00116208528650	2.27055257714811
H	2.15757468630119	11.14602034647102	3.03972770761986
H	1.84736065443375	12.23465013870709	1.67772386264965

Cartesian coordinates of **TS-*rac1-rac2-1-tBu*** (TPSS-D3BJ/def2-TZVP)

C	6.83702161404780	5.42402385332717	2.17710849952992
P	7.16126000602564	4.37727231231325	3.75816842765551
P	5.73592196344486	2.80096961127158	4.52949467428877
C	3.94989141789612	3.37307059144119	4.24105002810501
C	8.48770382780439	3.10583819378364	3.34974404024897
C	8.06486012819989	1.44310633678358	3.30833427457376
C	5.88586636047280	-0.46297519065750	4.12054714395775
B	9.27400957624638	0.53199872084243	4.09821473575257
H	8.96775563236094	-0.41774829883853	4.72377081962597
B	9.15861698368622	0.57377818503727	2.33190228000968
H	8.71738385168289	-0.33287637385564	1.71544337758771
B	10.73769289038657	0.72096569199927	3.11732106764126
H	11.52856106975804	-0.15801727546449	3.03698066083775
B	10.52189983018924	1.68032242004615	4.60559784386238
H	11.14253874094072	1.49704503420643	5.59781940866536
B	8.81399191886551	2.12233705635125	4.72079535098826
H	8.16479218996642	2.28391441563075	5.69013592619673
B	10.00200284438883	3.30372640147074	4.13500737954560
H	10.13936840298767	4.29778812238507	4.75908581164712

B	11.18492589883668	2.43767321186538	3.14024156943086
H	12.30383898499992	2.82202191185185	3.07192941767033
B	10.32473565062009	1.76487509868825	1.73234586772771
H	10.80957792477914	1.66222861356475	0.65623673229074
B	8.62130535741902	2.19622308096492	1.87798679888866
H	7.83019109577463	2.35686427170080	1.02625668282067
B	9.87129114658078	3.34904733246626	2.37164376014142
H	9.98300186409490	4.34865697243372	1.76092578019207
P	6.21411292461351	1.12907732770596	3.11610254986984
C	6.66080574853321	-1.60499009349902	3.43386484291725
C	4.38845206361356	-0.76208557714242	3.91244068143885
C	6.18961111547374	-0.38742811794406	5.61972849241450
C	6.65029982422310	4.72660425394511	0.82776415220380
C	8.05776933782736	6.37510195795707	2.13340831263676
C	5.63289416349590	6.33872137935524	2.47278004041076
H	6.43083350375370	-1.64565276756525	2.36367126296923
H	6.34562341230577	-2.55452473884892	3.88499430934182
H	7.73980051598735	-1.51708285549339	3.55111495741506
H	4.10419071183466	-0.69818150414425	2.85607500929368
H	3.75694912707262	-0.08713111610181	4.49052179902615
H	4.18364700814756	-1.78275732995380	4.25742947312937
H	7.24394512170252	-0.18924003445880	5.81749776339134
H	5.93008429939800	-1.34521012196394	6.08987288841828
H	5.60139441308505	0.40007242718517	6.10100335051906
H	7.58937316824654	4.31126879808759	0.46077089053294
H	6.30207923972561	5.46416424059070	0.09232569206382
H	5.91463461778367	3.91927619052584	0.87688237392134
H	4.67523899921016	5.82085304063570	2.43143763405850
H	5.61878421168057	7.12759290184628	1.71068840038875
H	5.73202946106292	6.82615941188830	3.44902947512418
H	8.99376373105192	5.85508337080471	1.93886288575542
H	8.15631266551742	6.92823312777532	3.07290717423075

H	7.89486671431190	7.09895345878527	1.32442606880841
C	3.01842588973981	2.43456459462426	5.03511739762059
C	3.49612535562028	3.39326081091979	2.77824708258476
C	3.86021315603575	4.74931742493262	4.93361741032168
H	2.84299579344590	5.14425144805603	4.81837949435412
H	4.55863296811154	5.48011918069391	4.52898679188130
H	4.06620784013323	4.64619235989147	6.00402996828355
H	2.03651327295497	2.91541220479282	5.12791481713625
H	3.39897886620466	2.24064860996639	6.04321177115555
H	2.86870696302244	1.48397191816263	4.52208142924430
H	2.47093958636314	3.78123561572896	2.70974358794943
H	3.50534745538368	2.38101506117339	2.36205958043210
H	4.13946958087002	4.00953283947555	2.15052182887392

Cartesian coordinates of **TS-*rac1-meso2-1-tBu*** (TPSS-D3BJ/def2-TZVP)

C	6.66931479763759	10.42362072364985	0.90081844812391
P	5.28705537295243	9.87555845788400	2.04441041434155
P	3.46102275441414	7.92822777500063	3.02427049408431
P	3.24705337530300	9.65346184797820	1.63470373024860
C	4.65414447031653	8.47555788229790	4.41215822716860
C	0.87824184078561	7.19835323961320	2.71021920753639
H	-0.09903740625827	6.90529672905848	3.11315621270009
H	1.29277075001395	6.34680316682634	2.16054681989335
H	0.72181883888852	8.01732647103963	2.00107857447960
C	5.73356672498606	9.56786114591134	3.80024805361271
C	6.01168474826852	10.68618120186029	-0.46304964152768
H	6.80359577729663	10.93386298021217	-1.18008039668779
H	5.31190616027251	11.52337222402059	-0.42310705053519
H	5.48042084364469	9.80195330270322	-0.82740824774050
C	7.34442759200107	11.69639577592936	1.43413252803965
H	7.77803467337754	11.53494591419064	2.42438040388526

H	6.62935340944599	12.52122243731121	1.49994419025603
H	8.15467014165796	11.98633105137117	0.75223037526861
C	1.79975266794232	7.61559484776324	3.87467396537362
C	2.00115645620889	6.39849625237191	4.79937804125794
H	1.02079631981466	6.05929803604558	5.15730059087949
H	2.61307266911588	6.64372621121871	5.66959268640197
H	2.47523059336782	5.56783942501180	4.26575949609428
C	1.17066764385252	8.77954383305332	4.64365769168143
H	0.96826731069783	9.62254799482966	3.98069708044452
H	1.80745300032168	9.12838763380263	5.45726348172626
H	0.21467942782214	8.45561483800870	5.07662405040299
C	7.68710189385837	9.27673257572369	0.75730168779983
H	8.48360604223358	9.59503964400717	0.07174953373461
H	7.20724247483686	8.38315827353700	0.35013482112485
H	8.14647476628075	9.01825928952516	1.71307591833034
B	4.43126002074030	8.73278062221089	6.08735969208372
H	3.37475395047594	8.51646364314652	6.56466608220702
B	5.44146140679306	7.39779881595167	5.50531120527520
H	5.05058054252515	6.28264204568517	5.54867054192776
B	6.28308708071973	10.64230069920188	5.02316020688973
H	6.51456098075946	11.75591314692999	4.69860907414291
B	7.15810684869478	9.61117764875935	6.16759356524941
H	8.08099585918148	10.03379205424812	6.77938422531907
B	5.48350356253239	10.09838039188661	6.51150707215437
H	5.17656173738671	10.86649661760959	7.35998704104207
B	7.13405473145318	7.93403560139622	5.54804056805155
H	8.02357698773188	7.16814388762782	5.70907505852454
B	7.29478767679198	9.30602616794070	4.42512360628110
H	8.22658705898173	9.53478289840281	3.73652089877556
B	6.00815825497241	8.42669771627504	6.83633892386974
H	6.08063549854132	8.00086788885949	7.93991025663003
B	4.60666017209726	10.09680701293003	4.98511502131076

H	3.70737197366790	10.75565037828039	4.62846892571022
B	6.25424689479035	7.92583561859577	4.03683463467142
H	6.37631959647916	7.26955074738259	3.06567378990853
C	2.20629484804177	11.27295635510314	1.81371592091426
C	2.79917660527857	12.13947479399324	0.68691738079886
C	2.25081416147644	12.07469265944102	3.11090513211804
C	0.76465081861233	10.89091002032182	1.43914164798267
H	3.27652156474266	12.36738772725660	3.35242470952649
H	1.83843904385694	11.52386493983539	3.95882176020446
H	1.65798791196194	12.99143644516025	2.98531304967762
H	0.73376508671229	10.30834225013519	0.51118754762837
H	0.17563026485086	11.80399637989485	1.28612806696071
H	0.27399777011261	10.30884123616230	2.22381073798927
H	2.78851532118112	11.62269177295801	-0.27886280210279
H	3.82983537853943	12.42574202107327	0.92230616066529
H	2.20445425795912	13.05691861358735	0.59248890921237

Cartesian coordinates of **TS-*rac2-meso1-1-tBu*** (TPSS-D3BJ/def2-TZVP)

C	6.22674386115613	10.62490009976324	1.14672196322265
P	5.65011220486231	9.19558119396376	2.21425823948210
P	3.88889554854523	7.07464278910947	3.69169917866840
P	4.65562635737768	7.43822750633184	1.64033859744782
C	4.90848126333083	8.24561388254376	4.78344780440234
C	1.43466527525769	6.56101659093450	2.75398818527434
H	1.88424580323260	6.36770262798463	1.77382862576104
H	0.37701802800812	6.80703197495859	2.59957850420253
H	1.49375634144694	5.64633158233536	3.35286202232681
C	5.98175011091253	9.27026819413905	4.00873917132806
C	5.38444680086226	11.87286742586175	1.46703822254669
H	5.72147128616506	12.70616094040173	0.83614562557321
H	5.49385896130960	12.17287122216593	2.51167306949529

H	4.32557470331221	11.68636488791803	1.26938092315577
C	7.72092589414010	10.90227446408558	1.36822881717911
H	8.32339078614462	10.02232786682889	1.12761198505072
H	7.92507863129641	11.18936332626051	2.40299737196277
H	8.03103281374022	11.73197856138436	0.71916858994837
C	2.12263693034104	7.75006729195290	3.46100815937409
C	1.47281916814677	7.95662365986523	4.83746024934369
H	0.38815944680654	8.05379785907782	4.70322849717262
H	1.83578913905978	8.86599200413129	5.31928908491585
H	1.65818503161403	7.11044213685271	5.50802520333348
C	1.94836185393000	9.00399531188289	2.59687459091817
H	2.35893617241471	8.85232006414279	1.59453220573312
H	2.42900502631949	9.87772538001807	3.03768887401936
H	0.87473607367859	9.21433105183327	2.49996826873759
C	5.96679290338895	10.17814489696066	-0.30095087653104
H	6.20281790917162	11.01572570737281	-0.96833270179463
H	4.91862070874320	9.90255223191915	-0.45384376567673
H	6.59573255622288	9.32794938044382	-0.57703335975281
B	4.47456561643457	8.88270074178530	6.32597554473286
H	3.39450587455165	8.66391265624291	6.74293487432856
B	5.65272808117819	7.57317932860597	6.18289552485533
H	5.34977533345900	6.46431902597762	6.45948922307865
B	6.28872534424298	10.64695164146559	4.95356351991869
H	6.47327647223085	11.67832851019719	4.40655598170546
B	7.10350269965184	10.04178464971588	6.41231401422629
H	7.89642712277703	10.71684549476277	6.97811755557029
B	5.35435573910291	10.41357133753879	6.45466259942942
H	4.90103049151890	11.33990764320946	7.03808428532897
B	7.28217395644776	8.27738616726830	6.25621107277808
H	8.19707508527712	7.66028680195996	6.68727029709297
B	7.47974809757363	9.33015471688113	4.83793116751269
H	8.45129034101904	9.45325129282413	4.17572326148057

B	5.98151602973234	8.94926129472639	7.25740327094621
H	5.96084140131027	8.82002230217707	8.43513063428652
B	4.65979243623751	9.94023127118821	4.91704929600869
H	3.78257878295991	10.43494344548382	4.31098199201523
B	6.57913859162377	7.82239813744435	4.70841321749852
H	6.87671440488117	6.95824345662870	3.97973640034689
C	5.71133409586870	5.91689738234643	1.16098662774056
C	6.84692329447349	5.45724855060561	2.06820949948744
C	6.27055411436608	6.27349468641691	-0.22606889727863
C	4.64992735305002	4.80715511978318	1.03542758520822
H	7.34532647717524	4.59196014026949	1.60990011874089
H	6.48097174512751	5.15325364077964	3.05248865768361
H	7.59371256873014	6.24647119384589	2.19655513239831
H	5.48067592692696	6.60800500761701	-0.90787414711618
H	6.75483602385337	5.39240945554590	-0.66521674475562
H	7.02074806863819	7.06821812147796	-0.14830121181071
H	3.83641640577378	5.10095226256961	0.36229522373478
H	4.21971958493697	4.56031912736023	2.01226889457288
H	5.11640484793098	3.90085328187404	0.62957420143278

Cartesian coordinates of **TS-*meso1-meso2-1-tBu*** (TPSS-D3BJ/def2-TZVP)

C	5.01910708422257	8.13811156612585	4.76077287562680
P	3.85208438747231	7.12185484552285	3.69634340000590
P	5.12436389671427	7.43145453638562	2.00571210547743
C	4.97692392382678	6.39394293352234	0.45276089017755
C	1.40430764167255	6.83000347284740	2.72298709135868
H	1.86402453726021	6.60454892273589	1.75426252511714
H	0.36949784103858	7.14222571618002	2.53794415780661
H	1.38947006617528	5.91146198879077	3.31869330454369
C	6.27178056475014	9.10902960076929	4.00479587812800
C	4.90839476174225	11.62483899746953	2.00690179478098

H	4.77936530021629	12.51752486392445	1.37957956295524
H	5.15784246050771	11.96029303163208	3.01477829999061
H	3.95542416226675	11.09543722118054	2.03434217938796
C	6.01304687901028	10.76367011649914	1.39958307922681
C	7.34758329842122	11.54101067042194	1.40402166996237
H	8.14806770350102	10.96356518177393	0.92994965760281
H	7.66274785883640	11.79210125782560	2.42066443953047
H	7.21933629089105	12.47730785260039	0.84602964618052
C	2.14926803912333	7.97287241034886	3.45009047232879
C	1.46102932042849	8.23025618475319	4.79764218645867
H	0.38752447192239	8.38304328085181	4.62653223170940
H	1.85742711895166	9.12304749533728	5.28406116571473
H	1.57510313317885	7.38291475795796	5.48274750816778
C	2.11247086689114	9.21866407416866	2.56838212493209
H	2.72609212357941	9.08210575690504	1.67080852523454
H	2.46991437896728	10.09874634212274	3.10477780318796
H	1.07900093875125	9.41436839300516	2.25415393123010
C	5.64497256667106	10.40705953216696	-0.05028030341360
H	4.67519144178072	9.90188508233552	-0.09126859577166
H	6.39676835512721	9.75546526803388	-0.51255522035506
H	5.58565412528541	11.32537753169740	-0.64696364438229
B	4.56434776939924	8.84616959721773	6.23824524905825
H	3.44458793711651	8.73429868436858	6.58515272806387
B	5.64740455529785	7.45111865891075	6.19786076965924
H	5.26015778376309	6.37057653935486	6.47947200569604
B	6.59386307707197	10.45623663248218	4.97879711444637
H	6.87887073007206	11.47023536292622	4.44395646880610
B	7.25105530876868	9.81719973886636	6.50214894846019
H	8.05334767128790	10.43736039532875	7.11556460153352
B	5.54043576810439	10.31437730274997	6.39789496637641
H	5.10636918651508	11.27955999883563	6.93101126404057
B	7.30957519142630	8.04258192988704	6.35906593382410

H	8.14685845596036	7.36687955349593	6.85499773511671
B	7.68293867043986	9.05848970655584	4.96051874372302
H	8.70846850148879	9.09463029491248	4.37398347245573
B	6.00155122069471	8.82478982836168	7.27040389440117
H	5.88475221721671	8.72155770974107	8.44524325600526
B	4.93041702572970	9.84074244358771	4.81036478996008
H	4.09642509278186	10.36780071038017	4.17940316963347
B	6.67352630334312	7.60890533635554	4.76192347504251
H	6.98644716074875	6.69685310692613	4.08959963999860
P	6.49735043495152	9.07035871403819	2.14877299177790
C	6.37964843534493	6.35919109289686	-0.17962447728765
C	3.95090068617895	6.93384973737654	-0.55394538038112
C	4.57521203830945	4.98266791235265	0.91944877237973
H	6.71523019677365	7.35983186863841	-0.46880980056953
H	6.34655677523661	5.73833176253934	-1.08358917407551
H	7.11361205452790	5.93842115324080	0.51264433932542
H	5.32082009446807	4.56674038757617	1.60220302270025
H	4.49330073889616	4.32942945544326	0.04182948770849
H	3.60726851989088	4.98630546529782	1.43027092680868
H	4.22700764683891	7.93067224073265	-0.90590277451455
H	2.95208307929722	6.98941260935354	-0.11246294474217
H	3.90389413287502	6.26462518337686	-1.42353395833219

Cartesian coordinates of *meso-3* (TPSS-D3BJ/def2-SVP)

C	0.53102520466484	6.43333009299536	4.54807961191249
C	-7.07543856692025	5.26393721031947	5.75454017929491
C	-1.97474727305636	8.65515650200416	1.43429699404919
H	-2.48494117341072	9.16628763010255	0.59592423182081
H	-2.56911249721962	7.76653436579018	1.70531829334084
H	-0.99077288787964	8.31948174482229	1.07692384878737
C	-2.96703186084351	9.01694947919563	6.93724861124617

C	-3.25915154189257	10.12349988325179	3.03157130587473
H	-3.75385701366166	10.58965676230540	2.15977139517951
H	-3.19441464553223	10.87434590401981	3.83667067924880
H	-3.90544068693355	9.29847535739363	3.38395453322712
C	-1.85745965427280	9.62241038616682	2.61892639019472
C	-6.54005037925260	6.16454943787982	2.83333564480317
C	-1.40636612797931	4.12220465127665	5.15397680429280
C	-6.49022104438491	4.76499374050014	2.17969687604425
H	-6.79573781978329	4.84799464938142	1.12025705686458
H	-7.16847793865638	4.05267485586892	2.67513146854573
H	-5.46748324773516	4.35043119822123	2.21119755186107
C	-0.32325017981907	3.22183387303244	5.78530952985631
H	-0.62871941935387	2.16420006124049	5.68148151910706
H	-0.20512086510240	3.43864954523282	6.86148630348324
H	0.65626573969710	3.34323189368498	5.29709640209936
C	0.40284470055149	7.95793225118720	3.85705042327361
C	-2.74287668935222	3.90844599994028	5.90043550531550
H	-3.55896718995267	4.49761019989921	5.44733520627536
H	-2.66837697408274	4.18391714052151	6.96713856927476
H	-3.02193400906552	2.84036770894015	5.83914393793520
C	-3.44673253881040	10.29167730900025	6.58310402280443
H	-4.31699486742804	10.37899508475009	5.92498870793186
C	-7.47739996328501	6.18012058306799	7.11990597601024
C	-0.97481175075297	10.84062852436940	2.27420774976163
H	0.04087784691041	10.54169114956103	1.97204216604751
H	-0.89294106516773	11.52615619887250	3.13597439701959
H	-1.43135414680703	11.39639452764421	1.43401577961617
C	-1.66768829845210	11.33640933706004	7.86617619178061
H	-1.15959686512994	12.23834258993651	8.22286005385917
C	-7.00687586466480	10.50663620496858	7.21194457808450
H	-6.62878924574667	10.58628810241484	6.17753333819356
H	-6.14394246593564	10.50700212744298	7.90189972448457

H	-7.61568701379504	11.40439231159381	7.42451789455260
C	-7.93995247338463	6.78046303937958	2.74243150120244
H	-8.18018011571404	6.97243985102202	1.67967782725827
H	-7.98658287424245	7.74352312633142	3.27979029986501
H	-8.71375069544113	6.11193069105476	3.14690945508735
C	-2.80433546809722	11.44518456720572	7.05217536877081
H	-3.18807441099651	12.43219320176975	6.77212988728513
C	-7.88693972890323	9.24880661864666	7.39009836721157
C	-1.18504780080826	10.06903603864745	8.22519457485511
H	-0.29865619017692	9.97842253725623	8.86167113350629
C	-1.59948015791613	3.82822112292262	3.66076603203250
H	-2.34782659941898	4.51058623598297	3.22078224783902
H	-1.96986445389120	2.79252679657811	3.54210218548922
H	-0.66201488929488	3.91941290545161	3.09283090922639
C	-5.52072905714902	7.08049736050513	2.12249872617844
H	-5.74512887457491	7.10065750329773	1.04035249565391
H	-4.48601421269396	6.71824430117179	2.25682683024662
H	-5.57603587339437	8.11442147113666	2.50461231507398
C	-1.83663273266312	8.91388793439923	7.77675604467226
H	-1.46084846652227	7.92376860001481	8.05761011229320
C	-8.98489582287475	9.23113466351369	6.32153965836601
H	-8.55519845816486	9.14111259859980	5.30858987852117
H	-9.55000795078887	10.18122790866285	6.36798791343685
H	-9.69800175724881	8.40846054653934	6.47679059952410
C	-8.48521593063326	9.25957417124592	8.81465190927392
H	-9.13114558367167	10.14964928438750	8.93061897169596
H	-7.69048548281076	9.30925336451604	9.57907501595866
H	-9.09842763232212	8.36610724319368	9.01052284337519
B	-6.90620343615640	3.61327145926718	6.17698230707127
H	-6.07555830347973	2.99360564065596	5.57995625869375
B	0.46430220028016	6.57423838862518	2.83938336215456
H	-0.53488623158379	6.23635310244056	2.28580526828326

B	-7.59228127397913	5.16938865969257	8.49745726812932
H	-7.24502962322881	5.64580500069945	9.53763918603800
B	3.01059809832638	7.67649654088748	4.79778555717804
H	3.87616765968780	8.07765036677026	5.52248687277709
B	-6.34173290635067	4.89152165912209	7.26993036902110
H	-5.19668247223246	5.19776721669041	7.40654721139422
B	1.32153260319690	7.76988149488091	5.30888490180007
H	0.82885315951298	8.18809914562932	6.31163834651882
B	-8.94457637441664	4.06500841814782	8.15823368303899
H	-9.63546658476398	3.65157747583556	9.04582818523096
B	3.17920613130608	6.23407903354911	3.75427915183507
H	4.18232441434037	5.57879063028688	3.72328749106308
B	1.58898661917384	5.44980806471048	3.63768447921958
H	1.37089537767995	4.28055783583666	3.56198593561163
B	2.10334130687429	6.18671078199537	5.17195940752083
H	2.19080489241214	5.52391392659651	6.16418045097258
B	-8.35466037341052	4.21603002366002	5.34431892980538
H	-8.55172681399015	3.98107382109413	4.19145884677431
B	2.15415872925347	6.47087886180721	2.30200801642461
H	2.40856614968034	6.00460375814297	1.22788850205536
B	1.88730601262584	8.79873821313080	3.98448350365106
H	1.82143602649960	9.98373776439965	4.13578618501511
B	3.04470031900136	7.85199625443373	3.01860131447505
H	3.94827696574722	8.39087106913867	2.44420808758566
B	-8.66883927539897	5.86930804694937	5.92667210978486
H	-9.02106061587899	6.75562039413385	5.22573804322063
B	-8.51974242428135	3.10165250203955	6.72184435884155
H	-8.89733033077400	1.97756913396257	6.54843344394524
B	1.37236561601310	8.05607201096013	2.45427395071080
H	1.00519294978532	8.72842043871945	1.54133187164561
B	-7.25861859563799	3.51833304739127	7.91921437589023
H	-6.71185850258640	2.71486719756857	8.61942651256750

B	-9.61807690754219	4.50928095380152	6.55749939923390
H	-10.77906758270163	4.41549301240517	6.27669688724979
B	-9.04078709735527	5.77227252949545	7.66491729034432
H	-9.72012565387320	6.63017613527514	8.13984659996243
P	-1.19023605610303	8.90257030562361	4.26145488072382
P	-3.65989243049755	7.43203445665521	6.32419317601017
P	-2.48140182040840	7.06515916709130	4.41938481370531
P	-5.62121948142007	8.02984128432046	5.36696750406677
P	-0.95174887229484	5.92147913883231	5.60518714918170
P	-6.60341615332504	7.83255856622965	7.37585060409328
P	-5.77819506363301	5.94189681112875	4.56987539222884

References

- [1] W. L. F. Armarego, C. L. L. Chai, *Purification of Laboratory Chemicals*, Butterworth-Heinemann, Oxford, **2009**.
- [2] A. Kreienbrink, M. B. Sárosi, E. G. Rys, P. Lönnecke, E. Hey-Hawkins, *Angew. Chem. Int. Ed.* **2011**, *50*, 4701–4703; *Angew. Chem.* **2011**, *123*, 4798–4800.
- [3] D. Heift, Z. Benkő, H. Grützmacher, *Dalton Trans.* **2013**, *43*, 831–840.
- [4] *CrysAlis Pro: Data Collection and Data Reduction Software Package*, Agilent Technologies, **n.d.**
- [5] G. M. Sheldrick, *Acta Crystallogr. A* **2008**, *64*, 112–122.
- [6] K. Brandenburg, H. Putz, *DIAMOND*, Crystal Impact GbR, Bonn, Germany, **2006**.
- [7] F. Neese, *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2018**, *8*:e1327.
- [8] F. Neese, *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2*, 73–78.
- [9] F. Neese, F. Wennmohs, A. Hansen, U. Becker, *Chem. Phys.* **2009**, *356*, 98–109.
- [10] S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456–1465.
- [11] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.
- [12] E. Glendening, A. Reed, J. Carpenter, F. Weinhold, *NBO Version 31 n.d.*
- [13] M. Frisch, G. Trucks, H. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. Petersson, et al., *Gaussian 09 Revis. B01 Gaussian Inc Wallingford CT* **2009**.
- [14] J. Tao, J. P. Perdew, V. N. Staroverov, G. E. Scuseria, *Phys. Rev. Lett.* **2003**, *91*, 146401.
- [15] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.
- [16] D. G. Liakos, M. Sparta, M. K. Kesharwani, J. M. L. Martin, F. Neese, *J. Chem. Theory Comput.* **2015**, *11*, 1525–1539.
- [17] C. Riplinger, B. Sandhoefer, A. Hansen, F. Neese, *J. Chem. Phys.* **2013**, *139*, 134101.
- [18] L. Goerigk, A. Hansen, C. Bauer, S. Ehrlich, A. Najibi, S. Grimme, *Phys. Chem. Chem. Phys.* **2017**, *19*, 32184–32215.
- [19] L. Goerigk, S. Grimme, *Phys. Chem. Chem. Phys.* **2011**, *13*, 6670–6688.
- [20] S. Borucki, Z. Kelemen, M. Maurer, C. Bruhn, L. Nyulási, R. Pietschnig, *Chem. Eur. J.* **2017**, *23*, 10438–10450.
- [21] A. Kreienbrink, S. Heinicke, T. T. Duong Pham, R. Frank, P. Lönnecke, E. Hey-Hawkins, *Chem. Eur. J.* **2014**, *20*, 1434–1439.
- [22] A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098–3100.
- [23] J. P. Perdew, *Phys. Rev. B* **1986**, *33*, 8822–8824.