

Sizing the Role of London Dispersion in the Dissociation of all-*meta tert*-Butyl Hexaphenylethane

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Supporting information

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Experiments

Determination of the dissociation energy

The free dissociation energy (ΔG_d^{298}) is connected to the equilibrium constant K via the van't Hoff plot. To determine K the dynamic $^1\text{H-NMR}$ technique was used. For the equilibrium between a radical $\mathbf{1}\bullet$ and a symmetric dimer $\mathbf{1}_2$ the equilibrium constant K is defined by

$$K_x = \frac{X_{\mathbf{1}\bullet}^2}{X_{\mathbf{1}_2}} \quad (1)$$

where X_i is the molar fraction. The molar fraction can be derived from the intensity of the corresponding peaks of $\mathbf{1}\bullet$ and $\mathbf{1}_2$ because the Intensity I_i is proportional to the amount of substance n_i and the number of hydrogen atoms H_i in the molecule

$$I_i \sim n_i H_i \Rightarrow n_i \sim \frac{I_i}{H_i} \quad (2)$$

The molar fraction becomes

$$X_i = \frac{n_i}{\sum n_i} = \frac{\frac{I_i}{H_i}}{\sum \frac{I_i}{H_i}} \quad (3)$$

Dimer $\mathbf{1}_2$ carries the double amount of hydrogen atoms than radical $\mathbf{1}\bullet$ so that the molar fraction becomes

$$X_{\mathbf{1}_2} = \frac{I_{\mathbf{1}_2}}{I_{\mathbf{1}_2} + 2I_{\mathbf{1}\bullet}} \quad (4.1)$$

and

$$X_{\mathbf{1}\bullet} = \frac{2I_{\mathbf{1}\bullet}}{I_{\mathbf{1}_2} + 2I_{\mathbf{1}\bullet}} \quad (4.2)$$

By plugging (4.1) and (4.2) in (1) and final transformation K is obtained as

$$K = \frac{4I_{\mathbf{1}\bullet}^2}{I_{\mathbf{1}_2}(I_{\mathbf{1}_2} + 2I_{\mathbf{1}\bullet})} \quad (5)$$

The van't Hoff plot (6) delivers now the enthalpy ΔH_d and the entropy ΔS_d of the dissociation as the slope and the y-interception, respectively, by plotting $\ln K$ versus $\frac{1}{T}$ with R , the gas constant and T , the temperature.

$$\ln K = -\frac{\Delta H_d}{R} \left(\frac{1}{T}\right) + \frac{\Delta S_d}{R} \quad (6)$$

The intensities of the $^1\text{H-NMR}$ spectra at temperatures from 4 °C to 65 °C (Table S1) were obtained by integration of the corresponding peaks. The final values and errors were determined by linear regression within the van't Hoff plot (Figure S1 and Figure S2).

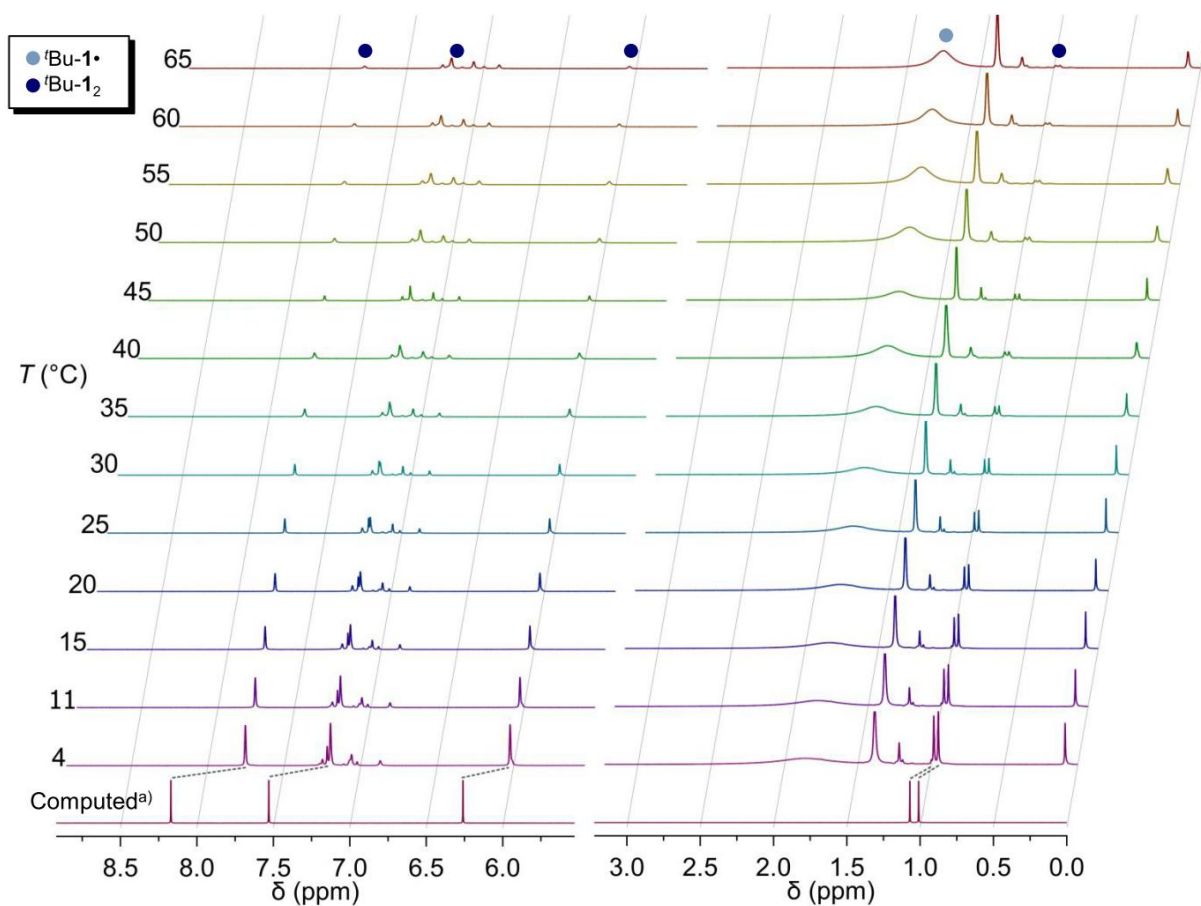


Figure S1. The equilibrium constant was obtained by the temperature dependence of the equilibrium between $t\text{Bu-1}\cdot$ and $t\text{Bu-1}_2$. To determine the molar fraction the broad $t\text{Bu-1}\cdot$ peak at 1.88 ppm and the two $t\text{Bu-1}_2$ at 0.95; 0.98 ppm were used. On the bottom is depicted the ${}^3\text{B3LYP-D3(BJ)/6-31G(d,p)/C-PCM:cyclohexane}$ ${}^1\text{H-NMR}$ spectrum of $t\text{Bu-1}_2$ at 25 $^\circ\text{C}$.

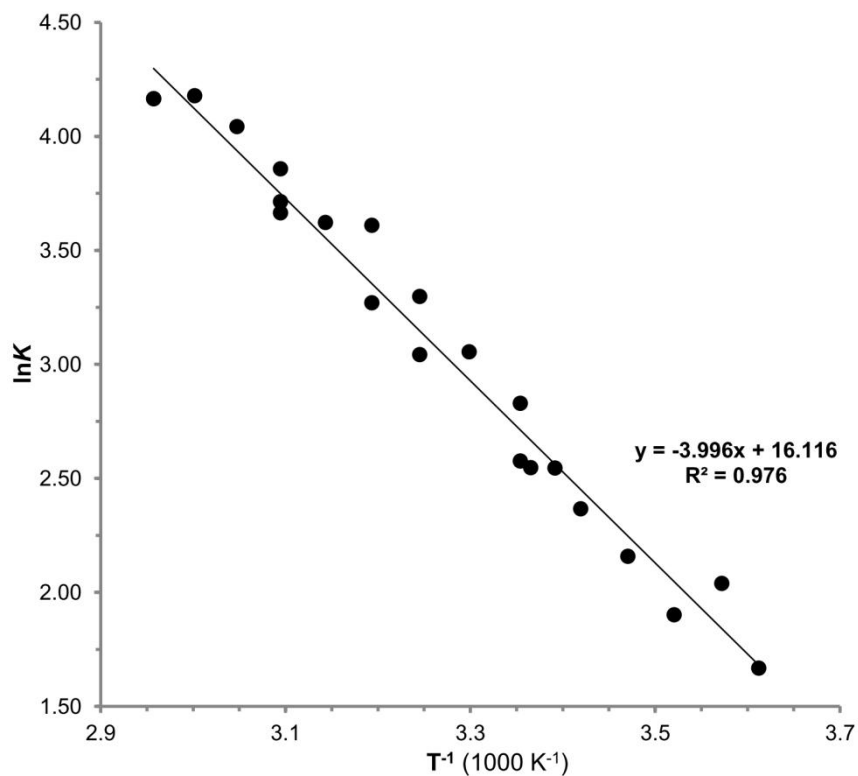


Figure S2. Van't Hoff plot of the equilibrium between $t\text{Bu-1}_2$ and $t\text{Bu-1}\cdot$ derived from VT ${}^1\text{H-NMR}$.

Table S1. Measured intensities (integrals I) of the in Figure S1 indicated peaks and the resulting equilibrium constant K .

T [$^{\circ}\text{C}$] ^{a)}	I (^t Bu-1•) ^{b)}	I (^t Bu-1 ₂) ^{b)}	$\ln(K)$ ^{c)}
65.0	32.7	1	4.17
65.0	32.7	1	4.17
60.0	33.1	1	4.18
55.0	29.0	1	4.04
50.0	24.2	1	3.86
50.0	20.0	1	3.66
50.0	21.0	1	3.71
45.0	19.2	1	3.62
40.0	19.0	1	3.61
40.0	13.6	1	3.27
35.0	14.0	1	3.30
35.0	11.0	1	3.04
30.0	11.1	1	3.06
25.0	8.94	1	2.83
25.0	7.04	1	2.58
24.0	6.85	1	2.55
21.7	6.84	1	2.55
19.3	5.79	1	2.37
15.0	4.78	1	2.16
10.9	3.79	1	1.90
6.8	4.29	1	2.04
3.7	3.08	1	1.67

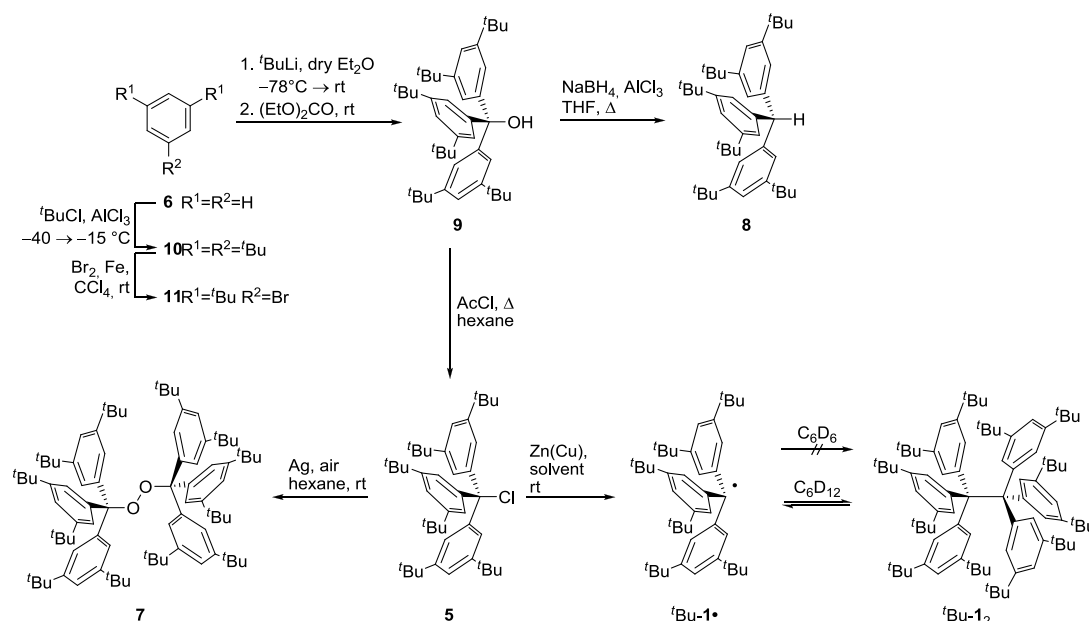
^{a)} Multiple listing of temperature entries result from temperature cycles to show the reversibility of the intensity change. Temperatures were determined with the internal NMR temperature sensor. ^{b)} Manual integration. ^{c)} Determined by equation (5).

Table S2. Thermodynamic data derived from the van't Hoff plot from the equilibrium between ^tBu-1₂ and ^tBu-1•.

$\Delta H_{\text{d}}^{298}$	7.9(3)	kcal mol ⁻¹
$\Delta S_{\text{d}}^{298}$	32.0(9)	cal K ⁻¹ mol ⁻¹
$\Delta G_{\text{d}}^{298}$	-1.6(5)	kcal mol ⁻¹

Experimental procedures

General information: All chemicals were purchased from Aldrich, Alfa Aesar, Acros Organics or Tokyo Chemical Industry in reagent grade or better quality and used without further purification if not mentioned different. For reactions under inert atmosphere nitrogen was used without purification. If not mentioned otherwise, dry solvents were obtained from drying system MBraun MB-SRS 800 and contained less than 15 ppm water. For reactions in the glovebox (MBraun Unilab Glovebox, N₂ filled; O₂ and H₂O levels were kept below 0.1 ppm) benzene-*d*₆ and cyclohexane-*d*₁₂ were dried by distillation from Na/benzophenone in a nitrogen atmosphere onto sodium and were then degassed with 15 to 20 freeze-pump-thaw cycles. The solvent then was brought into the glove box and the piece of sodium was scratched at the glass wall to permanently show a shiny surface. In case the surface got stained, scratching was repeated daily till it stayed shiny and were further stored and used so. For glovebox reaction grease was exchanged by Glindemann PTFE Sealing Rings. All solvents and hygroscopic chemicals used in the glove box were dried previously and all used materials and chemicals were stored at least two days before usage inside the glove box to lose traces of water and oxygen. Analytical thin-layer chromatography (TLC) was performed on plastic-backed silica gel 60 coated with a fluorescence indicator. Visualization of TLC plate was performed by UV (254 nm), iodine or phosphomolybdic acid stain. Column chromatography was performed using Merck silica gel 60 (0.040–0.063 mm). ¹H and ¹³C NMR spectra were measured with Bruker spectrometer Avance II 200 Hz (AV 200), Avance II 400 MHz (AV 400) and Avance III 600 MHz (AV 600), with and without TMS as the internal standard. Chemical shifts are reported in parts per million (ppm). Used GC-MS analyses were performed with a Quadrupol-MS HP MSD 5971(EI) and HP 5890A GC equipped with a J & W Scientific fused silica GC column (30 m × 0.250 mm, 0.25 micron DB-5MS stationary phase: 5% phenyl and 95% methyl silicone) using He (4.6 grade) as carrier gas. The EPR spectrum was recorded with a Varian combination of an E-101 Microwave Bridge, VHF-3400 Magnet and E-9 EPR Spectrometer.



Scheme S1. Complete synthesis route.

1,3,5-Tri-*tert*-butylbenzene 10¹

In a 500 mL one necked flask a mixture of 15.6 g (0.2 mol; 1 equiv.) benzene and 200 mL (1.8 mol; 9 equiv.) was cooled to $-40\text{ }^{\circ}\text{C}$ with a stirred acetone/liq. nitrogen bath. Then over 40 min 13.3 g (0.1 mol; 0.5 equiv.) yellow aluminium(III)chloride was added in portions. This yellow suspension was warmed to $-15\text{ }^{\circ}\text{C}$, stirred for further 2 h at this temperature and put on 200 mL ice. Thereafter, 50 mL of dichloromethane were added, the organic phase separated, washed with 250 mL brine, dried over Na₂SO₄ and concentrated *in vacuo* to give 50.3 g of a pale yellow, solid crude product (the product was a liquid at $55\text{ }^{\circ}\text{C}/15\text{ mbar}$ and congealed while cooling to rt). The product was recrystallized from 135 mL methanol at max. $60\text{ }^{\circ}\text{C}$ (otherwise the product melts to give a clear emulsion that do not result in white crystals but in a congealed pale yellow block) to give 34.9 g (71%) of 1,3,5-tri-*tert*-butylbenzene as white needles.

m.p. 71–72 °C. IR (KBr): 714 (m), 873 (m), 900 (m), 1249 (s), 1362 (s), 1598 (s), 1761 (w), 1780 (w), 2865 (s), 2901 (s), 2964 (vs), 3076 (w) cm⁻¹. ¹H NMR (400 MHz, CDCl₃): δ = 7.27 (s, 3H), 1.35 (s, 27H) ppm. ¹³C NMR (100 MHz, CDCl₃): δ = 149.9, 119.5, 35.0, 31.6 ppm. MS (EI): m/z = 246 (10%, M⁺), 231 (100%, [M⁺] – CH₃), 57 (32%, C₄H₉⁺).

1-Bromo-3,5-di-*tert*-butylbenzene 11¹

In a 100 mL one necked flask where dissolved 10.0 g (41 mmol; 1 equiv.) 1,3,5-tri-*tert*-butylbenzene in 25 mL CCl₄ and then added 2.8 g (50 mmol; 1.3 equiv.) iron powder. Thereafter a solution of 4.4 mL (85 mmol; 2.1 equiv.) Br₂ in 8 mL CCl₄ was added in 30 min at rt and the brown solution stirred for 2 h, poured on 50 mL ice, decanted in a separation funnel and separated between 100 mL aqueous Na₂S₂O₃ solution and 50 mL CHCl₃. The aqueous layer than was again extracted with 50 mL CHCl₃, the combined organic layers dried over Na₂SO₄ and concentrated *in vacuo* to give 21.4 g of a brown oil. After distillation over a 15 cm Vigreux column 9.4 g (86%) of 1-bromo-3,5-di-*tert*-butylbenzene were collected as a yellow oil with b.p. 115 °C/30 mbar.

IR (ATR): 549 (w), 703 (m), 751 (m), 841 (m), 863 (m), 1247 (m), 1280 (m), 1364 (m), 1407 (m), 1476 (m), 1564 (s), 1598 (s), 2716 (vw), 2746 (vw), 2869 (s), 2905 (s), 2964 (vs), 3080 (w) cm⁻¹. ¹H NMR (400 MHz, CDCl₃): δ = 7.32 (s, 3H), 1.30 (s, 18H) ppm. ¹³C NMR (100 MHz, CDCl₃): δ = 153.2, 125.9, 122.3, 121.2, 35.2, 31.4 ppm. MS (EI): m/z = 270.0 (16%, M⁺), 268.0 (16%, M⁺), 255.0 (94%, [M⁺] – CH₃), 253.0 (100%, [M⁺] – CH₃).

Tri(3,5-di-*tert*-butylphenyl)methanol 9²

(0.25 g to 10 g scale) In a dried, argon flushed 250 mL Schlenk flask with septum were placed 37 mmol (3 equiv.) 1-bromo-3,5-di-*tert*-butylbenzene and dissolved with 50 mL dry diethylether. After cooling to –78 °C (acetone/liq. nitrogen) 44.6 mL (76 mmol; 6.1 equiv.) of a 1.7 M *tert*-butyllithium solution in pentane were added dropwise over 30 min, the white suspension was further stirred for 10 min and then allowed to warm to rt during 35 min. To the yellow reaction mixture was added a solution of 1.47 g (12 mmol; 1 equiv.) diethylcarbonate in 3 mL dry diethylether dropwise within 10 min and further stirred for 2 h at rt to result in a cloudy brown suspension. After addition of 100 mL water and 30 mL 2 M aqueous HCl, the layers were separated and the aqueous layer extracted with diethylether (3x30 mL). The combined organic layers were dried over Na₂SO₄ and concentrated carefully *in vacuo* to give 7.72 g of a yellow, glassy solid. Purification by column chromatography (silica gel, hexane/diethylether 20:1→10:1, r_f(10:1) = 0.28) gave pure product as a white solid in 78–84% yield.

m.p. 162 °C. IR (KBr): 727 (m), 880 (m), 1248 (m), 1362 (m), 1477 (m), 1595 (m), 2866 (m), 2903 (m), 2963 (s), 3438 (m, broad), 3581 (w) cm⁻¹. ¹H NMR (400 MHz, CDCl₃): δ = 7.28 (t, ⁴J = 1.7 Hz, 3H), 7.04 (d, ⁴J = 1.7 Hz, 6H), 2.76 (s, 1H), 1.23 (s, 54H) ppm. ¹³C NMR (100 MHz, CDCl₃): δ = 149.7, 146.8, 122.8, 120.5, 83.6, 35.0, 31.6 ppm. ¹H NMR (400 MHz, C₆D₆): δ = 7.53 (d, ⁴J = 1.8 Hz, 6H), 7.48 (t, ⁴J = 1.8 Hz, 3H), 2.63 (s, 1H), 1.26 (s, 54H) ppm. ¹³C NMR (100 MHz, C₆D₆): δ = 150.2, 147.7, 123.4, 120.7, 83.7, 35.1, 31.7 ppm. ¹H NMR (200 MHz, C₆D₁₂): δ = 7.25 (t, ⁴J = 1.7 Hz, 3H), 7.06 (d, ⁴J = 1.7 Hz, 6H), 2.34 (s, 1H), 1.21 (s, 54H) ppm. ¹³C NMR (50 MHz, C₆D₁₂): δ = 145.0, 148.2, 123.5, 120.4, 83.7, 35.4, 31.9 ppm.

Tris(3,5-di-*tert*-butylphenyl)methyl chloride 5³

In a nitrogen flushed 25 mL two-necked Schlenk flask with condenser and septum were solved 504 mg (1 equiv./0.8 mmol) tris(3,5-di-*tert*-butylphenyl)methanol in 8 ml dry benzene (stored over 3 Å molecular sieves) and refluxed. Than 0.2 mL (3.5 equiv./2.9 mmol) acetyl chloride where in two steps added within 5 min and the yellow solution was refluxed for 30 min. After cooling to rt the solvent and reactants were removed *in vacuo* and the remaining yellow solid was recrystallized from dry hexane (freshly distilled from sodium/benzophenone) with 3 drops acetyl chloride (rt to –20 °C). Schlenk filtration gave 433 mg (83%) white needles which contained traces of the carbinol and were used without further purification.

¹H NMR (600 MHz, C₆D₆): δ = 7.49 (s, 9H), 1.23 (s, 54H) ppm. ¹³C NMR (150 MHz, C₆D₆): δ = 150.3, 146.2, 125.4, 121.3, 84.4, 35.1, 31.6 ppm. ¹H NMR (400 MHz, C₆D₁₂): δ = 7.28 (t, ⁴J = 1.8 Hz, 3H), 6.99 (d, ⁴J = 1.9 Hz, 6H), 1.20 (s, 54H) ppm. ¹³C NMR (100 MHz, C₆D₁₂): δ = 149.9, 146.7, 125.5, 120.9, 82.8, 35.4, 31.8 ppm.

Bis(tri(3,5-di-*tert*-butylphenyl)methyl)peroxide 7⁴

In a 25 mL round bottom flask were placed 49 mg (1 equiv./0.08 mmol) tris(3,5-di-*tert*-butylphenyl)methyl chloride and 56 mg (0.52 mmol; 6.4 equiv.) silver powder, suspended in 3 mL dry hexane (stored over 3 Å MS) and stirred for 65 min in air. Then the colorless suspension was filtered through celite and the filtrate was concentrated *in*

vacuo to give crude white product. Recrystallization from chloroform gave 23.2 mg (49%) of bis(tri(3,5-dialkylphenyl)methyl)peroxides as colorless crystals.

m.p. 246–252 °C (decomp.). IR (KBr): 3076 (w), 2962 (s), 2865 (s), 1596 (m), 1477 (m), 1463 (m), 1431 (m), 1362 (m), 11248 (m), 1205 (m), 880 (m) cm^{-1} . ^1H NMR (400 MHz, C_6D_6): δ = 7.48 (t, 3J = 1.7 Hz, 6H), 7.29 (broad), 1.21 (s, 108H) ppm. ^{13}C NMR (100 MHz, C_6D_6): δ = 149.4, 144.0, 125.8 (broad), 120.7, 95.1, 35.0, 31.7 ppm. ^1H NMR (400 MHz, C_6D_{12}): δ = 8.25–5.50 (d, very broad), 7.25 (t, 3J = 1.7 Hz, 2H), 1.21 (s, 36H) ppm. ^{13}C NMR (100 MHz, C_6D_{12}): δ = 149.5, 144.4, 126.1 (broad), 120.7, 35.2, 31.9 ppm. MS (ESI): m/z = 1214 (100%; $[\text{M}^+] + \text{Na}$), 1215 (93%; $[\text{M}^+] + \text{Na}$), 1216 (39%; $[\text{M}^+] + \text{Na}$). HRMS (ESI): m/z (found) = 1213,9656u ($[\text{M}^+] + \text{Na}$) \equiv 1190,9758 (M^+); m/z (calc.) = 1190,9758 (M^+).

Tri(3,5-di-*tert*-butylphenyl)methane **8**⁵

In an argon flushed 10 mL two neck round bottom flask with condenser and septum were suspended 203 mg (1 equiv./0.29 mmol) tris(3,5-dialkylphenyl)methanol, 54.6 mg (1.45 mmol; 5 equiv.) NaBH_4 and 111.4 mg (0.81 mmol; 2.8 equiv.) yellow AlCl_3 suspended with 3 mL dry THF (distilled from Na/benzophenone) at rt. The suspension turned brown and got colorless again after 5 min. After decrease of the vigorous hydrogen development the mixture was heated to reflux for 2 h. The cooled mixture was then quenched by dropwise addition of water, then further 10 mL water were added and the resulting colorless clear two layers were extracted with hexane (3x30 mL). The combined organic layers were dried with Na_2SO_4 and the solvent removed *in vacuo* to give crude product as a colorless film. Further purification by column filtration over silica gel with hexane gave 173 mg (89%) of pure tris(3,5-dialkylphenyl)methane as colorless film that slowly solidified. Large crystals were grown from isothermal evaporation of pentane.

m.p. 184.5 °C. IR (KBr): 717 (m), 874 (m), 1246 (m), 1362 (m), 1430 (m), 1460 (m), 1478 (m), 1596 (m), 2865 (s), 2903 (s), 2963 (s), 3086 (w) cm^{-1} . ^1H NMR (400 MHz, C_6D_6): δ = 7.43 (t, 4J = 1.7 Hz, 3H), 7.36 (d, 4J = 1.7 Hz, 6H), 5.79 (s, 1H), 1.27 (s, 54H) ppm. ^{13}C NMR (100 MHz, CDCl_3): δ = 150.7 (q), 144.6 (q), 124.5, 120.0, 59.0, 35.0 (q), 31.6 ppm. ^1H NMR (400 MHz, C_6D_{12}): δ = 7.19 (t, 4J = 1.7 Hz, 3H), 6.88 (d, 4J = 1.7 Hz, 6H), 5.41 (s, 1H), 1.22 (s, 54H) ppm. ^{13}C NMR (100 MHz, CDCl_3): δ = 150.4, 145.0, 124.7, 119.7, 58.7, 35.3, 31.9 ppm. MS (EI): m/z = 580 (10%, M^+), 581 (4.8%, M^+), 582 (1.3%, M^+). HRMS E.A.: (found) C 88.83 H 11.22 (calc.) C 88.90 H 11.10.

Tri(3,5-di-*tert*-butylphenyl)methyl radical **4**Bu-1⁶

Inside a glovebox in a tube-like 10 mL glass flask with a joint and a glass stirring bar where placed 16.7 mg (1 equiv./27 μmol) tris(3,5-dialkylphenyl)methyl chloride and 35.5 mg (20 equiv./543 μmol) Zn(Cu). These were suspended with 0.9 mL dry, degassed benzene- d_6 , then stirred 2 h at rt and finally the stirring was stopped for the solids to settle down. After 0.65 mL of the supernatant, clear orange solution was transferred *via* syringe to a flame sealable NMR test tube, a Schlenk attachment with plug were attached, the valve closed and the set up brought out of the glove box. Now the solution was frozen in a cooling bath (-20 °C), vacuum applied and then immediately the NMR test tube flame sealed.

^1H NMR (600 MHz, C_6D_6): δ = 1.83 (s, 108H, very broad) ppm.

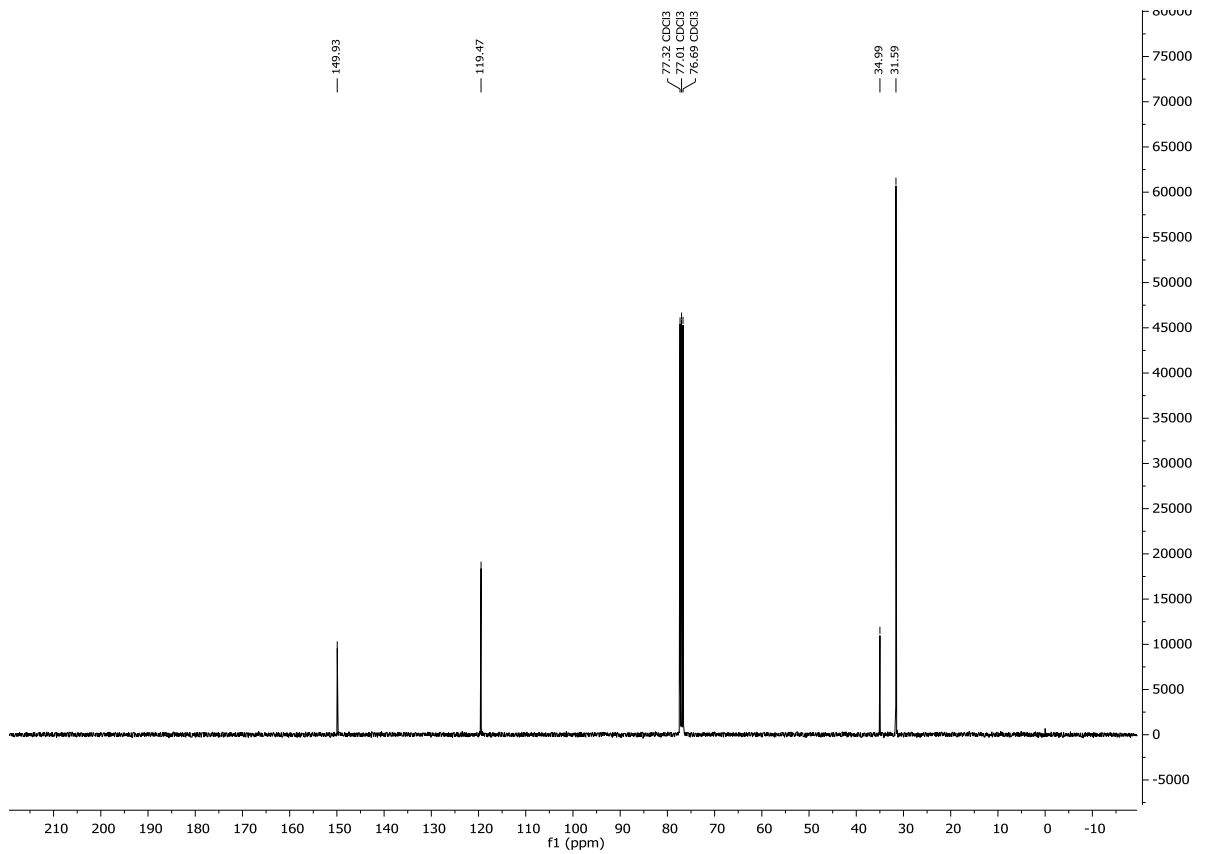
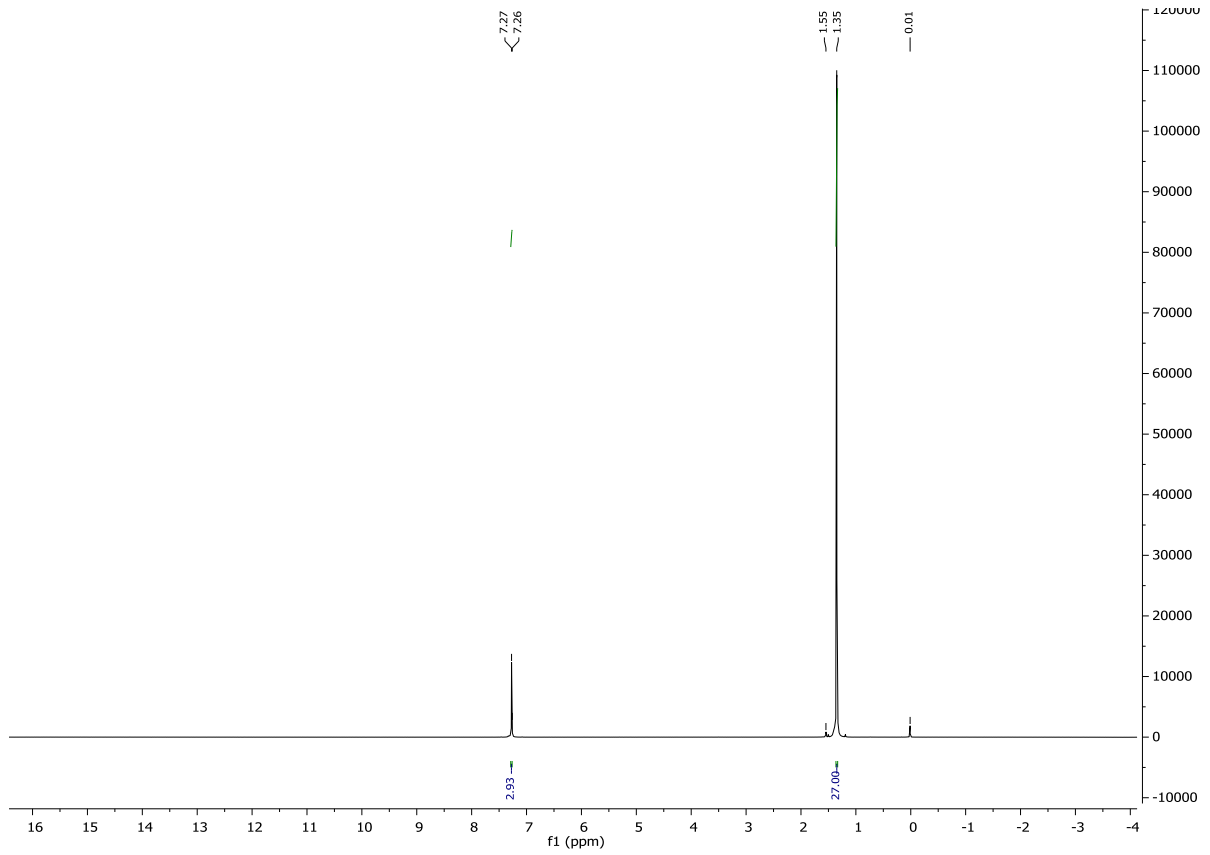
Hexa(3,5-di-*tert*-butylphenyl)ethane **4**Bu-1₂⁷

Inside a glovebox in a tube like 10 mL glass flask with a joint and a glass stirring bar where placed 16.7 mg (1 equiv./27 μmol) tris(3,5-di-*tert*-butylphenyl)methylchlorid and 35.5 mg (20 equiv./540 μmol) Zn(Cu). These were suspended with 0.8 mL dry, degassed cyclohexane- d_{12} , then stirred 6 h at rt and finally the stirring was stopped for the solids to settle down. After 0.65 mL of the supernatant, clear orange solution were transferred *via* a 1 mL syringe to a flame-sealable NMR test tube, a Schlenk attachment with stopper was attached, the valve closed and the set up brought out of the glove box. Now the solution was frozen in a cooling bath (-20 °C), vacuum applied and then immediately the NMR test tube flame sealed. The NMR test tube was kept away from light and did not show signs of decomposition within 5 weeks.

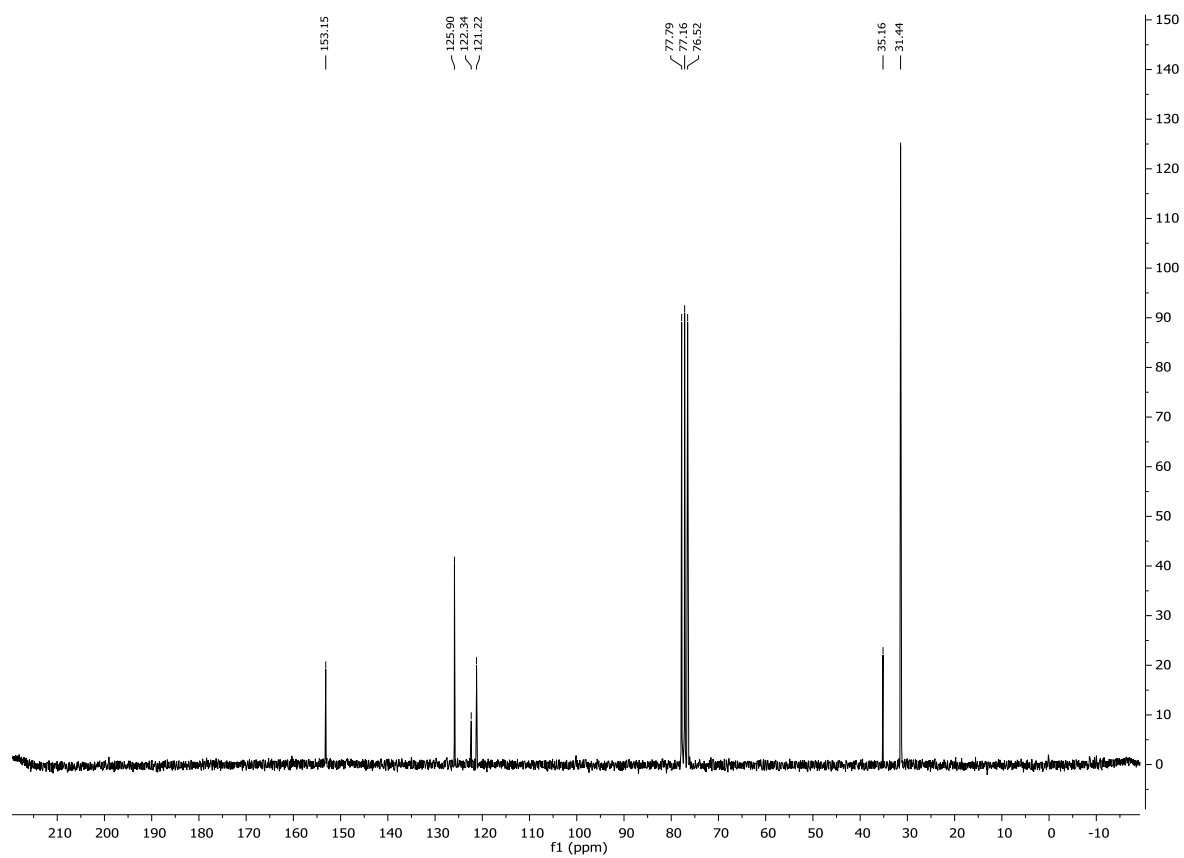
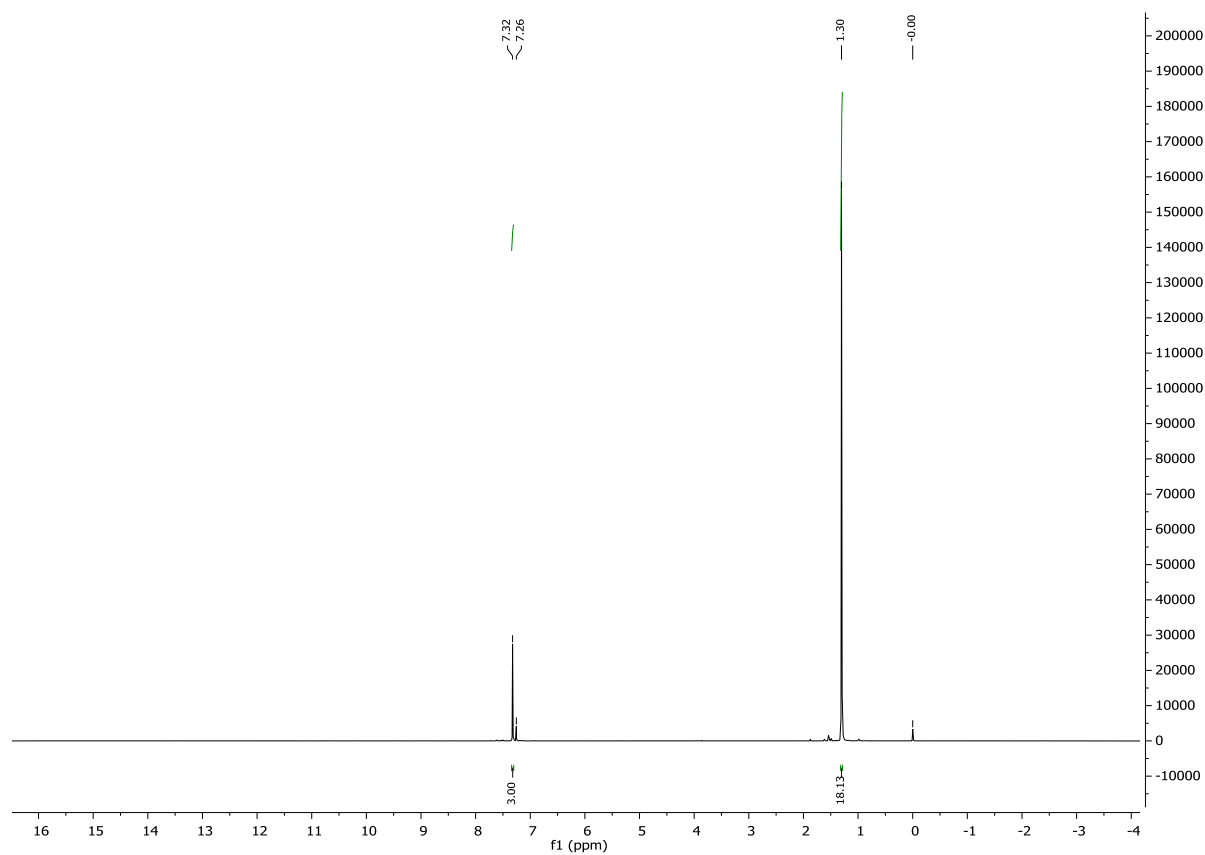
^1H NMR (600 MHz, C_6D_{12}): δ = 7.75 (s, 3H), 7.19 (s, 3H), 6.02 (s, 3H), 0.98 (s, 27H), 0.95 (s, 27H) ppm. ^{13}C NMR (150 MHz, C_6D_6): δ = 151.1 (q), 149.9 (q), 149.5 (q), 128.6 (t), 128.1 (t), 120.3 (t), 71.5 (q), 35.3 (q), 35.2 (q), 32.1 (p), 31.8 (p) ppm.

Spectra

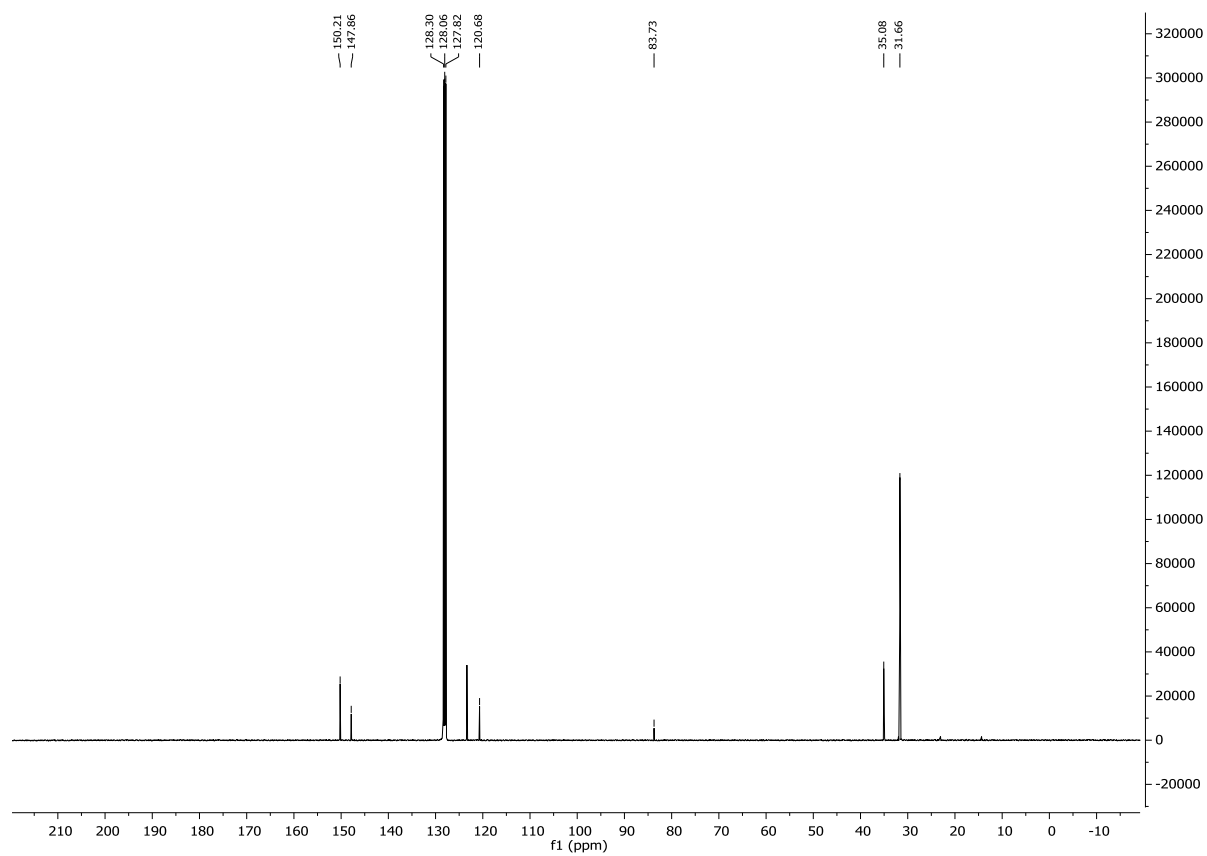
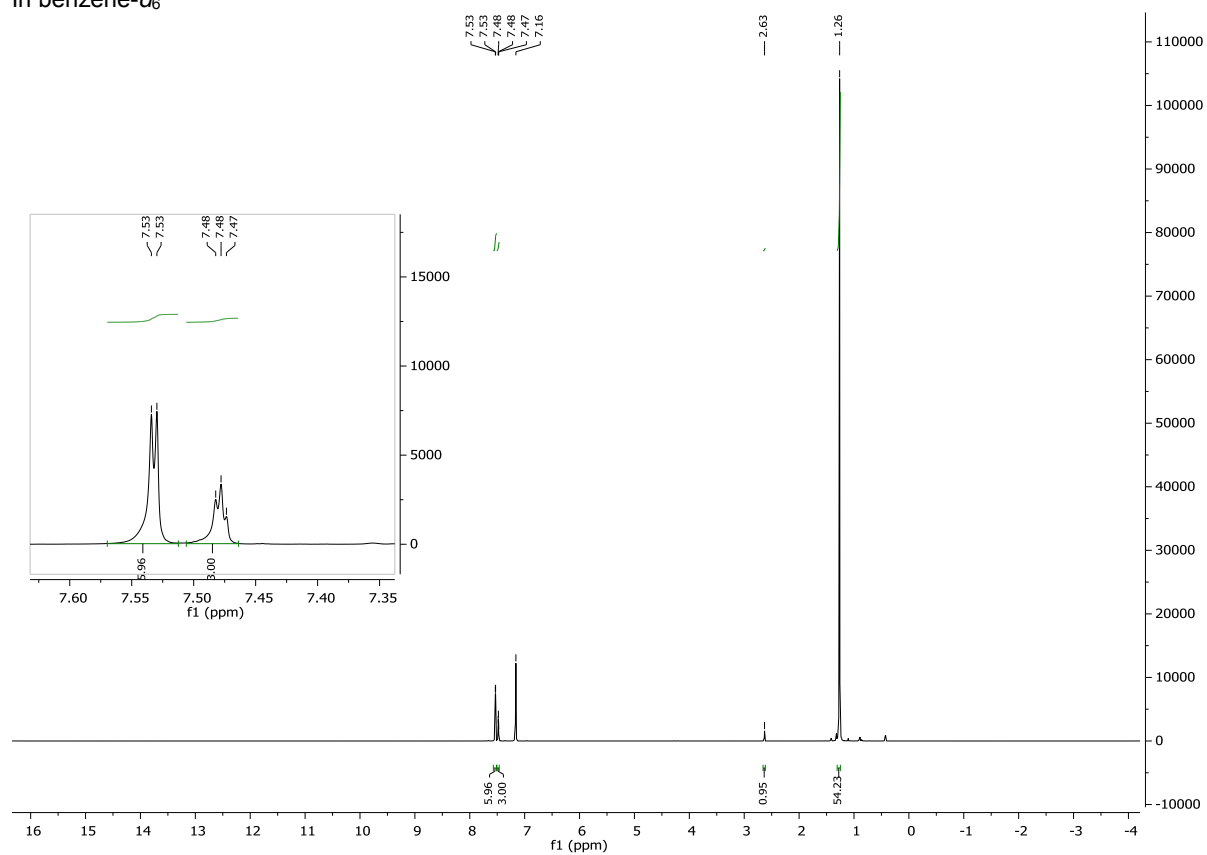
1,3,5-Tri-*tert*-butylbenzene 10:



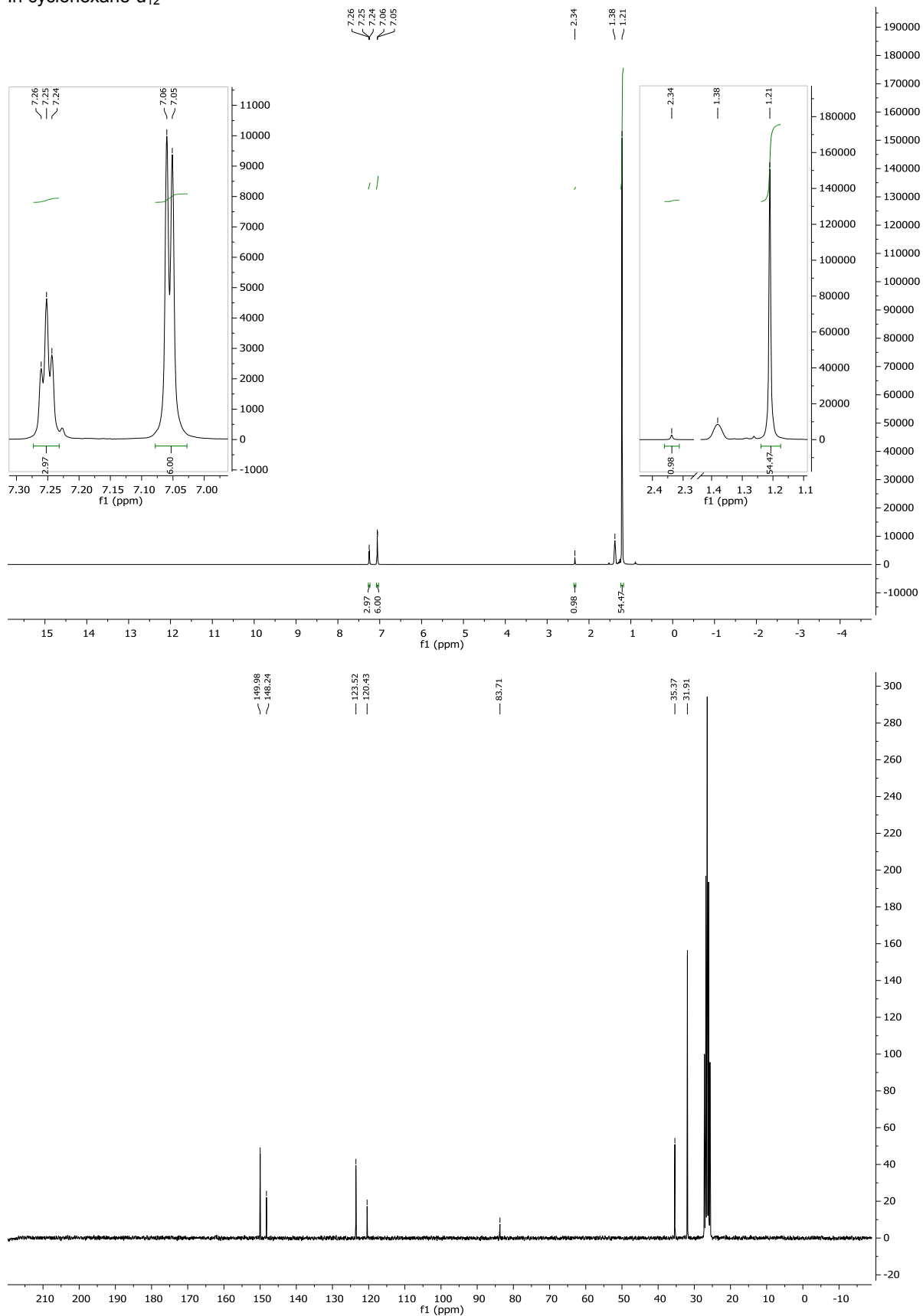
1-Bromo-3,5-di-*tert*-butylbenzene 11:



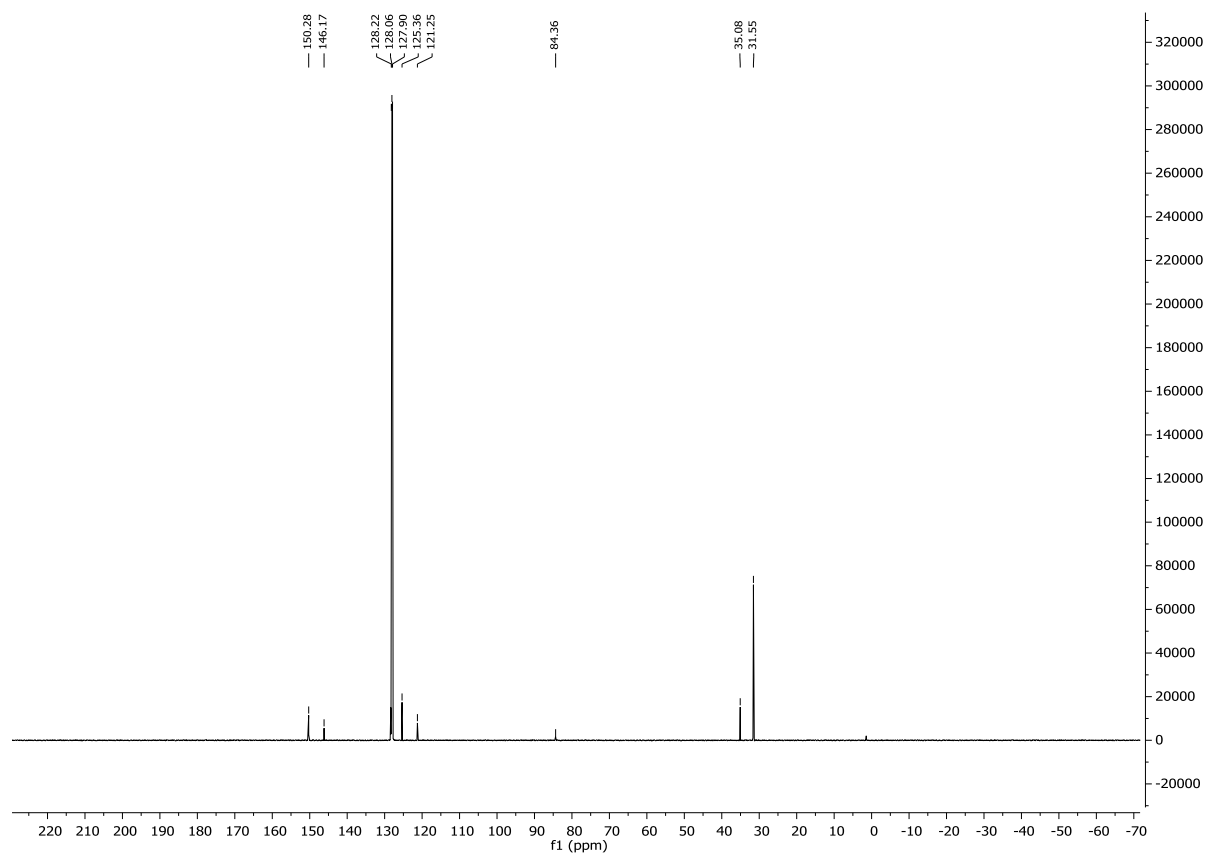
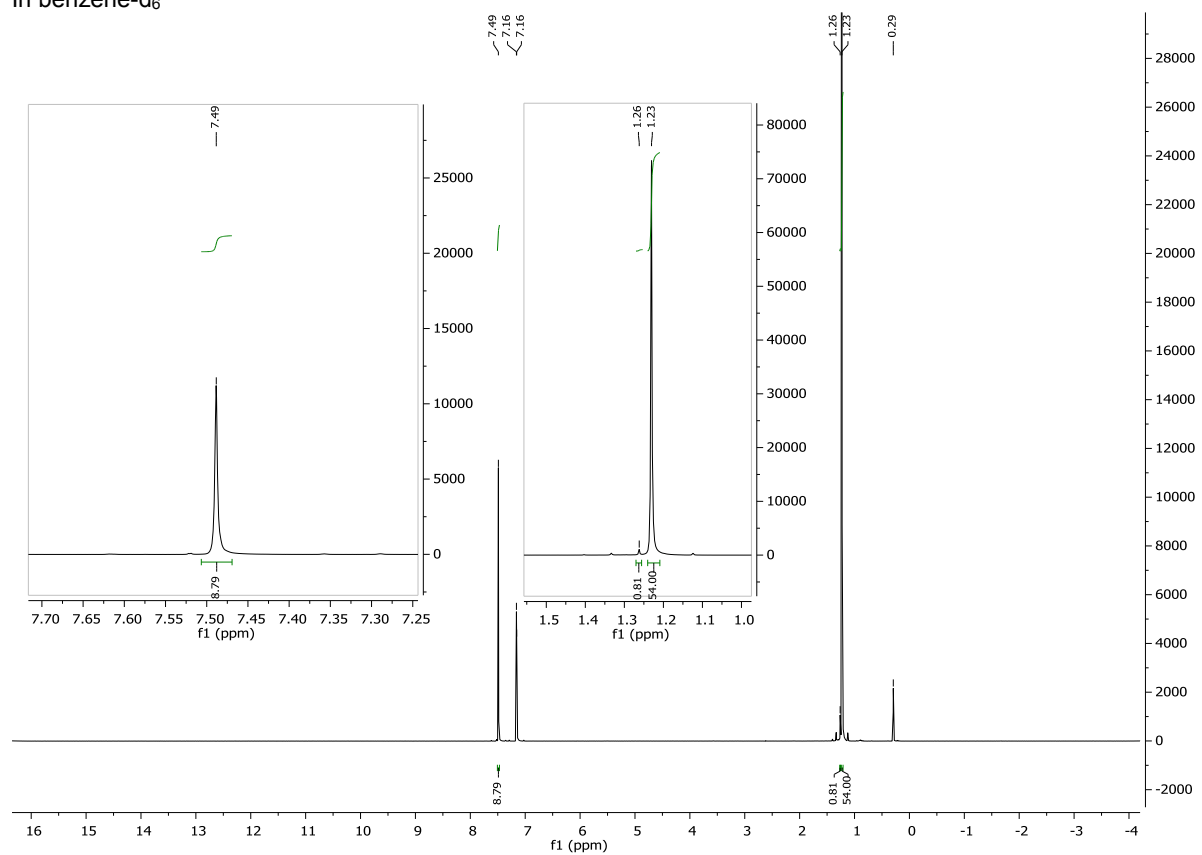
Tri(3,5-di-*tert*-butylphenyl)methanol 9:
In benzene-*d*₆



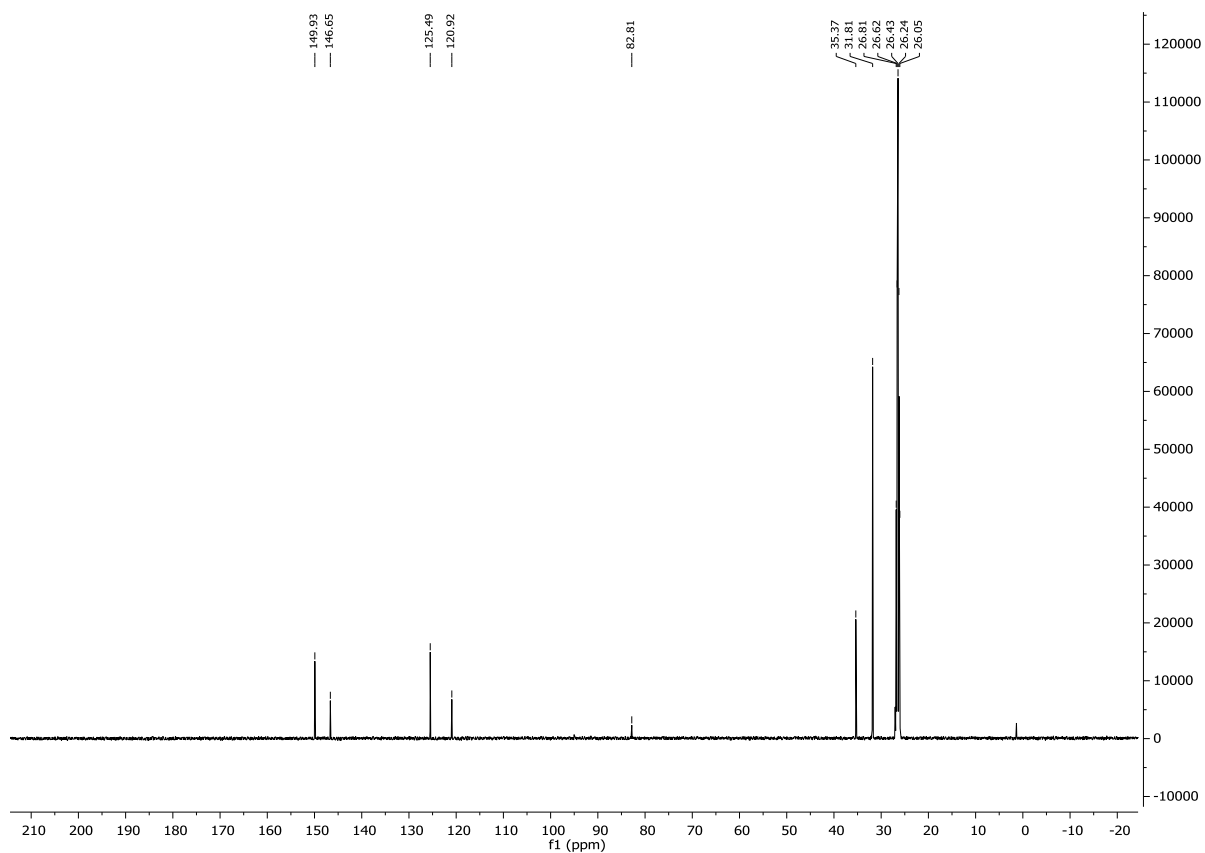
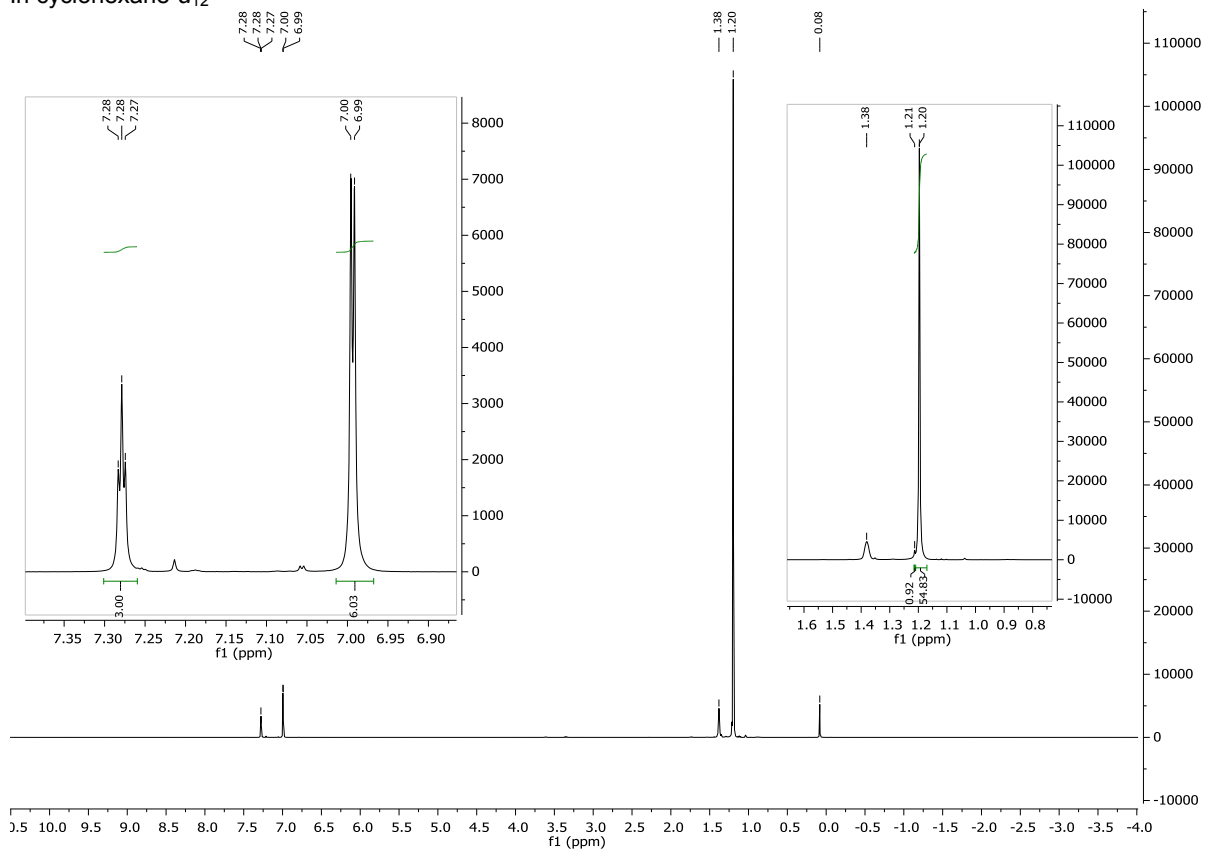
In cyclohexane- d_{12}



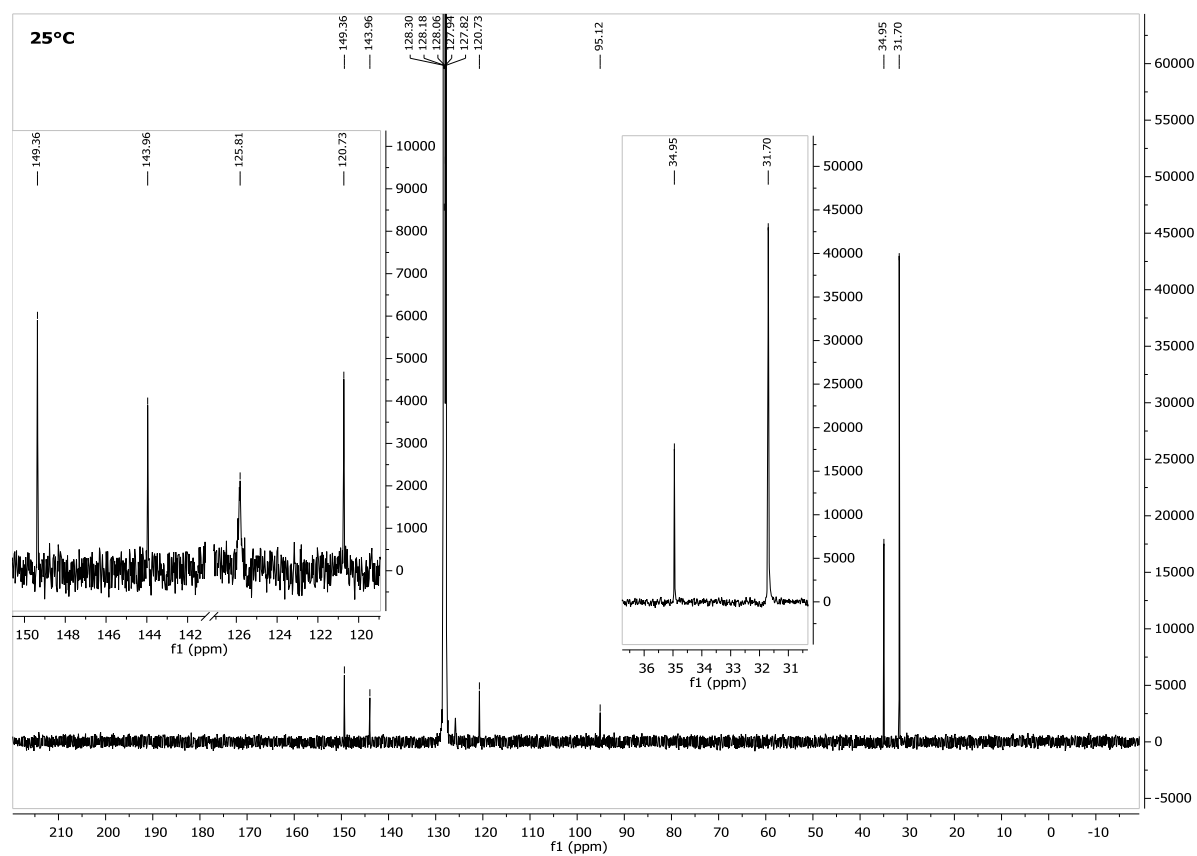
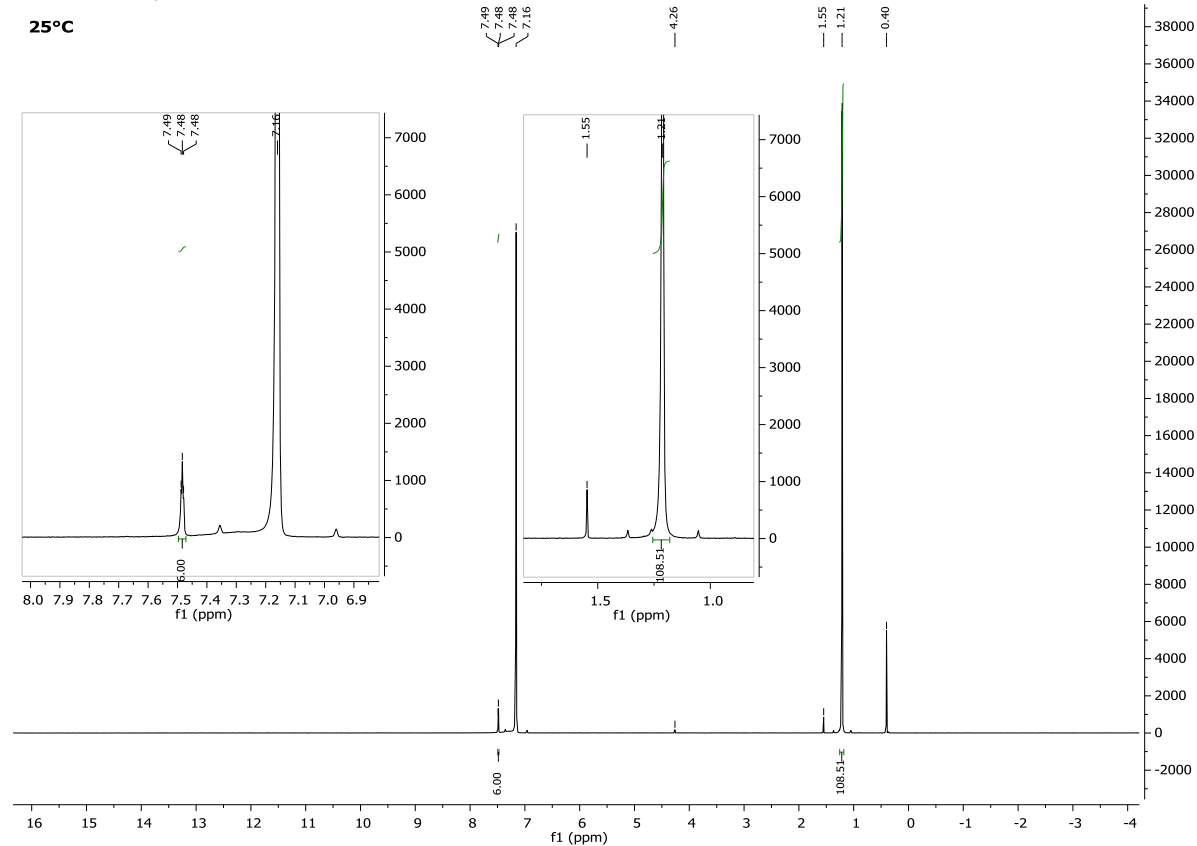
Tri(3,5-di-*tert*-butylphenyl)methyl chloride 5:
In benzene- d_6

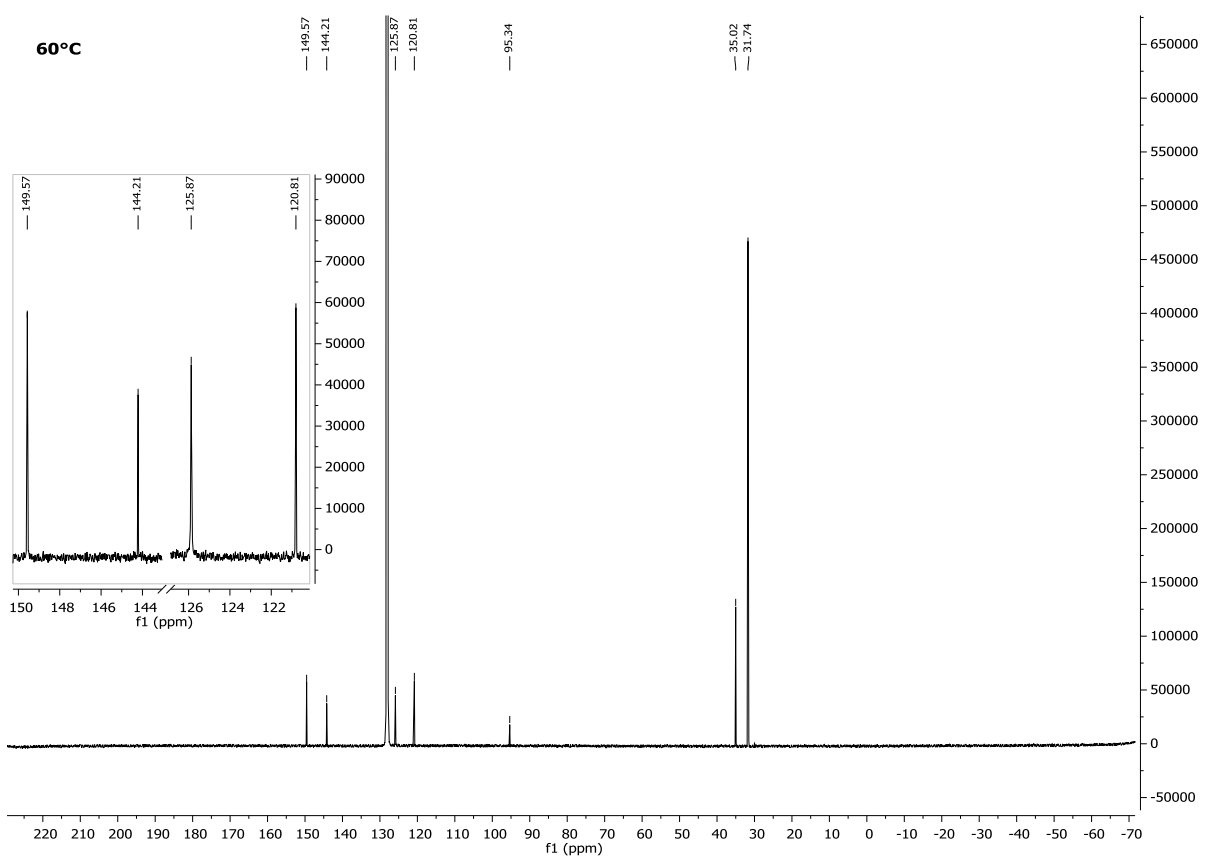
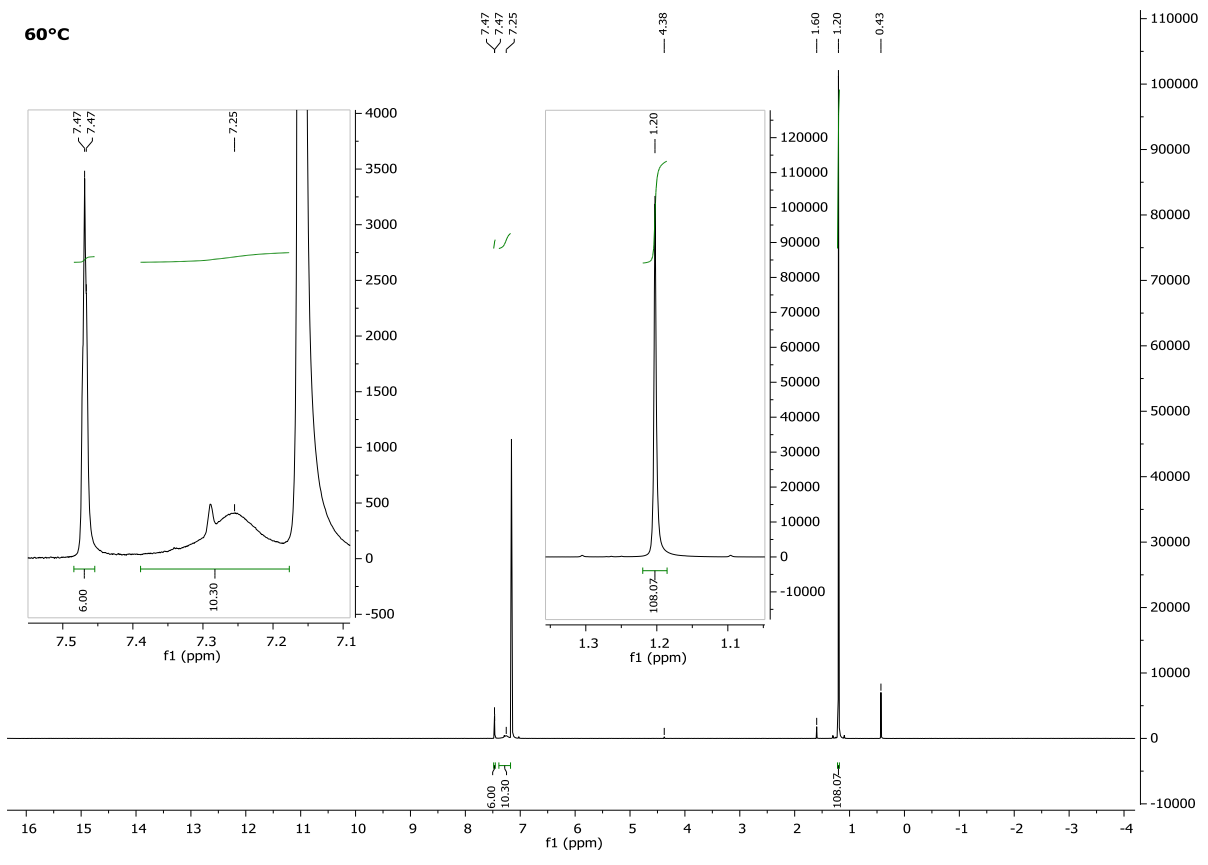


In cyclohexane-d₁₂

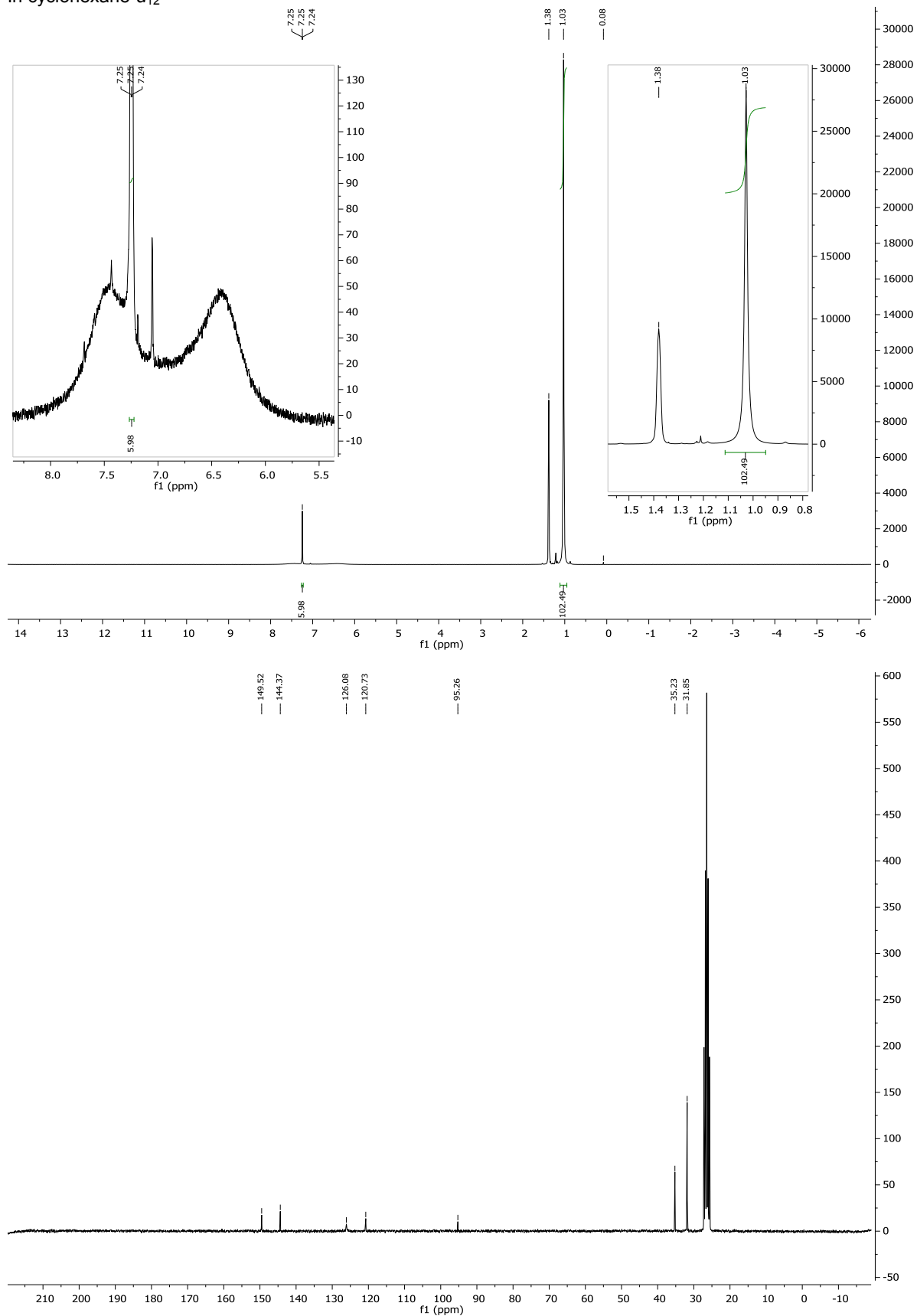


Bis(tri(3,5-di-*tert*-butylphenyl)methyl)peroxide 7:
In benzene- d_6

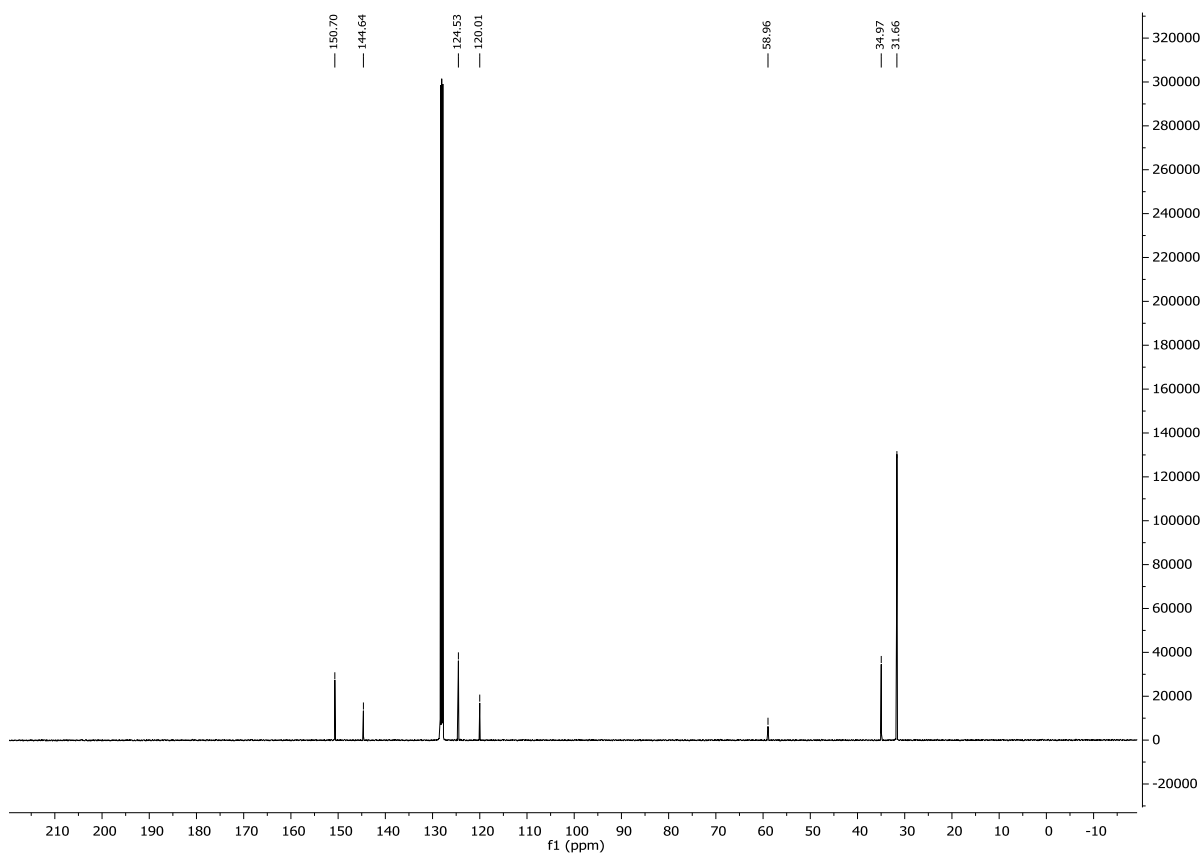
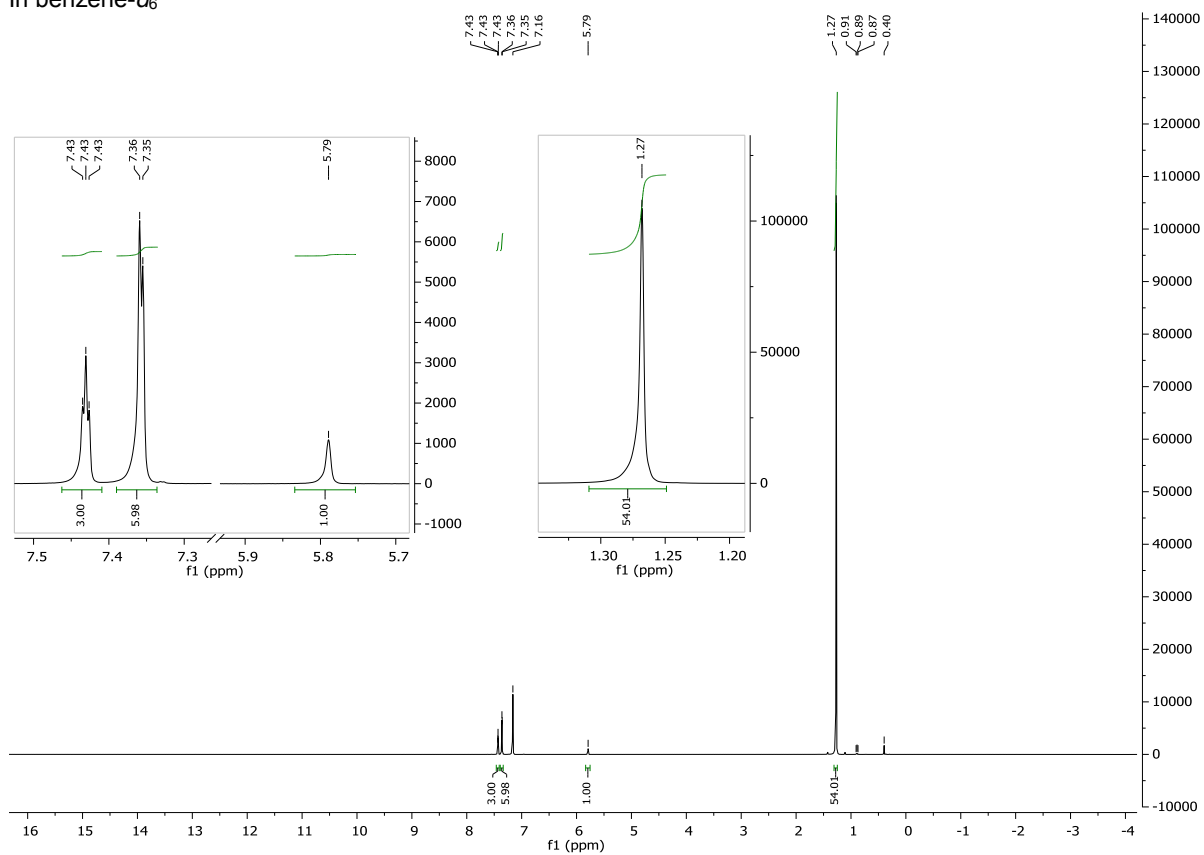




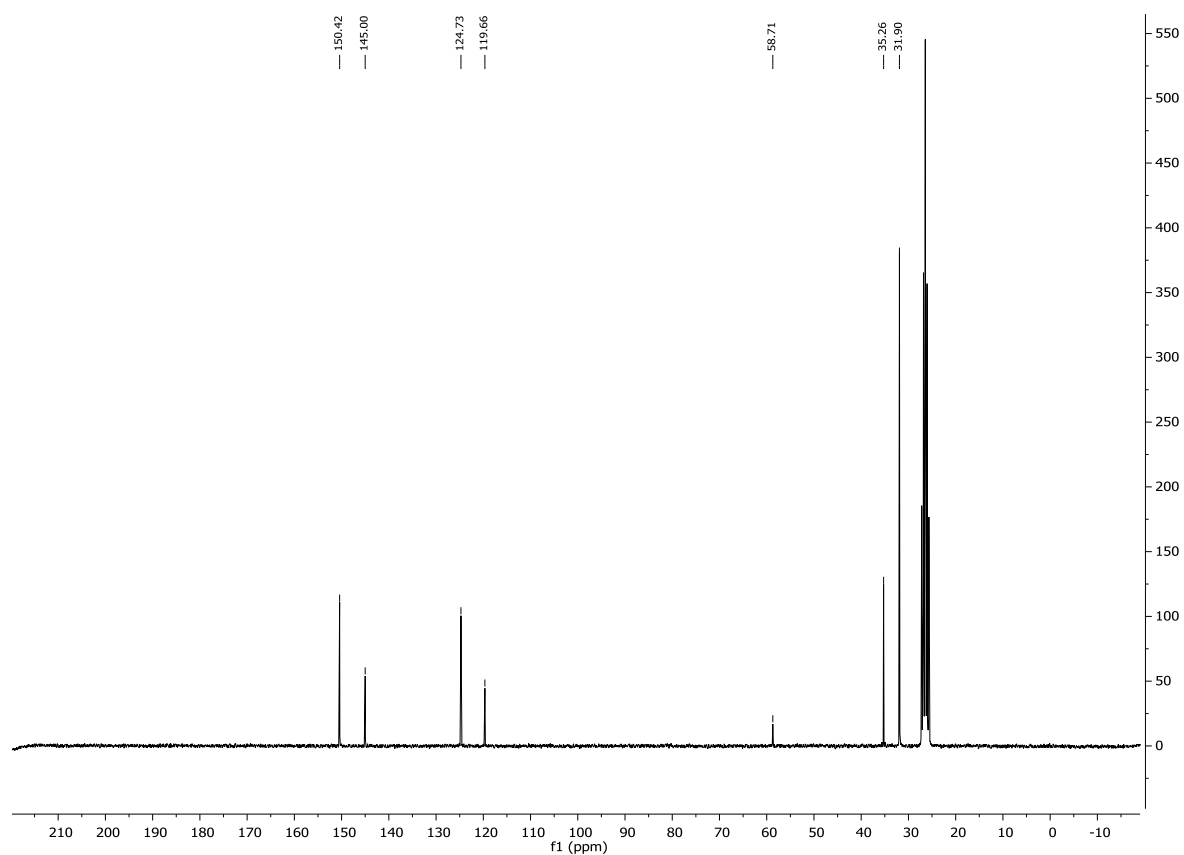
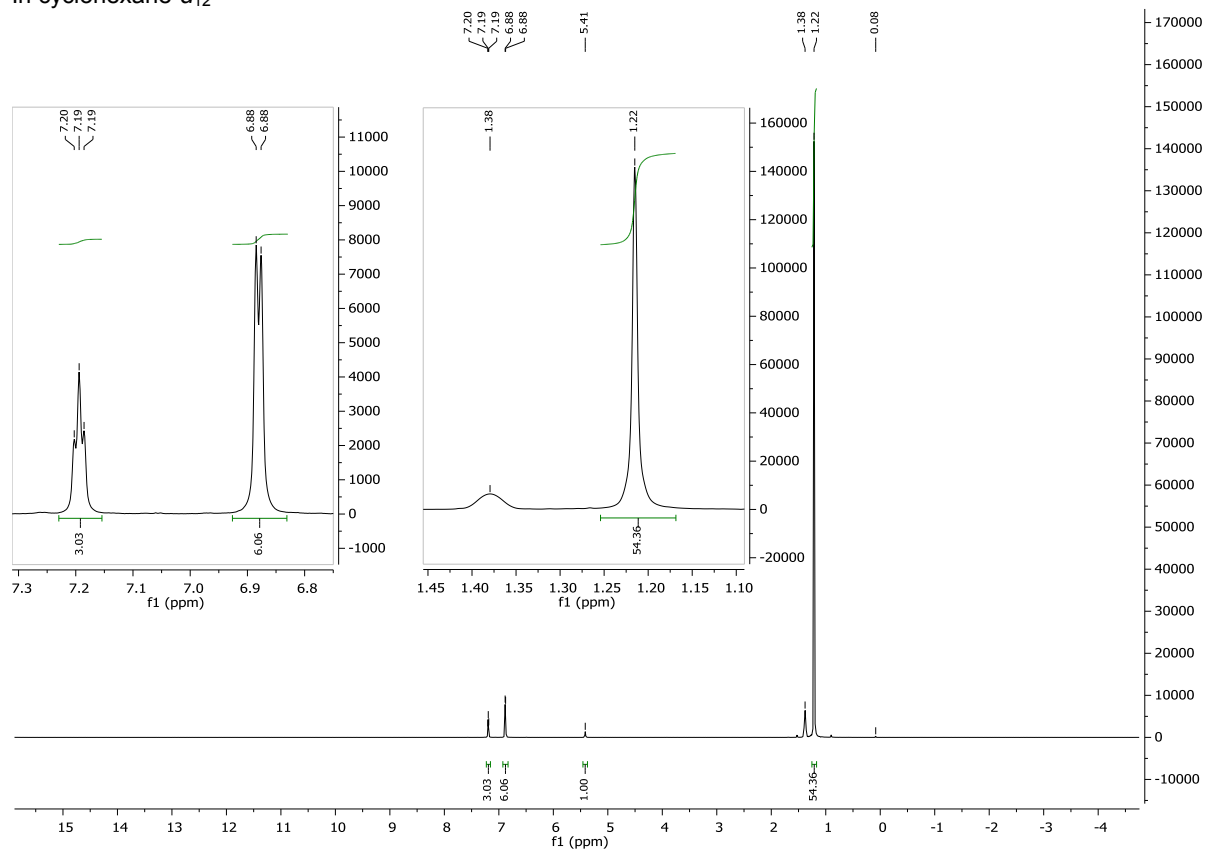
In cyclohexane- d_{12}



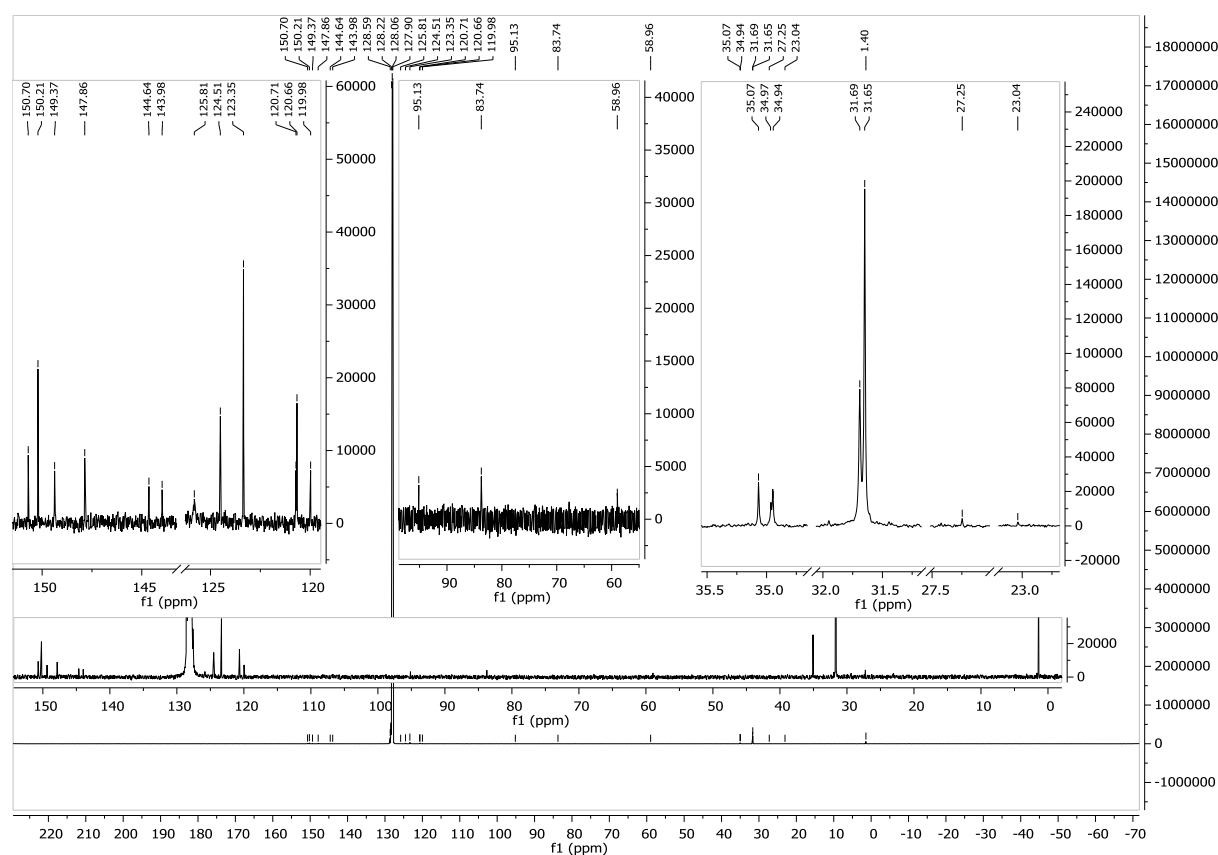
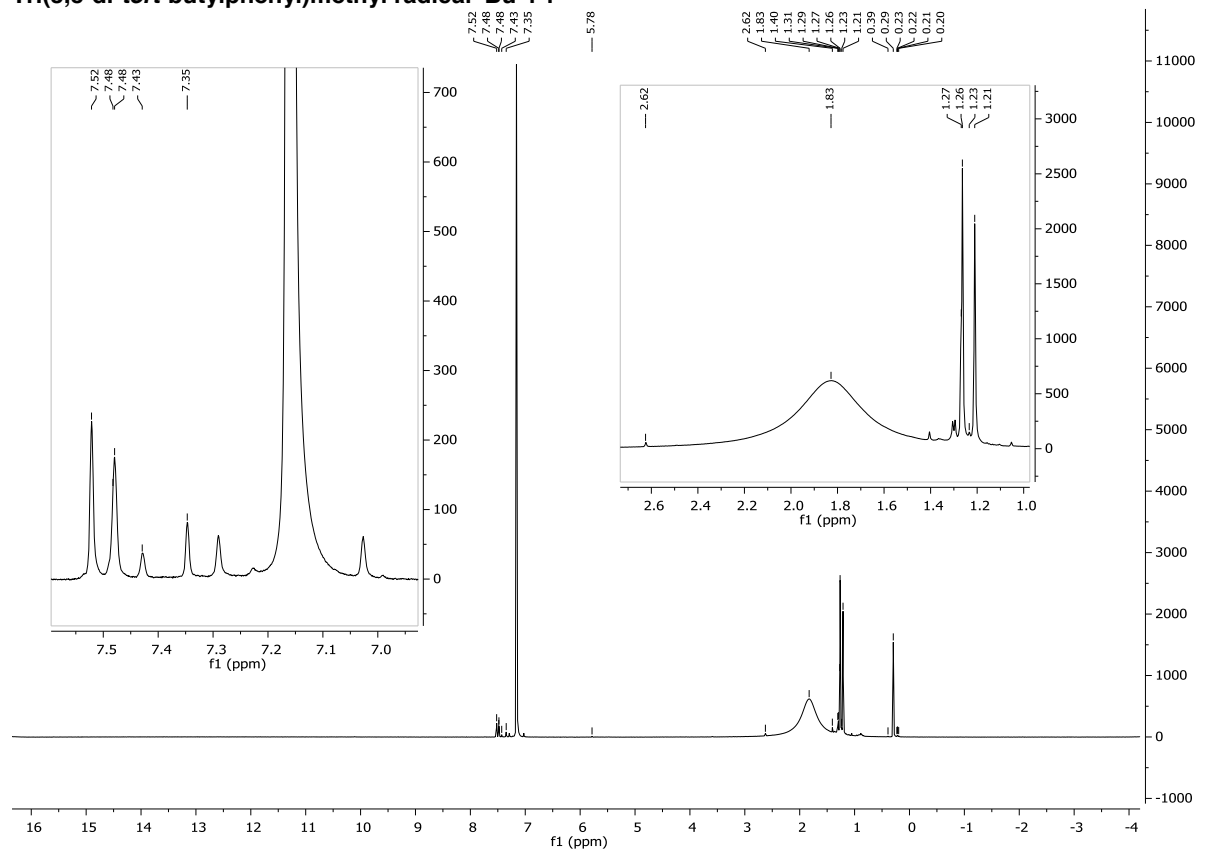
Tri(3,5-di-*tert*-butylphenyl)methane 8:
In benzene-*d*₆

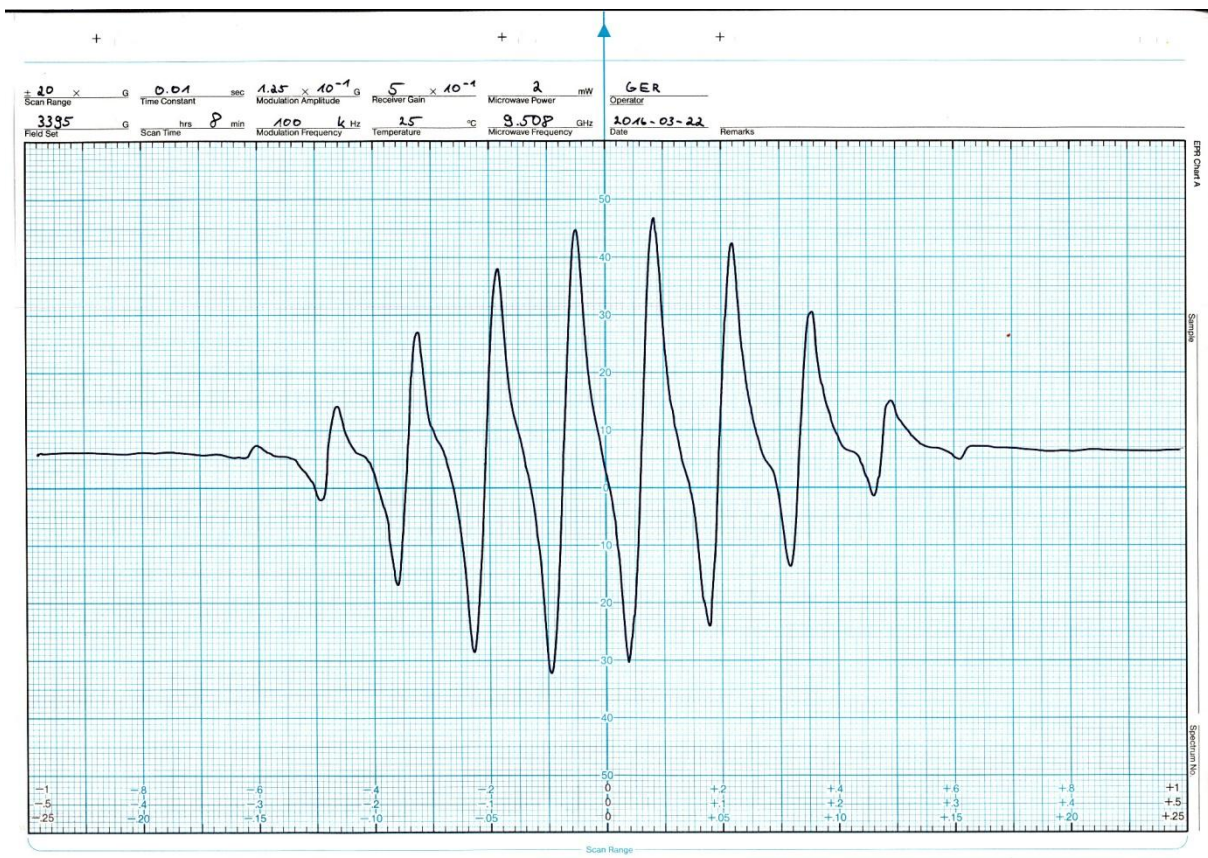
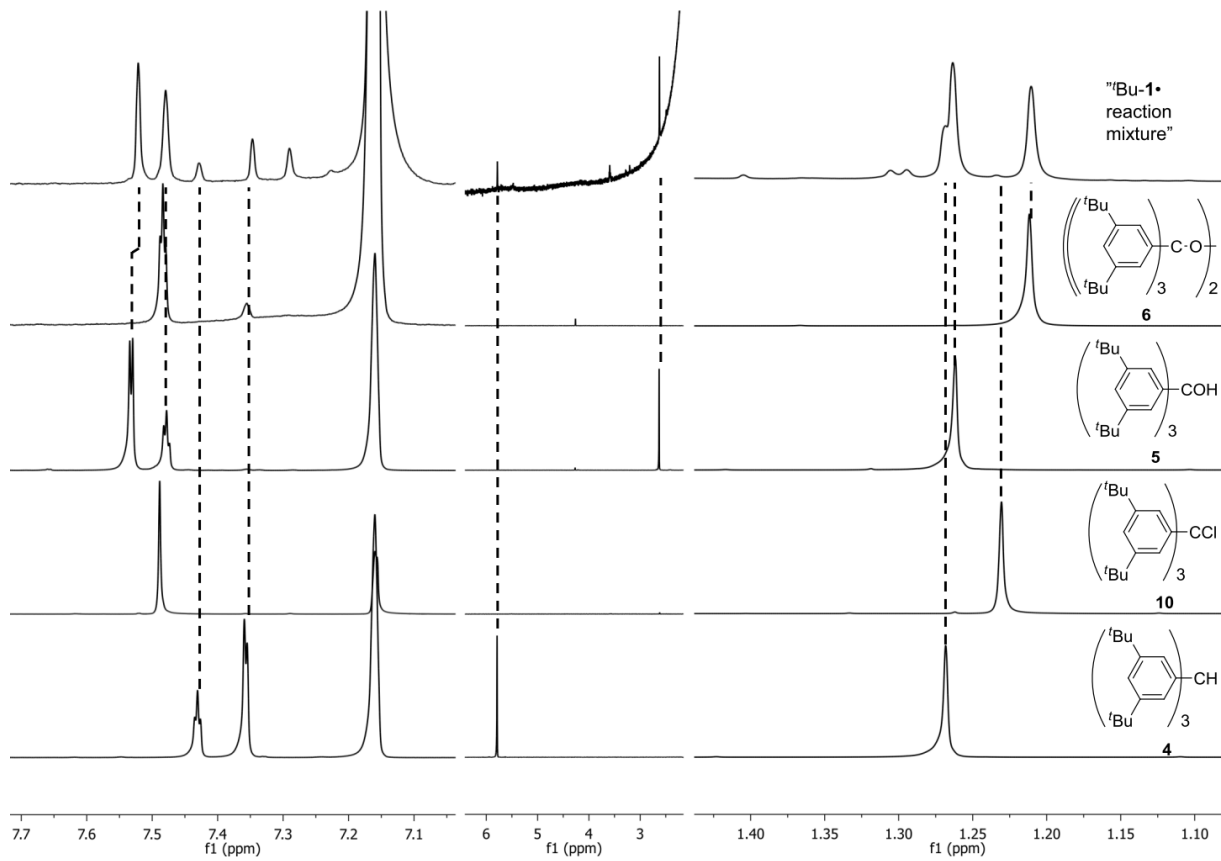


In cyclohexane- d_{12}

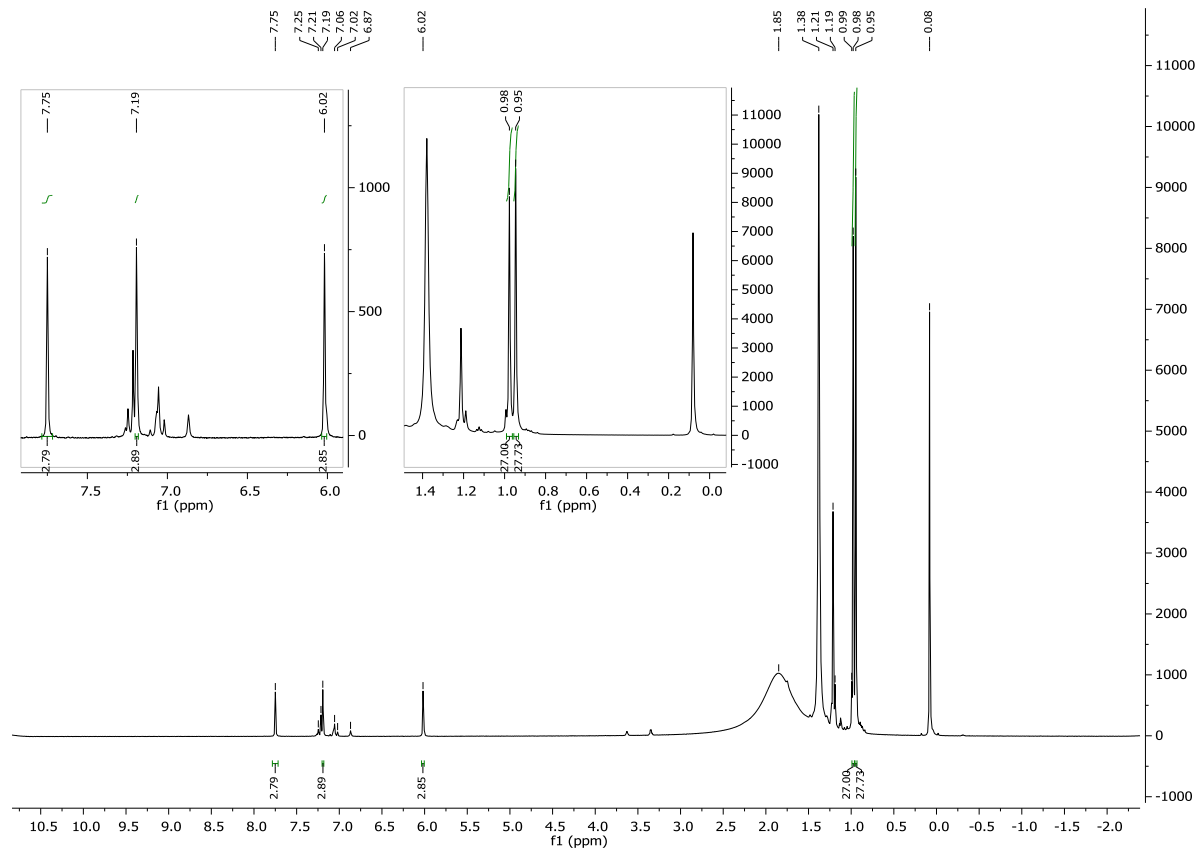


Tri(3,5-di-*tert*-butylphenyl)methyl radical ^tBu-1•:

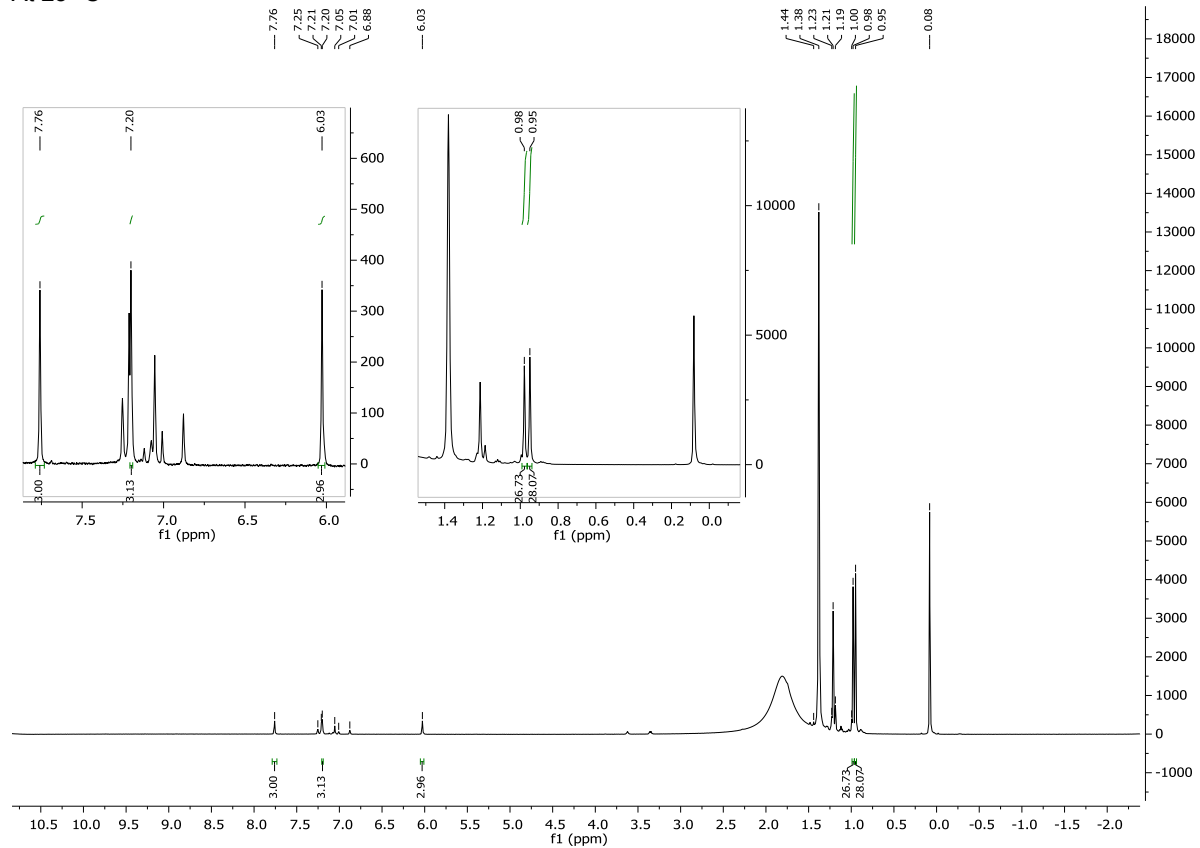


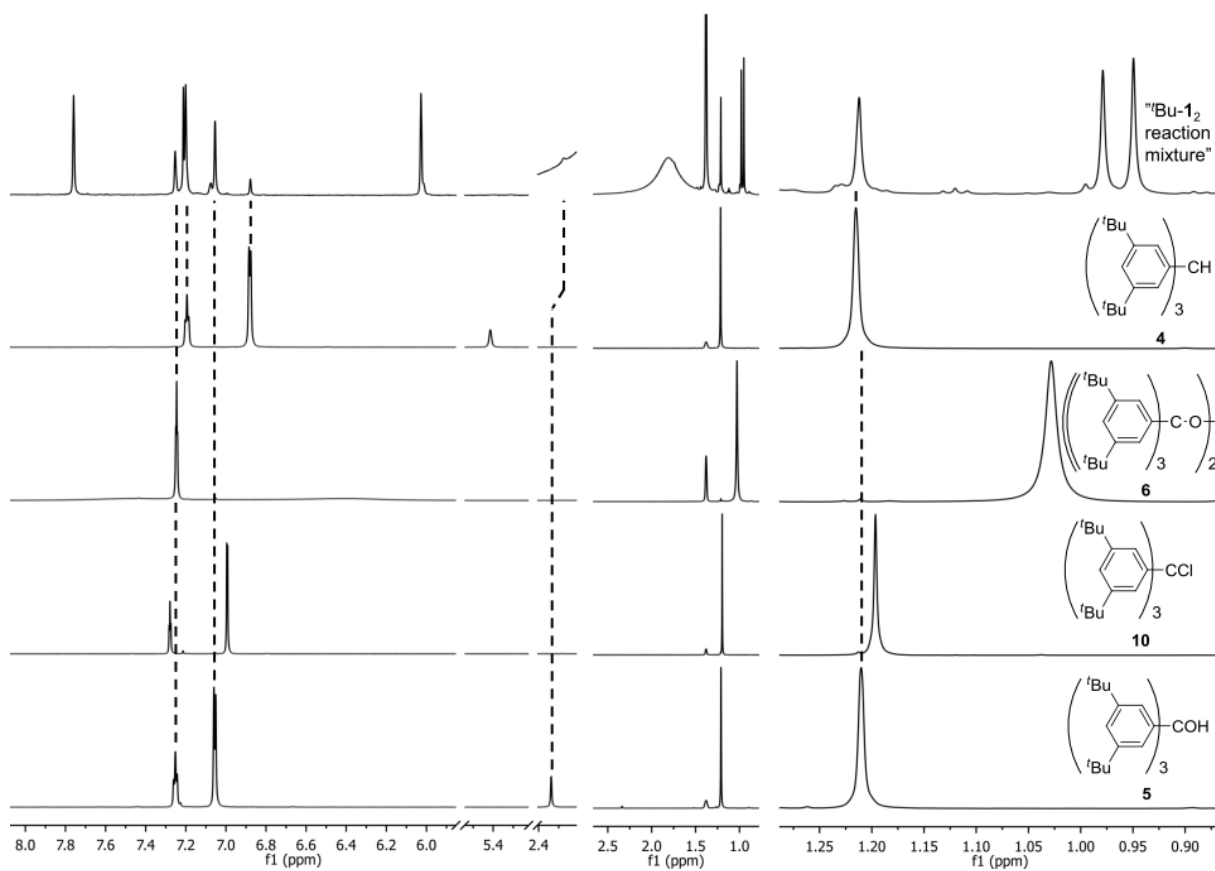
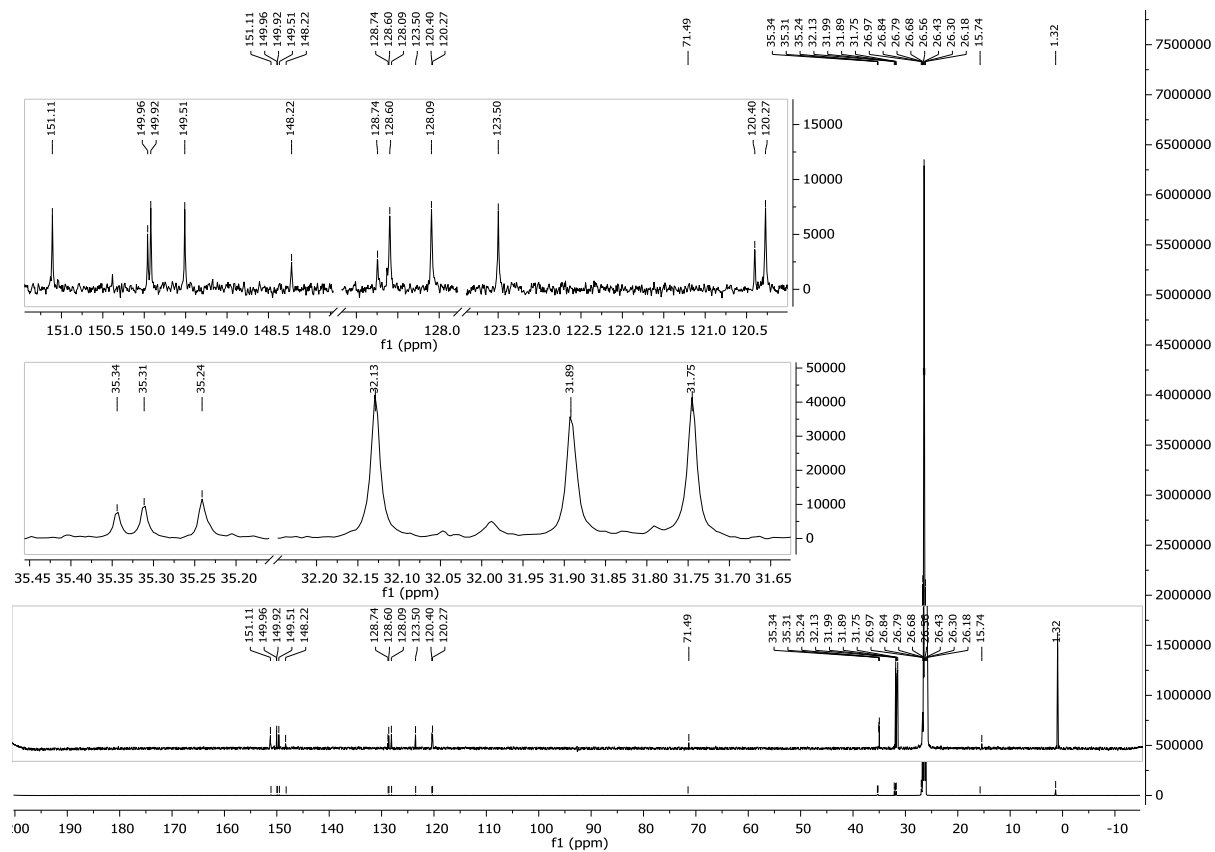


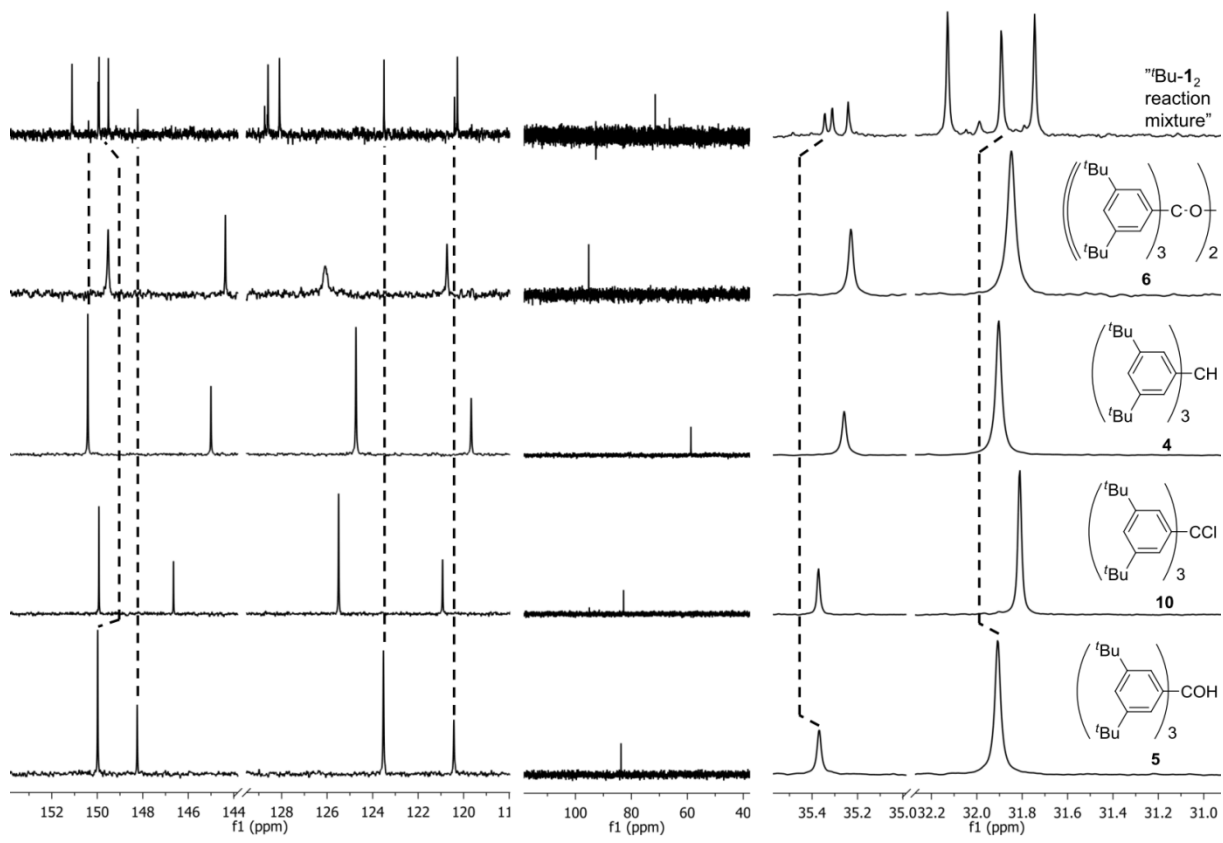
Hexa(3,5-di-*tert*-butylphenyl)ethane ^tBu-1₂:
At 3.8 °C



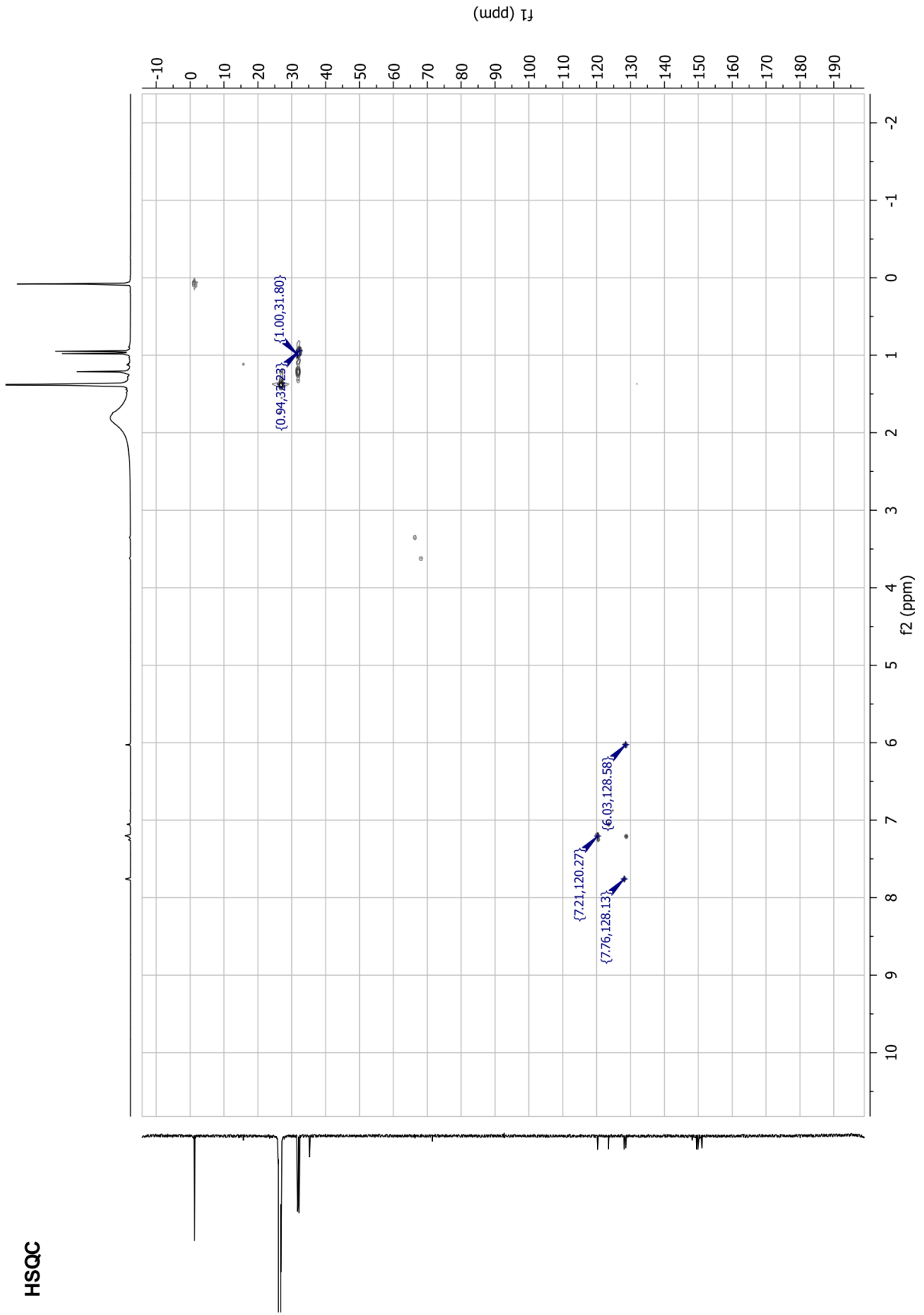
At 25 °C



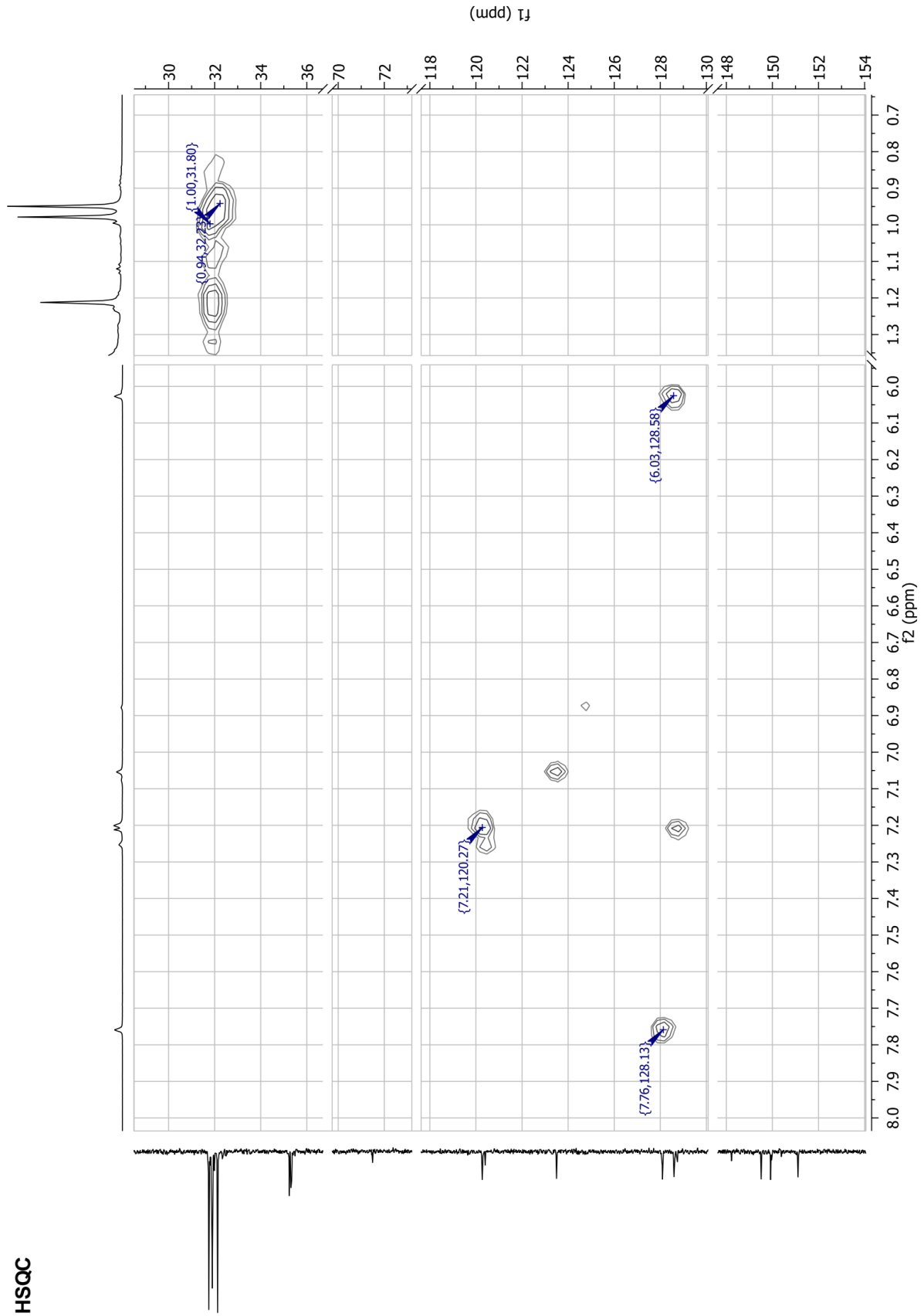


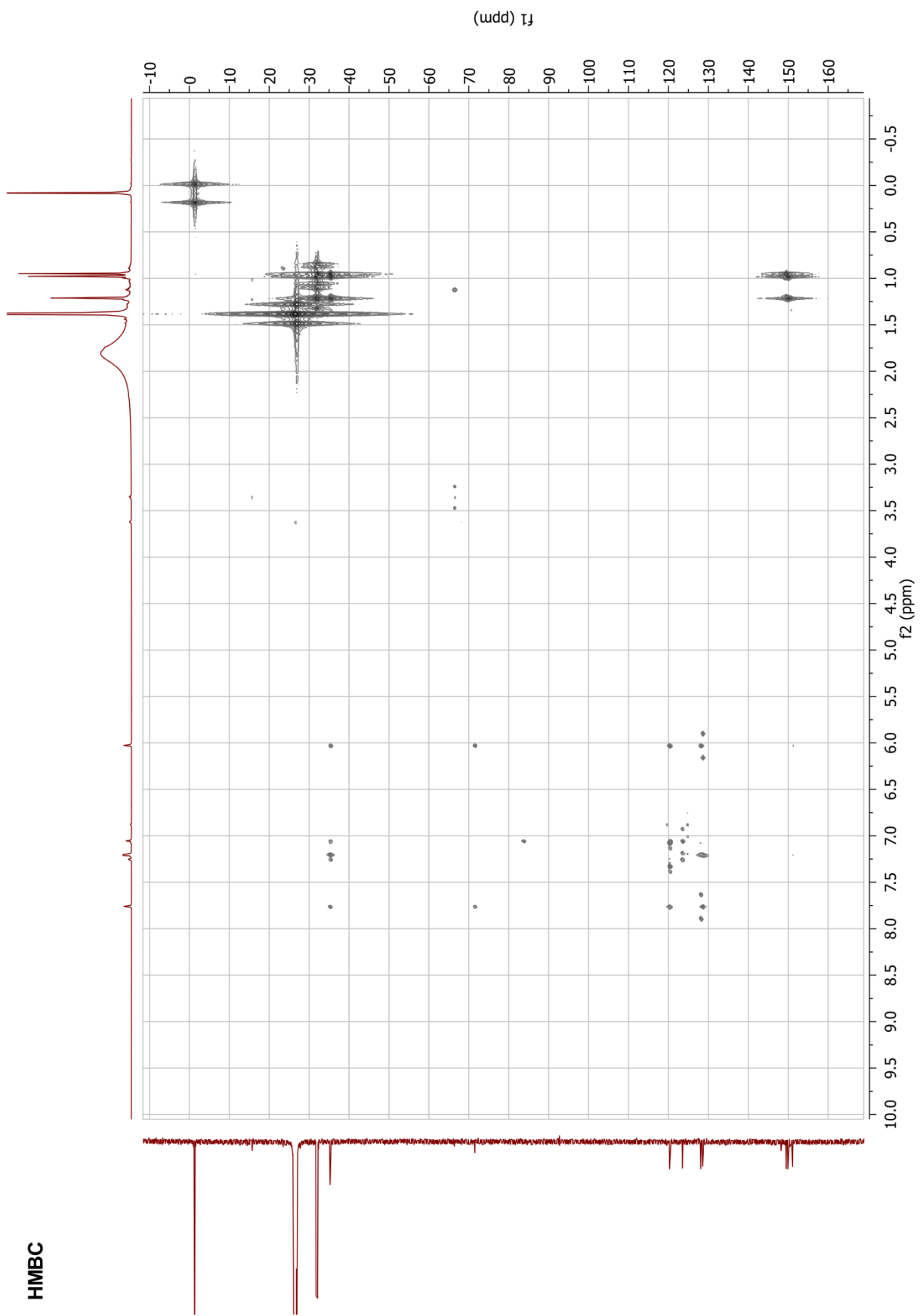


HSQC

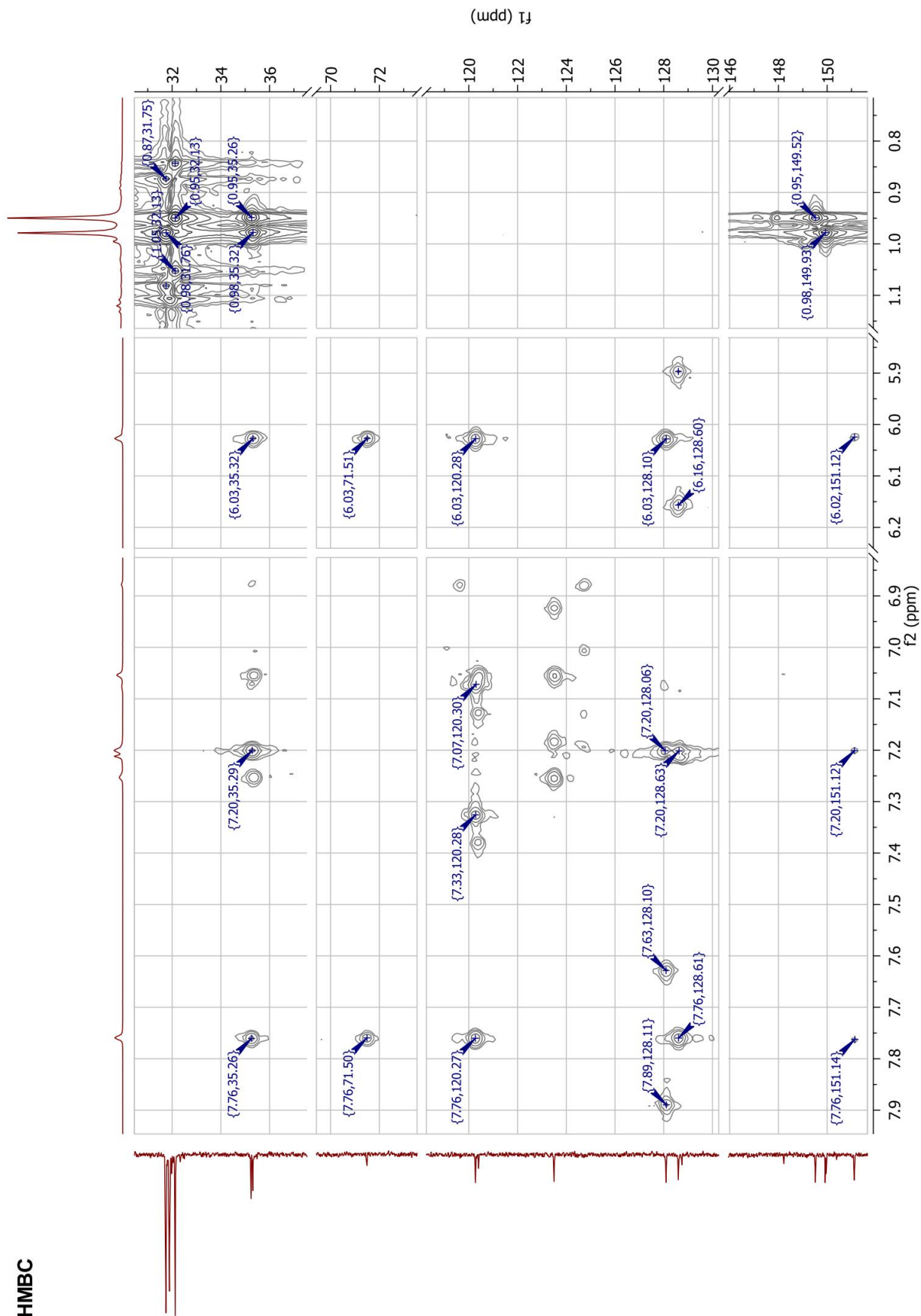


HSQC





HMBC



Computations

For the computations Gaussian 09, Revision D.01 was used.⁸ Dissociation energies were derived through $\Delta E = 2 \cdot E(\text{R-1}\bullet) - E(\text{R-1}_2)$ with $E = D_e, H_d^{298}, S_d^{298}, G_d^{298}$.

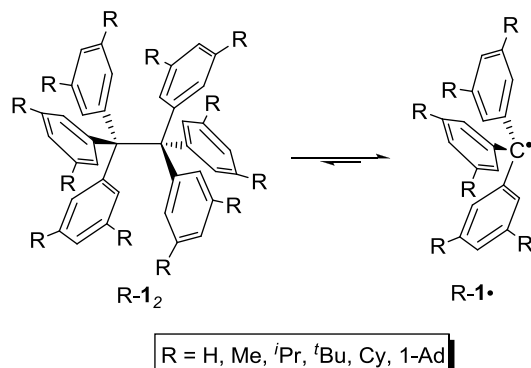


Figure S3. Nomenclature of the computed compounds.

Overview

Table S3. Computed free energies ΔG_d^{298} for the equilibrium between R-1₂ and R-1• with C-PCM:cyclohexane as solvent model in kcal mol⁻¹. Dispersion corrections were obtained via $E_{\text{disp}} = D_e(\text{B3LYP-D3(BJ)}) - D_e(\text{B3LYP})$. The isotropic polarizability α of R-1₂ is the average value of B3LYP-D3(BJ) and M06-2X; basis set: cc-pVDZ.

Prop.	R =	H	Me	<i>i</i> Pr	<i>t</i> Bu	Cy	1-Ad
ΔG_d^{298} ^[a]	M06-2X	-5.2	-8.3	-0.3	-5.1	3.1	12.8
	B3LYP-D3(BJ)	-8.1	-8.3	7.8	10.5	19.1	33.0
E_{disp} ^[a]		31.1	41.5	61.2	67.7	67.3	98.3
α ^[b]	averaged	0.7	1.0	1.4	1.7	2.1	2.8
R_{CC} ^[c]	M06-2X	1.692	1.712	1.669	1.666	1.700	1.663
	B3LYP-D3(BJ)	1.701	1.725	1.665	1.662	1.703	1.662

^[a]Kcal mol⁻¹ ^[b]nm³; max. deviation $\Delta\alpha = 0.02$ nm³; ^[c]Å.

Dissociation Energies

Table S4. H-1₂ → 2 H-1•

		D_e	ΔH_d^0	ΔH_d^{298}	ΔS_d^{298}	$T\Delta S_d^{298}$	ΔG_d^{298}	α
		kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹ K ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	nm ³
<i>Vacuum</i>	B3LYP	-18.22	-22.18	-21.58	55.19	16.45	-38.04	0.59
	B3LYP-D3(BJ)	12.99	8.46	9.05	55.17	16.45	-7.40	0.58
	M06-2X	17.22	12.31	12.90	57.61	17.18	-4.28	0.57
<i>C-PCM: CyH</i>	B3LYP	-18.98	-23.05	-22.46	53.42	15.93	-38.39	0.69
	B3LYP-D3(BJ)	12.16	7.70	8.29	55.09	16.43	-8.14	0.69
	M06-2X	16.18	11.39	11.98	57.48	17.14	-5.15	0.67

Table S5. Me-1₂ → 2 Me-1•

		D_e	ΔH_d^0	ΔH_d^{298}	ΔS_d^{298}	$T\Delta S_d^{298}$	ΔG_d^{298}	α
		kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹ K ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	nm ³
<i>Vacuum</i>	B3LYP	-17.97	6.98	-25.25	34.33	10.24	-35.49	0.81
	B3LYP-D3(BJ)	20.61	12.09	12.68	37.84	11.28	1.40	0.81
	M06-2X	21.47	16.21	16.80	81.45	24.28	-7.48	0.79
<i>C-PCM: CyH</i>	B3LYP	-19.05	-23.26	-22.67	68.23	20.34	-43.01	0.96
	B3LYP-D3(BJ)	19.40	14.54	15.13	78.74	23.48	-8.34	0.95
	M06-2X	20.03	15.08	15.67	80.33	23.95	-8.28	0.93

Table S6. ⁱPr-1₂ → 2 ⁱPr-1•

		D_e	ΔH_d^0	ΔH_d^{298}	ΔS_d^{298}	$T\Delta S_d^{298}$	ΔG_d^{298}	α
		kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹ K ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	nm ³
<i>Vacuum</i>	B3LYP	-26.10	-30.73	-30.14	82.13	24.49	-54.63	1.21
	B3LYP-D3(BJ)	35.16	27.49	28.08	51.06	15.22	12.86	1.20
	M06-2X	30.91	22.92	23.51	38.54	11.49	12.02	1.18
<i>C-PCM: CyH</i>	B3LYP	-27.26	-31.87	-31.27	76.68	22.86	-54.14	1.43
	B3LYP-D3(BJ)	33.93	28.03	28.62	70.01	20.87	7.75	1.42
	M06-2X	28.39	22.08	22.67	77.13	23.00	-0.32	1.40

Table S7. ^tBu-1₂ → 2 ^tBu-1•

		D_e	ΔH_d^0	ΔH_d^{298}	ΔS_d^{298}	$T\Delta S_d^{298}$	ΔG_d^{298}	α
		kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹ K ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	nm ³
<i>Vacuum</i>	B3LYP	-28.44	-30.49	-29.89	86.07	25.66	-55.56	1.41
	B3LYP-D3(BJ)	39.40	37.37	37.96	111.22	33.16	4.81	1.40
	M06-2X	28.94	30.15	30.75	110.46	32.93	-2.19	1.38
<i>C-PCM: CyH</i>	B3LYP	-29.81	-31.81	-31.21	84.65	25.24	-56.45	1.67
	B3LYP-D3(BJ)	37.90	34.23	34.82	81.63	24.34	10.49	1.66
	M06-2X	27.30	29.14	29.74	116.71	34.80	-5.06	1.64

Table S8. Cy-1₂ → 2 Cy-1•

		D_e	ΔH_d^0	ΔH_d^{298}	ΔS_d^{298}	$T\Delta S_d^{298}$	ΔG_d^{298}	α
		kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹ K ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	nm ³
<i>Vacuum</i>	B3LYP	-19.84	-24.00	-23.40	53.78	16.03	-39.44	1.79
	B3LYP-D3(BJ)	47.74	41.87	42.46	86.15	25.69	16.77	1.78
	M06-2X	34.18	34.81	35.40	110.82	33.04	2.36	1.75

	B3LYP	-21.15	-16.67	-16.08	115.52	34.44	-50.52	2.09
<i>C-PCM:CyH</i>	B3LYP-D3(BJ)	46.12	41.86	42.46	78.51	23.41	19.05	2.08
	M06-2X	33.46	29.57	30.16	90.64	27.03	3.14	2.05

Table S9. Ad-1₂ → 2 Ad-1•

		D_e	ΔH_d^0	ΔH_d^{298}	ΔS_d^{298}	$T\Delta S_d^{298}$	ΔG_d^{298}	α
		kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹ K ⁻¹	kcal mol ⁻¹	kcal mol ⁻¹	nm ³
<i>Vacuum</i>	B3LYP	-28.82	-41.36	-40.76	-2.63	-0.78	-39.98	2.40
	B3LYP-D3(BJ)	60.70	55.48	56.07	104.44	31.14	24.93	2.38
	M06-2X	40.99	37.49	38.08	77.61	23.14	14.94	2.36
<i>C-PCM:CyH</i>	B3LYP	-32.85	-36.61	-36.02	56.57	16.87	-52.89	2.85
	B3LYP-D3(BJ)	65.42	59.03	59.63	89.31	26.63	33.00	2.83
	M06-2X	38.68	38.23	38.83	87.32	26.04	12.79	2.81

Energies

Energies of the optimized structures are given in hartree. Throughout cc-pVDZ was used as basis set. Symmetry for dimers was restricted to S_6 , for radical monomers to C_3 .

Table S10. Radical monomers R-1• in gas phase in hartree.

H-1•		
method	electronic energy	ZPVE
B3LYP	-733.0764598	0.277351
B3YLP-D3(BJ)	-733.1568231	0.277795
M06-2X	-732.7935605	0.278935
Me-1•		
method	electronic energy	ZPVE
B3LYP	-968.9813788	0.438957
B3YLP-D3(BJ)	-969.0952808	0.439616
M06-2X	-968.5820561	0.442479
iPr-1•		
method	electronic energy	ZPVE
B3LYP	-1440.746265	0.778034
B3YLP-D3(BJ)	-1440.940249	0.780041
M06-2X	-1440.128500	0.783835
tBu-1•		
method	electronic energy	ZPVE
B3LYP	-1676.609727	0.944188
B3YLP-D3(BJ)	-1676.854105	0.946712
M06-2X	-1675.902194	0.952281
Cy-1•		
method	electronic energy	ZPVE
B3LYP	-2141.201519	1.176190
B3YLP-D3(BJ)	-2141.493126	1.177676
M06-2X	-2140.318802	1.183848
Ad-1•		
method	electronic energy	ZPVE
B3LYP	-3070.299518	1.608311
B3YLP-D3(BJ)	-3070.782260	1.615265
M06-2X	-3069.168355	1.625587

Table S11. Radical monomers R-1• with C-PCM:cyclohexane in hartree.

H-1•		
method	electronic energy	ZPVE
B3LYP	-733.0787485	0.277293
B3YLP-D3(BJ)	-733.1590829	0.277742
M06-2X	-732.7964368	0.278896

	Me-1•	
method	electronic energy	ZPVE
B3LYP	-968.9838193	0.438955
B3YLP-D3(BJ)	-969.0976825	0.439616
M06-2X	-968.5851891	0.439509
	ⁱPr-1•	
method	electronic energy	ZPVE
B3LYP	-1440.748523	0.777475
B3YLP-D3(BJ)	-1440.942455	0.779511
M06-2X	-1440.13230	0.782526
	^tBu-1•	
method	electronic energy	ZPVE
B3LYP	-1676.612119	0.943492
B3YLP-D3(BJ)	-1676.856469	0.946265
M06-2X	-1675.905340	0.951729
	Cy-1•	
method	electronic energy	ZPVE
B3LYP	-2141.204065	1.175433
B3YLP-D3(BJ)	-2141.495535	1.176557
M06-2X	-2140.322113	1.182930
	Ad-1•	
method	electronic energy	ZPVE
B3LYP	-3070.304520	1.610998
B3YLP-D3(BJ)	-3070.779891	1.612403
M06-2X	-3069.172026	1.623864

Table S12. Dimers R-1₂ in gas phase in hartree.

	H-1₂	
method	electronic energy	ZPVE
B3LYP	-1466.123877	0.560584
B3YLP-D3(BJ)	-1466.334350	0.562632
M06-2X	-1465.614561	0.565697
	Me-1₂	
method	electronic energy	ZPVE
B3LYP	-1937.934124	0.88536
B3YLP-D3(BJ)	-1938.223412	0.88806
M06-2X	-1937.198322	0.89488
	ⁱPr-1₂	
method	electronic energy	ZPVE
B3LYP	-2881.450942	1.563903
B3YLP-D3(BJ)	-2881.936535	1.569315
M06-2X	-2880.306254	1.575694
	^tBu-1₂	
method	electronic energy	ZPVE
B3LYP	-3353.17413	1.893794
B3YLP-D3(BJ)	-3353.770992	1.900866
M06-2X	-3351.850503	1.909038
	Cy-1₂	
method	electronic energy	ZPVE
B3LYP	-4282.371419	2.357848
B3YLP-D3(BJ)	-4283.062331	2.365418
M06-2X	-4280.69208	2.374363
	Ad-1₂	
method	electronic energy	ZPVE
B3LYP	-6140.553102	3.225925
B3YLP-D3(BJ)	-6141.661258	3.241213
M06-2X	-6138.402039	3.256664

Table S13. Dimers R-1₂ with C-PCM:cyclohexane in hartree.

H-1 ₂		
method	electronic energy	ZPVE
B3LYP	-1466.127253	0.560676
B3YLP-D3(BJ)	-1466.337552	0.562399
M06-2X	-1465.618663	0.565398
Me-1 ₂		
method	electronic energy	ZPVE
B3LYP	-1937.937282	0.88472
B3YLP-D3(BJ)	-1938.226278	0.88733
M06-2X	-1937.202304	0.89283
ⁱ Pr-1 ₂		
method	electronic energy	ZPVE
B3LYP	-2881.453611	1.562604
B3YLP-D3(BJ)	-2881.93898	1.568258
M06-2X	-2880.309852	1.576509
^t Bu-1 ₂		
method	electronic energy	ZPVE
B3LYP	-3353.176729	1.892288
B3YLP-D3(BJ)	-3353.773333	1.899777
M06-2X	-3351.854193	1.907694
Cy-1 ₂		
method	electronic energy	ZPVE
B3LYP	-4282.374429	2.352386
B3YLP-D3(BJ)	-4283.064564	2.361481
M06-2X	-4280.697544	2.375467
Ad-1 ₂		
method	electronic energy	ZPVE
B3LYP	-6140.556687	3.226542
B3YLP-D3(BJ)	-6141.664032	3.239013
M06-2X	-6138.405688	3.252795

H	-1.762767000	1.655971000	-1.243394000	C	-1.011963000	2.186029000	-0.655367000
H	2.315497000	0.698616000	-1.243394000	C	-1.017270000	3.575689000	-0.681539000
H	4.659437000	-2.690457000	-0.008165000	C	1.269060000	-0.728437000	0.020652000
H	0.561570000	-2.352656000	1.253608000	C	2.399138000	-0.216629000	-0.655367000
H	-2.318245000	0.689995000	1.253608000	C	3.605273000	-0.906863000	-0.681539000
H	-0.552729000	-2.354587000	-1.243394000	C	3.696851000	-2.134378000	-0.009395000
H	-4.659723000	-2.689962000	-0.008165000	C	2.605484000	-2.670898000	0.674094000
H	2.046088000	4.095477000	2.536393000	C	1.400948000	-1.963565000	0.679607000
H	1.940449000	5.440626000	1.375569000	C	-3.615807000	-0.920966000	0.674094000
H	3.075438000	4.098182000	1.094104000	C	-2.400971000	-0.231474000	0.679607000
H	-1.609233000	5.003017000	-2.243482000	C	-1.265375000	-0.734820000	0.020652000
H	-2.636760000	5.021336000	-0.799473000	C	-1.387175000	-1.969400000	-0.655367000
H	-2.770731000	3.682609000	-1.965866000	C	-2.588003000	-2.668826000	-0.681539000
H	5.137356000	-1.107872000	-2.243482000	C	-3.696851000	-2.134378000	-0.009395000
H	5.666985000	-0.227167000	-0.799473000	C	0.000000000	0.000000000	0.025526000
H	4.574598000	0.558219000	-1.965866000	C	2.100323000	4.340234000	1.398125000
H	2.523743000	-3.819703000	2.536393000	C	-2.085675000	4.337286000	-1.423204000
H	3.741496000	-4.400791000	1.375569000	C	4.799038000	-0.362396000	-1.423204000
H	2.011410000	-4.712498000	1.094104000	C	2.708591000	-3.989050000	1.398125000
H	-4.569832000	-0.275774000	2.536393000	C	-4.808914000	-0.351184000	1.398125000
H	-5.681944000	-1.039835000	1.375569000	C	-2.713363000	-3.974891000	-1.423204000
H	-5.086848000	0.614317000	1.094104000	H	-0.000135000	5.362238000	-0.021928000
H	-3.528123000	-3.895145000	-2.243482000	H	1.778830000	1.655831000	1.223743000
H	-3.030225000	-4.794169000	-0.799473000	H	-1.789664000	1.635755000	-1.188714000
H	-1.803867000	-4.240828000	-1.965866000	H	2.311437000	0.732017000	-1.188714000
				H	4.643902000	-2.681002000	-0.021928000
				H	0.544577000	-2.368427000	1.223743000
				H	-2.323406000	0.712596000	1.223743000
				H	-0.521773000	-2.367772000	-1.188714000
				H	-4.643767000	-2.681236000	-0.021928000
				H	2.149819000	4.038762000	2.454679000
				H	1.935248000	5.424901000	1.359085000
				H	3.083918000	4.128910000	0.951968000
				H	-1.644376000	4.964702000	-2.212039000
				H	-2.635652000	5.005112000	-0.743269000
				H	-2.807912000	3.656545000	-1.892424000
				H	5.121746000	-1.058280000	-2.212039000
				H	5.652380000	-0.220015000	-0.743269000
				H	4.570617000	0.603450000	-1.892424000
				H	2.422761000	-3.881179000	2.454679000
				H	3.730478000	-4.388424000	1.359085000
				H	2.033782000	-4.735206000	0.951968000
				H	-4.572580000	-0.157583000	2.454679000
				H	-5.665726000	-1.036477000	1.359085000
				H	-5.117700000	0.606296000	0.951968000
				H	-3.477370000	-3.906423000	-2.212039000
				H	-3.016728000	-4.785098000	-0.743269000
				H	-1.762705000	-4.259995000	-1.892424000

B3LYP-D3(BJ)

C	0.000000000	4.276471000	0.005309000				
C	-1.012098000	3.593662000	-0.678299000				
C	-1.002135000	2.194630000	-0.676159000				
C	0.002070000	1.461687000	-0.008972000				
C	1.010812000	2.191785000	0.667269000				
C	1.018350000	3.584307000	0.684938000				
C	-1.266894000	-0.729051000	-0.008972000				
C	-2.403548000	-0.220503000	0.667269000				
C	-3.613276000	-0.910236000	0.684938000				
C	-3.703533000	-2.138236000	0.005309000				
C	-2.606153000	-2.673333000	-0.678299000				
C	-1.399537000	-1.965189000	-0.676159000				
C	3.618251000	-0.920329000	-0.678299000				
C	2.401673000	-0.229440000	-0.676159000				
C	1.264823000	-0.732637000	-0.008972000				
C	1.392735000	-1.971282000	0.667269000				
C	2.594926000	-2.674071000	0.684938000				
C	3.703533000	-2.138236000	0.005309000				
C	0.000000000	0.000000000	-0.010315000				
C	-2.097289000	4.340097000	-1.415878000				
C	2.090055000	4.347642000	1.423842000				
C	-4.810196000	-0.363780000	1.423842000				
C	-2.709990000	-3.986354000	-1.415878000				
C	4.807279000	-0.353744000	-1.415878000				
C	2.720141000	-3.983862000	1.423842000				
H	-0.000529000	5.370272000	0.011109000				
H	-1.777149000	1.653796000	-1.222064000				
H	1.785217000	1.644950000	1.207069000				
H	-2.317178000	0.723568000	1.207069000				
H	-4.650528000	-2.685594000	0.011109000				
H	-0.543655000	-2.365954000	-1.222064000				
H	2.320804000	0.712158000	-1.222064000				
H	0.531960000	-2.368519000	1.207069000				
H	4.651056000	-2.684678000	0.011109000				
H	-2.097602000	4.085007000	-2.488636000				
H	-1.971046000	5.429038000	-1.327597000				
H	-3.094972000	4.081229000	-1.023910000				
H	1.654935000	4.989898000	2.207729000				
H	2.650228000	5.008389000	0.741039000				
H	2.809656000	3.668476000	1.903588000				
H	-5.148846000	-1.061734000	2.207729000				
H	-5.662506000	-0.209030000	0.741039000				
H	-4.581822000	0.598996000	1.903588000				
H	-2.488919000	-3.859080000	-2.488636000				
H	-3.716162000	-4.421495000	-1.327597000				
H	-1.986962000	-4.720939000	-1.023910000				
H	4.586521000	-0.225927000	-2.488636000				
H	5.687208000	-1.007543000	-1.327597000				
H	5.081934000	0.639710000	-1.023910000				
H	3.493911000	-3.928165000	2.207729000				
H	3.012279000	-4.799359000	0.741039000				
H	1.772165000	-4.267472000	1.903588000				

M06-2X

C	0.000000000	4.268756000	-0.009395000				
C	1.010324000	3.591864000	0.674094000				
C	1.000024000	2.195039000	0.679607000				
C	-0.003686000	1.463257000	0.020652000				

Pr-1

B3LYP

C	0.007898000	4.279797000	-0.017282000				
C	0.989078000	3.599970000	0.721498000				
C	0.980125000	2.201578000	0.712001000				
C	0.000000000	1.467970000	0.001653000				
C	-0.977861000	2.197711000	-0.715668000				
C	-0.978964000	3.595773000	-0.744579000				
C	1.271300000	-0.733985000	0.001653000				
C	2.392204000	-0.252002000	-0.715668000				
C	3.603513000	-0.950079000	-0.744579000				
C	3.702464000	-2.146739000	-0.017282000				
C	2.623127000	-2.656552000	0.721498000				
C	1.416560000	-1.949602000	0.712001000				
C	-3.612205000	-0.943419000	0.721498000				
C	-2.396684000	-0.251976000	0.712001000				
C	-1.271300000	-0.733985000	0.001653000				
C	-1.414343000	-1.945708000	-0.715668000				
C	-2.624549000	-2.645694000	-0.744579000				
C	-3.710362000	-2.133058000	-0.017282000				
C	0.000000000	0.000000000	0.005231000				
C	-2.777845000	-3.932951000	-1.548479000				
C	-2.544237000	-3.706375000	-3.052535000				
C	-1.873731000	-5.056261000	-1.011066000				
C	-4.805269000	-0.439865000	1.527522000				
C	-5.272673000	0.951855000	1.068664000				
C	-4.518734000	-0.457477000	3.039872000				
C	4.794958000	-0.439209000	-1.548479000				
C	5.315716000	0.905431000	-1.011066000				
C	4.481933000	-0.350187000	-3.052535000				
C	2.783569000	-3.941552000	1.527522000				
C	1.812006000	-5.042197000	1.068664000				
C	2.655554000	-3.684600000	3.039872000				
C	2.021700000	4.381417000	1.527522000				
C	1.863180000	4.142077000	3.039872000				
C	3.460668000	4.090341000	1.068664000				
C	-2.017113000	4.372160000	-1.548479000				

C	-1.937696000	4.056561000	-3.052535000	C	1.950943000	-4.155198000	-2.955803000
C	-3.441984000	4.150829000	-1.011066000	C	3.504106000	-3.986851000	-0.961644000
H	0.011807000	5.374149000	-0.025173000	C	-2.084373000	-4.350976000	1.446125000
H	1.727470000	1.651023000	1.285999000	C	-1.956848000	-4.131865000	2.962012000
H	-1.728831000	1.643570000	-1.281075000	C	-3.495014000	-3.996350000	0.953633000
H	2.287789000	0.675427000	-1.281075000	H	0.008714000	-5.364806000	0.011717000
H	4.648246000	-2.697299000	-0.025173000	H	1.774133000	-1.641353000	-1.222723000
H	0.566093000	-2.321544000	1.285999000	H	-1.775314000	-1.637546000	-1.207754000
H	-2.293563000	0.670521000	1.285999000	H	2.305813000	-0.718694000	1.207754000
H	-0.558957000	-2.318997000	-1.281075000	H	4.641702000	2.689950000	0.011717000
H	-4.660052000	-2.676850000	-0.025173000	H	0.534387000	2.357121000	-1.222723000
H	-3.824214000	-4.262663000	-1.423295000	H	-2.308520000	-0.715767000	-1.222723000
H	-1.507016000	-3.391660000	-3.255243000	H	-0.530499000	2.356240000	1.207754000
H	-3.214334000	-2.926804000	-3.448371000	H	-4.650416000	2.674857000	0.011717000
H	-2.726527000	-4.634903000	-3.618879000	H	-3.738209000	4.372721000	1.247200000
H	-0.806975000	-4.799921000	-1.120746000	H	-1.601799000	3.370790000	3.222165000
H	-2.049266000	-5.995756000	-1.561374000	H	-3.346441000	3.035199000	3.321393000
H	-2.064193000	-5.245629000	0.057455000	H	-2.744990000	4.706654000	3.509197000
H	-5.634351000	-1.145014000	1.341360000	H	-0.678659000	4.701616000	1.150312000
H	-5.512200000	0.958873000	-0.006698000	H	-1.864827000	5.988699000	1.466684000
H	-4.497376000	1.715858000	1.244486000	H	-1.810106000	5.192644000	-0.130518000
H	-6.175311000	1.261331000	1.621474000	H	-5.666410000	1.039367000	-1.225491000
H	-4.223327000	-1.463258000	3.378570000	H	-5.395609000	-1.055791000	0.122877000
H	-5.412097000	-0.152448000	3.610099000	H	-4.402641000	-1.767476000	-1.169162000
H	-3.702566000	0.236681000	3.301348000	H	-6.113963000	-1.392340000	-1.476425000
H	5.603682000	-1.180535000	-1.423295000	H	-4.326126000	1.403122000	-3.303544000
H	4.560341000	1.701099000	-1.120746000	H	-5.467272000	0.043163000	-3.502201000
H	6.217111000	1.223162000	-1.561374000	H	-3.735375000	-0.273701000	-3.229145000
H	5.574944000	0.835171000	0.057455000	H	5.655993000	1.051023000	1.247200000
H	3.690772000	0.390716000	-3.255243000	H	4.411048000	-1.763072000	1.150312000
H	4.141853000	-1.320293000	-3.448371000	H	6.118779000	-1.379363000	1.466684000
H	5.377208000	-0.043790000	-3.618879000	H	5.402015000	-1.028724000	-0.130518000
H	3.808787000	-4.306984000	1.341360000	H	3.720089000	-0.298196000	3.222165000
H	1.925692000	-5.253141000	-0.006698000	H	4.301780000	1.380504000	3.321393000
H	0.762711000	-4.752771000	1.244486000	H	5.448577000	0.023904000	3.509197000
H	1.995311000	-5.978642000	1.621474000	H	3.733324000	4.387572000	-1.225491000
H	3.378882000	-2.925880000	3.378570000	H	1.783463000	5.200630000	0.122877000
H	2.838073000	-4.610790000	3.610099000	H	0.670641000	4.696537000	-1.169162000
H	1.646311000	-3.324857000	3.301348000	H	1.851180000	5.991018000	-1.476425000
H	1.825564000	5.451998000	1.341360000	H	3.378202000	3.044974000	-3.303544000
H	0.844445000	4.389138000	3.378570000	H	2.771016000	4.713214000	-3.502201000
H	2.574025000	4.763238000	3.610099000	H	1.630656000	3.371780000	-3.229145000
H	2.056255000	3.088176000	3.301348000	H	1.933087000	-5.426939000	-1.225491000
H	3.586508000	4.294269000	-0.006698000	H	0.947924000	-4.448096000	-3.303544000
H	3.734665000	3.036913000	1.244486000	H	2.696255000	-4.756378000	-3.502201000
H	4.180000000	4.717311000	1.621474000	H	2.104719000	-3.098079000	-3.229145000
H	-1.779468000	5.443198000	-1.423295000	H	3.612146000	-4.144839000	0.122877000
H	-2.183756000	3.000944000	-3.255243000	H	3.732000000	-2.929061000	-1.169162000
H	-0.927519000	4.247097000	-3.448371000	H	4.262784000	-4.598677000	-1.476425000
H	-2.650680000	4.678694000	-3.618879000	H	-1.917783000	-5.423745000	1.247200000
H	-3.753366000	3.098822000	-1.120746000	H	-2.118290000	-3.072594000	3.222165000
H	-4.167844000	4.772595000	-1.561374000	H	-0.955339000	-4.415703000	3.321393000
H	-3.510751000	4.410457000	0.057455000	H	-2.703587000	-4.730558000	3.509197000

B3LYP-D3(BJ)

C	0.005978000	-4.271011000	0.006705000
C	1.019270000	-3.587971000	-0.681550000
C	1.006784000	-2.191944000	-0.677896000
C	0.000000000	-1.461496000	-0.006617000
C	-1.004723000	-2.190079000	0.669708000
C	-1.011514000	-3.585992000	0.686864000
C	1.265693000	0.730748000	-0.006617000
C	2.399026000	0.224924000	0.669708000
C	3.611317000	0.916999000	0.686864000
C	3.695815000	2.140683000	0.006705000
C	2.597639000	2.676700000	-0.681550000
C	1.394888000	1.967873000	-0.677896000
C	-3.616909000	0.911272000	-0.681550000
C	-2.401672000	0.224072000	-0.677896000
C	-1.265693000	0.730748000	-0.006617000
C	-1.394303000	1.965155000	0.669708000
C	-2.599803000	2.668992000	0.686864000
C	-3.701793000	2.130329000	0.006705000
C	0.000000000	0.000000000	-0.009235000
C	-2.725870000	3.980608000	1.446125000
C	-2.599877000	3.760612000	2.962012000
C	-1.713434000	5.024946000	0.953633000
C	-4.818055000	0.366261000	-1.438473000
C	-5.204767000	-1.041219000	-0.961644000
C	-4.573978000	0.388033000	-2.955803000
C	4.810243000	0.370368000	1.446125000
C	5.208448000	-1.028596000	0.953633000
C	4.566724000	0.371253000	2.962012000
C	2.726219000	3.989428000	-1.438473000
C	1.700662000	5.028070000	-0.961644000
C	2.623035000	3.767165000	-2.955803000
C	2.091836000	-4.355689000	-1.438473000

M06-2X

C	-0.017450000	4.265052000	0.100908000
C	1.024271000	3.585767000	0.751930000
C	1.019405000	2.195136000	0.743279000
C	0.000000000	1.463430000	0.091615000
C	-1.019294000	2.184514000	-0.554622000
C	-1.042200000	3.580970000	-0.552474000
C	1.267367000	-0.731715000	0.091615000
C	2.401491000	-0.209522000	-0.554622000
C	3.622311000	-0.887913000	-0.552474000
C	3.702368000	-2.117414000	0.100908000
C	2.593230000	-2.679929000	0.751930000
C	1.391341000	-1.980399000	0.743279000
C	-3.617501000	-0.905839000	0.751930000
C	-2.410746000	-0.214737000	0.743279000
C	-1.267367000	-0.731715000	0.091615000
C	-1.382197000	-1.974992000	-0.554622000
C	-2.580111000	-2.693057000	-0.552474000
C	-3.684918000	-2.147638000	0.100908000
C	0.000000000	0.000000000	0.095868000
C	-2.667337000	-4.042061000	-1.242056000
C	-2.421966000	-3.918492000	-2.748614000
C	-1.698069000	-5.045281000	-0.609643000
C	-4.869903000	-0.355890000	1.414819000
C	-5.850088000	0.145575000	0.346698000
C	-4.595572000	0.741992000	2.439230000
C	4.834196000	-0.288951000	-1.242056000
C	5.218376000	1.052069000	-0.609643000
C	4.604497000	-0.138238000	-2.748614000
C	2.743161000	-4.039515000	1.414819000

C	2.798972000	-5.139112000	0.346698000	C	2.717918000	-3.975950000	1.516199000
C	1.655202000	-4.350878000	2.439230000	C	-1.343809000	5.282971000	-2.574307000
C	2.126742000	4.395405000	1.414819000	C	-2.835791000	5.311627000	-0.539913000
C	2.940370000	3.608886000	2.439230000	C	-3.064859000	3.502737000	-2.246913000
C	3.051116000	4.993537000	0.346698000	C	1.961058000	3.962114000	3.010308000
C	-2.166859000	4.331012000	-1.242056000	C	1.962673000	5.872118000	1.399843000
C	-2.182530000	4.056730000	-2.748614000	C	3.482743000	3.931710000	0.999128000
C	-3.520307000	3.993211000	-0.609643000	C	-4.411820000	-0.282731000	3.010308000
H	-0.031146000	5.359318000	0.114208000	C	-6.066740000	-1.236334000	1.399843000
H	1.798094000	1.641128000	1.267689000	C	-5.146332000	1.050289000	0.999128000
H	-1.801501000	1.629977000	-1.077034000	C	-3.903283000	-3.805258000	-2.574307000
H	2.312353000	0.745157000	-1.077034000	C	-3.182108000	-5.111680000	-0.539913000
H	4.656879000	-2.652685000	0.114208000	C	-1.501030000	-4.405614000	-2.246913000
H	0.522212000	-2.377759000	1.267689000	C	5.247092000	-1.477713000	-2.574307000
H	-2.320306000	0.736631000	1.267689000	C	6.017899000	-0.199946000	-0.539913000
H	-0.510851000	-2.375135000	-1.077034000	C	4.565889000	0.902877000	-2.246913000
H	-4.625732000	-2.706632000	0.114208000	C	2.450762000	-3.679383000	3.010308000
H	-3.692884000	-4.417497000	-1.093392000	C	4.104067000	-4.635784000	1.399843000
H	-1.399760000	-3.562126000	-2.950312000	C	1.663589000	-4.981999000	0.999128000
H	-3.123798000	-3.207153000	-3.207290000	H	-0.635242000	5.989495000	-2.115092000
H	-2.541140000	-4.894369000	-3.243162000	H	-2.082644000	5.873313000	-3.141963000
H	-0.656600000	-4.705657000	-0.729763000	H	-0.781203000	4.661746000	-3.289901000
H	-1.787937000	-6.031968000	-1.088741000	H	-2.174243000	6.015526000	-0.011752000
H	-1.894091000	-5.160642000	0.466423000	H	-3.361435000	4.710435000	0.219508000
H	-5.348388000	-1.200533000	1.939361000	H	-3.588086000	5.905907000	-1.085239000
H	-6.089033000	-0.642736000	-0.381653000	H	-3.626239000	2.864203000	-1.547050000
H	-5.408080000	0.991165000	-0.203721000	H	-2.575746000	2.850722000	-2.987205000
H	-6.788846000	0.488386000	0.807948000	H	-3.795499000	4.126214000	-2.786486000
H	-3.870889000	0.415545000	3.199052000	H	2.734721000	4.478424000	3.603274000
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B3LYP

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H	-4.531450000	6.064311000	4.103910000	H	5.302170000	-6.054929000	-1.665950000
H	-3.183650000	4.982451000	4.512060000	H	4.477130000	-7.298969000	-2.626810000
H	-5.489100000	4.302381000	0.925640000	H	2.040620000	-7.855439000	-2.163970000
H	-5.890000000	5.664371000	1.993240000	H	1.167360000	-7.010549000	-0.868920000
H	-2.332470000	7.125671000	3.552310000	H	3.586290000	-7.241379000	-0.290520000
H	-4.637390000	6.451281000	-0.026200000	H	4.050610000	-4.849299000	0.191800000
H	-4.324160000	7.665191000	2.139640000	H	2.346430000	-5.219429000	0.508140000
H	-2.835550000	7.699181000	1.173210000	H	2.174311000	5.932581000	0.191800000
H	-3.268278000	-7.241738000	-0.026200000	H	3.346943000	4.641783000	0.508140000
H	-3.846989000	-4.844921000	-0.361490000	H	1.003010000	4.531894000	-3.109320000
H	-2.092775000	-5.077389000	-0.458150000	H	0.778733000	5.868554000	-1.967940000
H	-0.981421000	-6.904890000	0.925640000	H	4.478073000	6.726508000	-0.290520000
H	-1.960489000	-7.933075000	1.993240000	H	3.662101000	2.758373000	-1.148950000
H	-4.476170000	-7.577428000	2.139640000	H	2.701116000	2.715369000	-2.640530000
H	-5.249911000	-6.305249000	1.173210000	H	2.592637000	7.619279000	-1.665950000
H	-4.627451000	-2.671660000	0.006110000	H	4.082528000	7.526793000	-2.626810000
H	-0.747761000	-6.173122000	3.299720000	H	2.138273000	6.612620000	-3.907550000
H	-1.312082000	-3.774880000	2.967550000	H	5.782700000	5.694949000	-2.163970000
H	-0.611242000	-4.479500000	1.495300000	H	5.487634000	4.516238000	-0.868920000
H	-2.276382000	0.787747000	-0.972770000	H	5.007427000	3.504821000	-3.098620000
H	-0.557326000	-2.366204000	1.353260000	H	4.407586000	5.624435000	-4.288440000
H	-5.004777000	-5.582814000	3.552310000	H	3.138569000	4.398537000	-4.490230000
H	-4.878809000	-3.860816000	1.775590000	H	-4.219872000	1.792286000	-1.148950000
H	-3.822294000	-3.419954000	3.128550000	H	-3.702136000	0.981551000	-2.640530000
H	-2.986122000	-6.956506000	4.103910000	H	-6.224921000	-1.083282000	0.191800000
H	-2.723104000	-5.248347000	4.512060000	H	-5.693373000	0.577646000	0.508140000
H	7.337247000	-1.542857000	3.552310000	H	-5.538977000	2.584149000	-3.098620000
H	5.782969000	-2.294765000	1.775590000	H	-4.426240000	-1.397315000	-3.109320000
H	4.872914000	-1.600227000	3.128550000	H	-5.471683000	-2.259874000	-1.967940000
H	8.800330000	-0.087763000	2.139640000	H	-7.823320000	2.160491000	-2.163970000
H	8.085461000	-1.393932000	1.173210000	H	-6.654994000	2.494311000	-0.868920000
H	7.517572000	0.892196000	4.103910000	H	-8.064364000	0.514871000	-0.290520000
H	5.906754000	0.265896000	4.512060000	H	-7.074697000	1.004864000	-4.288440000
H	4.627451000	-2.671660000	0.006110000	H	-5.378529000	0.518812000	-4.490230000
H	7.905668000	0.790457000	-0.026200000	H	-6.795834000	-1.454511000	-3.907550000
H	6.119319000	-0.909130000	-0.361490000	H	-7.894808000	-1.564350000	-1.665950000
H	5.443535000	0.726298000	-0.458150000	H	-8.559658000	-0.227824000	-2.626810000

Table S15. Radical monomers R-1• with C-PCM:cyclohexane.

H-1•				B3LYP-D3(BJ)			
B3LYP				B3LYP-D3(BJ)			
C	-0.004010000	4.307178000	0.005427000	H	-2.329657000	0.699405000	1.234155000
C	-0.996663000	3.600012000	-0.683838000	H	-4.465424000	-0.539046000	1.240133000
C	-0.999020000	2.206174000	-0.686651000	H	-4.673139000	-2.704562000	0.009750000
C	0.000000000	1.466289000	-0.004707000	H	-2.699121000	-3.605544000	-1.231082000
C	0.997743000	2.204276000	0.681372000	H	-0.562623000	-2.369203000	-1.243410000
C	0.991278000	3.597917000	0.689051000	H	4.472053000	-0.534735000	-1.231082000
C	-1.269844000	-0.733145000	-0.004707000	H	2.333102000	0.697356000	-1.243410000
C	-2.407830000	-0.238068000	0.681372000	H	0.559126000	-2.367245000	1.234155000
C	-3.611526000	-0.940487000	0.689051000	H	2.699539000	-3.597648000	1.240133000
C	-3.728121000	-2.157062000	0.005427000	H	4.678789000	-2.694776000	0.009750000
C	-2.619370000	-2.663142000	-0.683838000	C	-0.004917000	4.296865000	0.006150000
C	-1.411093000	-1.968263000	-0.686651000	C	-1.006721000	3.590478000	-0.670055000
C	3.616034000	-0.936871000	-0.683838000	C	-1.008149000	2.197761000	-0.674210000
C	2.410113000	-0.237910000	-0.686651000	C	0.000000000	1.461255000	-0.005351000
C	1.269844000	-0.733145000	-0.004707000	C	1.006337000	2.195937000	0.668266000
C	1.410088000	-1.966209000	0.681372000	C	0.999950000	3.588521000	0.675921000
C	2.620249000	-2.657430000	0.689051000	C	-1.265484000	-0.730627000	-0.005351000
C	3.732131000	-2.150116000	0.005427000	C	-2.404906000	-0.226455000	0.668266000
C	0.000000000	0.000000000	-0.006735000	C	-3.607725000	-0.928279000	0.675921000
H	-0.005650000	5.399338000	0.009750000	C	-3.718736000	-2.152691000	0.006150000
H	-1.772932000	4.140279000	-1.231082000	C	-2.606085000	-2.667085000	-0.670055000
H	-1.770479000	1.671848000	-1.243410000	C	-1.399324000	-1.971963000	-0.674210000
H	1.770531000	1.667840000	1.234155000	C	3.612806000	-0.923393000	-0.670055000
H	1.765885000	4.136693000	1.240133000	C	2.407391000	-0.225798000	-0.674210000
				C	1.265484000	-0.730627000	-0.005351000

C	1.398569000	-1.969482000	0.668266000	H	-1.760514000	1.661232000	-1.250226000
C	2.607775000	-2.660242000	0.675921000	H	1.761907000	1.660501000	1.245711000
C	3.723653000	-2.144174000	0.006150000	H	-2.318990000	0.695605000	1.245711000
C	0.000000000	0.000000000	-0.007596000	H	-4.655319000	-2.699398000	0.012870000
H	-0.006898000	5.388621000	0.011083000	H	-0.558412000	-2.355266000	-1.250226000
H	-1.790033000	4.131142000	-1.205907000	H	2.318926000	0.694034000	-1.250226000
H	-1.784513000	1.660025000	-1.219698000	H	0.557083000	-2.356107000	1.245711000
H	1.784507000	1.656180000	1.209165000	H	4.665407000	-2.681925000	0.012870000
H	1.781211000	4.127762000	1.216223000	H	-1.932507000	4.211658000	-2.562378000
H	-2.326548000	0.717338000	1.209165000	H	-2.030917000	5.429127000	-1.268894000
H	-4.465352000	-0.521307000	1.216223000	H	-3.074779000	3.984773000	-1.227329000
H	-4.663234000	-2.700285000	0.011083000	H	1.599271000	5.009938000	2.243239000
H	-2.682657000	-3.615785000	-1.205907000	H	2.631228000	5.023397000	0.803010000
H	-0.545368000	-2.375446000	-1.219698000	H	2.761600000	3.687444000	1.973785000
H	4.472690000	-0.515357000	-1.205907000	H	-5.138369000	-1.119959000	2.243239000
H	2.329881000	0.715421000	-1.219698000	H	-5.666004000	-0.232988000	0.803010000
H	0.542041000	-2.373519000	1.209165000	H	-4.574220000	0.547894000	1.973785000
H	2.684141000	-3.606455000	1.216223000	H	-2.681150000	-3.779429000	-2.562378000
H	4.670132000	-2.688337000	0.011083000	H	-3.686303000	-4.473389000	-1.268894000

M06-2X

C	-0.009750000	4.288822000	0.012618000	H	4.988304000	0.670450000	-1.227329000
C	-1.012910000	3.586257000	-0.657696000	H	3.539098000	-3.889978000	2.243239000
C	-1.011871000	2.195859000	-0.667674000	H	3.034776000	-4.790409000	0.803010000
C	0.000000000	1.462601000	-0.011210000	H	1.812620000	-4.235338000	1.973785000

B3LYP-D3(BJ)

C	1.008043000	2.191642000	0.655737000	symmetry c3			
C	0.999108000	3.581961000	0.669554000	C	0.006897000	4.277324000	-0.006857000
C	-1.266649000	-0.731300000	-0.011210000	C	1.018470000	3.592326000	0.676755000
C	-2.402039000	-0.222830000	0.655737000	C	1.006558000	2.193059000	0.673134000
C	-3.601623000	-0.925728000	0.669554000	C	0.000000000	1.461710000	0.006723000
C	-3.709354000	-2.152854000	0.012618000	C	-1.008356000	2.193915000	-0.668262000
C	-2.599294000	-2.670405000	-0.657696000	C	-1.013502000	3.587115000	-0.685942000
C	-1.395734000	-1.974236000	-0.667674000	C	1.265878000	-0.730855000	0.006723000
C	3.612285000	-0.915853000	-0.657696000	C	2.404164000	-0.223696000	-0.668262000
C	2.407605000	-0.221623000	-0.667674000	C	3.613284000	-0.915839000	-0.685942000
C	1.266649000	-0.731300000	-0.011210000	C	3.700823000	-2.144635000	-0.006857000
C	1.393996000	-1.968812000	0.655737000	C	2.601811000	-2.678184000	0.676755000
C	2.602515000	-2.656234000	0.669554000	C	1.395966000	-1.968235000	0.673134000
C	3.719104000	-2.135968000	0.012618000	C	-3.620281000	-0.914142000	0.676755000
C	0.000000000	0.000000000	-0.016349000	C	-2.402524000	-0.224825000	0.673134000
H	-0.013320000	5.379321000	0.022898000	C	-1.265878000	-0.730855000	0.006723000
H	-1.801381000	4.126989000	-1.183462000	C	-1.395808000	-1.970219000	-0.668262000
H	-1.793448000	1.657704000	-1.206270000	C	-2.599782000	-2.671276000	-0.685942000
H	1.792714000	1.650611000	1.186787000	C	-3.707720000	-2.132689000	-0.006857000
H	1.783454000	4.119209000	1.204777000	C	0.000000000	0.000000000	0.007022000
H	-2.325828000	0.727230000	1.186787000	C	2.098217000	4.337646000	1.423566000
H	-4.459067000	-0.515088000	1.204777000	C	-2.084153000	4.352231000	-1.424652000
H	-4.651969000	-2.701196000	0.022898000	C	4.811219000	-0.371186000	-1.424652000
H	-2.673387000	-3.623536000	-1.183462000	C	2.707403000	-3.985933000	1.423566000
H	-0.538890000	-2.382024000	-1.206270000	C	-4.805621000	-0.351714000	1.423566000
H	4.474768000	-0.503453000	-1.183462000	C	-2.727066000	-3.981045000	-1.424652000
H	2.332338000	0.724320000	-1.206270000	H	0.010081000	5.371015000	-0.013414000
H	0.533114000	-2.377841000	1.186787000	H	1.782784000	1.651722000	1.216665000
H	2.675612000	-3.604121000	1.204777000	H	-1.784467000	1.649737000	-1.208234000
H	4.665289000	-2.678125000	0.022898000	H	2.320947000	0.720525000	-1.208234000

Me-1•

B3LYP

C	-0.006662000	4.287189000	0.006765000	H	4.646395000	-2.694238000	-0.013414000
C	-1.004004000	3.602184000	-0.699047000	H	0.539041000	-2.369798000	1.216665000
C	-0.993409000	2.201336000	-0.691426000	H	-2.321826000	0.718075000	1.216665000
C	0.000000000	1.467202000	-0.005013000	H	-0.536481000	-2.370262000	-1.208234000
C	0.995313000	2.202665000	0.688949000	H	-4.656476000	-2.676777000	-0.013414000
C	0.999515000	3.597351000	0.708605000	H	2.010938000	4.176988000	2.511443000
C	-1.270634000	-0.733601000	-0.005013000	H	2.043519000	5.420259000	1.238347000
C	-2.405220000	-0.239366000	0.688949000	H	3.100939000	3.989299000	1.127207000
C	-3.615155000	-0.933070000	0.708605000	H	-1.647310000	4.996199000	-2.206017000
C	-3.709484000	-2.149364000	0.006765000	H	-2.643616000	5.012243000	-0.740753000
C	-2.617581000	-2.670585000	-0.699047000	H	-2.803564000	3.674202000	-1.906083000
C	-1.409709000	-1.960986000	-0.691426000	H	5.150490000	-1.071487000	-2.206017000
C	3.621585000	-0.931599000	-0.699047000	H	5.662538000	-0.216683000	-0.740753000
C	2.403118000	-0.240350000	-0.691426000	H	4.583735000	0.590857000	-1.906083000
C	1.270634000	-0.733601000	-0.005013000	H	2.611909000	-3.830018000	2.511443000
C	1.409908000	-1.963299000	0.688949000	H	3.672323000	-4.479869000	1.238347000
C	2.615640000	-2.664281000	0.708605000	H	1.904364000	-4.680141000	1.127207000
C	3.716146000	-2.137825000	0.006765000	H	-4.622847000	-0.346971000	2.511443000
C	0.000000000	0.000000000	-0.004517000	H	-5.715842000	-0.940390000	1.238347000
C	-2.064450000	4.349161000	-1.475296000	H	-5.005304000	0.690843000	1.127207000
C	2.053671000	4.364080000	1.473005000	H	-3.503180000	-3.924712000	-2.206017000
C	-4.806240000	-0.403509000	1.473005000	H	-3.018922000	-4.795560000	-0.740753000
C	-2.734259000	-3.962447000	-1.475296000	H	-1.780170000	-4.265059000	-1.906083000
C	4.798709000	-0.386714000	-1.475296000	M06-2X			
C	2.752569000	-3.960571000	1.473005000	C	0.000000000	4.269860000	-0.009813000
H	-0.010088000	5.381323000	0.012870000				

B3LYP-D3(BJ)

C	4.802300000	-0.365233000	-1.516549000			
C	2.788475000	-3.981117000	1.517091000			
C	-4.841986000	-0.424332000	1.517091000			
C	-2.717451000	-3.976297000	-1.516549000			
C	1.343952000	5.287149000	2.571361000	C	-0.007040000	4.266470000
C	2.838302000	5.310159000	0.538831000	C	1.033940000	3.586060000
C	3.063341000	3.503788000	2.250091000	C	1.018740000	2.194200000
C	-1.963719000	3.958761000	-3.010089000	C	-0.003150000	1.461180000
C	-1.961718000	5.871961000	-1.402749000	C	-1.019820000	2.185630000
C	-3.482559000	3.932631000	-0.996529000	C	-1.041340000	3.585840000
C	4.410247000	-0.278750000	-3.010089000	C	1.266994000	-0.727862000
C	6.066126000	-1.237083000	-1.402749000	C	2.402721000	-0.209625000
C	5.147038000	1.049669000	-0.996529000	C	3.626099000	-0.891093000
C	3.906830000	-3.807471000	2.571361000	C	3.698392000	-2.127138000
C	3.179581000	-5.113121000	0.538831000	C	2.588649000	-2.688448000
C	1.502699000	-4.404825000	2.250091000	C	1.390863000	-1.979355000
C	-5.250781000	-1.479678000	2.571361000	C	-3.622589000	-0.897612000
C	-6.017883000	-0.197038000	0.538831000	C	-2.409603000	-0.214845000
C	-4.566040000	0.901037000	2.250091000	C	-1.263844000	-0.733318000
C	-2.446528000	-3.680011000	-3.010089000	C	-1.382901000	-1.976005000
C	-4.104408000	-4.634878000	-1.402749000	C	-2.584759000	-2.694747000
C	-1.664479000	-4.982300000	-0.996529000	C	-3.691351000	-2.139332000
H	0.636602000	5.993069000	2.109381000	C	0.000000000	0.000000000
H	2.083422000	5.877969000	3.137511000	C	2.142040000	4.394990000
H	0.781231000	4.667999000	3.288861000	C	-2.181490000	4.312290000
H	2.177682000	6.014129000	0.009531000	C	4.825298000	-0.266919000
H	3.364581000	4.706998000	-0.218749000	C	2.735153000	-4.052556000
H	3.590432000	5.903948000	1.084731000	C	-4.877193000	-0.342434000
H	3.625541000	2.863548000	1.552341000	C	-2.643808000	-4.045371000
H	2.572141000	2.853349000	2.990871000	C	1.516440000	5.338960000
H	3.793211000	4.128158000	2.789531000	C	2.890230000	5.227790000
H	-2.737609000	4.475221000	-3.602399000	C	3.163170000	3.493530000
H	-2.088919000	2.876401000	-3.167129000	C	-2.134340000	3.949600000
H	-0.978489000	4.245930000	-3.412049000	C	-2.080820000	5.839510000
H	-2.758948000	6.352111000	-1.992009000	C	-3.533610000	3.862450000
H	-0.997888000	6.237870000	-1.790449000	C	4.487624000	-0.126407000
H	-2.065778000	6.216851000	-0.361739000	C	6.097574000	-1.117712000
H	-4.270999000	4.452122000	-1.566419000	C	5.111785000	1.128971000
H	-3.599849000	4.197801000	0.066941000	C	3.865455000	-3.982756000
H	-3.657369000	2.850251000	-1.095689000	C	3.082284000	-5.116908000
H	5.244459000	0.133228000	-3.602399000	C	1.443901000	-4.486151000
H	3.535496000	0.370857000	-3.167129000	C	-5.381895000	-1.356204000
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Ad-1•

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M06-2X

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C	1.265217000	-0.733960000	0.019140000	H	4.286959000	1.735931000	1.295130000
C	5.864394000	1.505929000	2.771750000	H	6.734125000	2.393587000	0.986930000
C	4.602708000	1.003084000	2.057880000	H	7.913115000	2.027057000	2.265210000
C	7.006704000	1.654707000	1.759380000	H	2.818350000	-6.615050000	-4.400010000
C	2.682660000	-5.660580000	-3.864820000	H	2.360900000	-4.910680000	-4.606290000
C	4.004830000	-5.226680000	-3.219230000	H	4.775880000	-5.106450000	-3.996260000
C	3.805640000	-3.888070000	-2.496230000	H	3.496200000	-3.107980000	-3.212210000
C	1.613080000	-5.816290000	-2.775940000	H	4.759650000	-3.559220000	-2.052410000
C	1.420430000	-4.476410000	-2.053250000	H	0.658330000	-6.115350000	-3.235510000
C	2.731990000	-4.014650000	-1.391120000	H	0.631020000	-4.575100000	-1.288020000
C	4.453100000	-6.289920000	-2.206980000	H	1.080570000	-3.714970000	-2.774830000
C	2.058550000	-6.885880000	-1.771050000	H	5.410830000	-5.992780000	-1.747710000
C	3.379190000	-6.452940000	-1.122160000	H	4.619960000	-7.251780000	-2.719620000
C	3.177160000	-5.114150000	-0.398720000	H	2.187380000	-7.854040000	-2.283060000
C	2.840404000	5.308576000	-0.398720000	H	1.284790000	-7.023680000	-0.996940000
C	2.110794000	4.373298000	-1.391120000	H	3.701180000	-7.211940000	-0.392280000
C	1.464347000	5.239816000	-2.496230000	H	4.116150000	-4.814440000	0.094640000
C	3.898815000	6.152935000	-1.122160000	H	2.413610000	-5.215550000	0.391680000
C	3.166470000	3.468334000	-2.053250000	H	2.111352000	5.971911000	0.094640000
C	3.220680000	7.001458000	-2.206980000	H	3.309994000	4.698023000	0.391680000
C	2.524022000	6.081625000	-3.219230000	H	0.943489000	4.581788000	-3.212210000
C	4.934072000	5.225697000	-1.771050000	H	5.901588000	5.901588000	-2.052410000
C	4.230515000	4.305114000	-2.775940000	H	4.395133000	6.811286000	-0.392280000
C	3.560876000	5.153542000	-3.864820000	H	3.646643000	2.834030000	-1.288020000
C	-4.586900000	1.008076000	-2.053250000	H	2.676973000	2.793286000	-2.774830000
C	-4.842784000	-0.358648000	-1.391120000	H	2.484484000	7.682306000	-1.747710000
				H	3.970245000	7.626893000	-2.719620000
				H	2.034375000	6.689259000	-3.996260000
				H	5.708108000	5.821347000	-2.283060000

H	5.440290000	4.624501000	-0.996940000	H	-5.462200000	-2.342368000	-2.052410000
H	4.966883000	3.627806000	-3.235510000	H	-7.895488000	2.032693000	-2.283060000
H	4.319626000	5.748288000	-4.400010000	H	-6.725080000	2.399179000	-0.996940000
H	3.072323000	4.499940000	-4.606290000	H	-8.096313000	0.400654000	-0.392280000
H	-4.277663000	1.741070000	-1.288020000	H	-7.137976000	0.866762000	-4.400010000
H	-3.757543000	0.921684000	-2.774830000	H	-5.433224000	0.410740000	-4.606290000
H	-6.227502000	-1.157471000	0.094640000	H	-6.810255000	-1.582809000	-3.996260000
H	-5.723604000	0.517527000	0.391680000	H	-7.895315000	-1.689527000	-1.747710000
H	-5.625214000	2.487544000	-3.235510000	H	-8.590206000	-0.375113000	-2.719620000
H	-4.439690000	-1.473808000	-3.212210000				

Dimers

Table S16. Dimers R-1₂ in gas phase.

H-1 ₂			B3LYP			M06-2X					
C	-2.228037000	3.438986000	2.543080000	C	-2.895756000	1.671866000	2.826882000	C	1.855256000	3.692895000	2.370669000
C	-1.198184000	3.636963000	1.619150000	C	1.418026000	0.331350000	1.405227000	C	2.560400000	2.837163000	1.524637000
C	-0.497253000	2.552231000	1.089870000	C	2.550874000	-0.432847000	1.054752000	C	1.981792000	1.659495000	1.063183000
C	-0.807850000	1.218562000	1.436900000	C	3.821829000	-0.125509000	1.537696000	C	0.660911000	1.297758000	1.399596000
C	-1.819381000	1.050420000	2.400150000	C	4.010234000	0.943507000	2.417917000	C	0.000000000	2.139032000	2.304112000
C	-2.521048000	2.135936000	2.939160000	C	2.895756000	1.671866000	2.826882000	C	0.580305000	3.320115000	2.774856000
C	1.459231000	0.090338000	1.436900000	C	1.622945000	1.362969000	2.334568000	C	0.793436000	-1.221244000	1.399596000
C	2.458924000	-0.845482000	1.089870000	C	0.000000000	-3.343731000	2.826882000	C	0.446268000	-2.546030000	1.063183000
C	3.748795000	-0.780824000	1.619150000	C	0.368893000	-2.086996000	2.334568000	C	1.176856000	-3.635953000	1.524637000
C	4.092268000	0.210044000	2.543080000	C	1.622945000	1.362969000	2.334568000	C	2.270513000	-3.453146000	2.370669000
C	3.110299000	1.115324000	2.939160000	C	0.000000000	-1.393722000	1.405227000	C	2.585151000	-2.162617000	2.774856000
C	1.819381000	1.050420000	2.400150000	C	-1.650294000	-1.992698000	1.054752000	C	1.852456000	-1.069516000	2.304112000
C	-0.589251000	-3.251260000	2.939160000	C	-2.019608000	-3.247047000	1.537696000				
C	0.000000000	-2.100840000	2.400150000	C	-1.188016000	-3.944718000	2.417917000				
C	-0.651380000	-1.308900000	1.436900000	C	0.000000000	0.000000000	0.850251000				
C	-1.961670000	-1.706750000	1.089870000	C	2.822218000	-3.001211000	-2.417917000				
C	-2.550611000	-2.856140000	1.619150000	C	2.895756000	-1.671866000	-2.826882000				
C	-1.864231000	-3.649030000	2.543080000	C	1.991839000	-0.724027000	-2.334568000				
C	0.000000000	0.000000000	0.864810000	C	0.995971000	-1.062371000	-1.405227000				
C	2.228037000	-3.438986000	-2.543080000	C	0.900580000	-2.425545000	-1.054752000				
C	2.521048000	-2.135936000	-2.939160000	C	1.802221000	-3.372556000	-1.537696000				
C	1.819381000	-1.050420000	-2.400150000	C	0.422055000	1.393722000	-1.405227000				
C	0.807850000	-1.218562000	-1.436900000	C	1.650294000	1.992698000	-1.054752000				
C	0.497253000	-2.552231000	-1.089870000	C	2.019608000	3.247047000	-1.537696000				
C	1.198184000	-3.636963000	-1.619150000	C	1.188016000	3.944718000	-2.417917000				
C	0.651380000	1.308900000	-1.436900000	C	0.000000000	3.343731000	-2.826882000				
C	1.961670000	1.706750000	-1.089870000	C	-0.368893000	2.086996000	-2.334568000				
C	2.550611000	2.856140000	-1.619150000	C	-2.895756000	-1.671866000	-2.826882000				
C	1.864231000	3.649030000	-2.543080000	C	-1.622945000	-1.362969000	-2.334568000				
C	0.589251000	3.251260000	-2.939160000	C	-1.418026000	-0.331350000	-1.405227000				
C	0.000000000	2.100840000	-2.400150000	C	-2.550874000	0.432847000	-1.054752000				
C	-3.110299000	-1.115324000	-2.939160000	C	-3.821829000	0.125509000	-1.537696000				
C	-1.819381000	-1.050420000	-2.400150000	C	-4.010234000	-0.943507000	-2.417917000				
C	-1.459231000	-0.090338000	-1.436900000	C	0.000000000	0.000000000	-0.850251000				
C	-2.458924000	0.845482000	-1.089870000	H	-3.532634000	3.741198000	2.792385000				
C	-3.748795000	0.780824000	-1.619150000	H	-1.696561000	4.413188000	1.223392000				
C	-4.092268000	-0.210044000	-2.543080000	H	-0.109155000	2.768038000	0.399198000				
C	0.000000000	0.000000000	-0.864810000	H	-2.082027000	-0.297879000	2.690825000				
H	-2.777916000	4.287287000	2.957110000	H	-3.661725000	1.355379000	3.538310000				
H	-0.923981000	4.647937000	1.308070000	H	2.451769000	-1.289488000	0.399198000				
H	0.314513000	2.763191000	0.402090000	H	4.670213000	-0.737329000	1.223392000				
H	-2.079463000	0.056744000	2.754520000	H	5.006289000	1.188752000	2.792385000				
H	-3.302601000	1.946827000	3.679100000	H	3.004655000	2.493458000	3.538310000				
H	2.235737000	-1.653972000	0.402090000	H	0.783043000	1.952028000	2.690825000				
H	4.487222000	-1.523777000	1.308070000	H	0.657070000	-3.848837000	3.538310000				
H	5.101857000	0.262103000	2.957110000	H	1.298984000	-1.654149000	2.690825000				
H	3.337302000	1.886723000	3.679100000	H	-2.342614000	-1.478550000	0.399198000				
H	1.088874000	1.772496000	2.754520000	H	-2.973653000	-3.675859000	1.223392000				
H	-0.034701000	-3.833550000	3.679100000	H	-1.473655000	-4.929949000	2.792385000				
H	0.990590000	-1.829240000	2.754520000	H	3.532634000	-3.741198000	-2.792385000				
H	-2.550250000	-1.109220000	0.402090000	H	3.661725000	-1.355379000	-3.538310000				
H	-3.563241000	-3.124159000	1.308070000	H	2.082027000	0.297879000	-2.690825000				
H	-2.323941000	-4.549390000	2.957110000	H	0.109155000	-2.768038000	-0.399198000				
H	2.777916000	-4.287287000	-2.957110000	H	1.696561000	-4.413188000	-1.223392000				
H	3.302601000	-1.946827000	-3.679100000	H	2.342614000	1.478550000	-0.399198000				
H	2.079463000	-0.056744000	-2.754520000	H	2.973653000	3.675859000	-1.223392000				
H	-0.314513000	-2.763191000	-0.402090000	H	-1.473655000	4.929949000	-2.792385000				
H	0.923981000	-4.647937000	-1.308070000	H	-0.657070000	3.848837000	-3.538310000				
H	2.550250000	1.109220000	-0.402090000	H	-1.298984000	1.654149000	-2.690825000				
H	3.563241000	3.124159000	-1.308070000	H	-3.004655000	-2.493458000	-3.538310000				
H	2.323941000	4.549390000	-2.957110000	H	-0.783043000	-1.952028000	-2.690825000				
H	0.034701000	3.833550000	-3.679100000	H	-2.451769000	1.289488000	-0.399198000				
H	-0.990590000	1.829240000	-2.754520000	H	-4.670213000	0.737329000	-1.223392000				
H	-3.337302000	-1.886723000	-3.679100000	H	-5.006289000	-1.188752000	-2.792385000				
H	-1.088874000	-1.772496000	-2.754520000								
H	-2.235737000	1.653972000	-0.402090000								
H	-4.487222000	1.523777000	-1.308070000								
H	-5.101857000	-0.262103000	-2.957110000								
B3LYP-D3(BJ)			M06-2X								
C	-2.822218000	3.001211000	2.417917000	C	1.855256000	3.692895000	2.370669000				
C	-1.802221000	3.372556000	1.537696000	C	2.560400000	2.837163000	1.524637000				
C	-0.900580000	2.425545000	1.054752000	C	1.981792000	1.659495000	1.063183000				
C	-0.995971000	1.062371000	1.405227000	C	0.660911000	1.297758000	1.399596000				
C	-1.991839000	0.724027000	2.334568000	C	0.000000000	2.139032000	2.304112000				

C	-3.165457000	-1.157498000	2.774856000	C	-1.037555000	3.693831000	-1.607861000
C	-1.852456000	-1.069516000	2.304112000	C	-2.062590000	3.511758000	-2.550822000
C	-1.454346000	-0.076513000	1.399596000	C	-2.416429000	2.231453000	-2.973349000
C	-2.428061000	0.886535000	1.063183000	C	-1.753757000	1.121832000	-2.415530000
C	-3.737256000	0.798790000	1.524637000	C	-0.724280000	-3.208416000	-2.973349000
C	-4.125769000	-0.239749000	2.370669000	C	-0.094656000	-2.079714000	-2.415530000
C	0.000000000	0.000000000	0.845722000	C	-0.706332000	-1.280032000	-1.440499000
C	-1.855256000	-3.692895000	-2.370669000	C	-2.028129000	-1.628449000	-1.079978000
C	-0.580305000	-3.320115000	-2.774856000	C	-2.680174000	-2.745464000	-1.607861000
C	0.000000000	-2.139032000	-2.304112000	C	-2.009977000	-3.542134000	-2.550822000
C	-0.660911000	-1.297758000	-1.399596000	C	0.000000000	0.000000000	-0.864097000
C	-1.981792000	-1.659495000	-1.063183000	C	-4.719805000	1.998012000	1.184939000
C	-2.560400000	-2.837163000	-1.524637000	C	-3.490631000	-2.015317000	4.014287000
C	1.454346000	0.076513000	-1.399596000	C	4.090232000	3.088465000	1.184939000
C	2.428061000	-0.886535000	-1.063183000	C	0.000000000	4.030634000	4.014287000
C	3.737256000	-0.798790000	-1.524637000	C	3.490631000	-2.015317000	4.014287000
C	4.125769000	0.239749000	-2.370669000	C	0.629573000	-5.086477000	1.184939000
C	3.165457000	1.157498000	-2.774856000	C	3.490631000	2.015317000	-4.014287000
C	1.852456000	1.069516000	-2.304112000	C	4.719805000	-1.998012000	-1.184939000
C	-2.585151000	2.162617000	-2.774856000	C	-0.629573000	5.086477000	-1.184939000
C	-1.852456000	1.069516000	-2.304112000	C	-3.490631000	2.015317000	-4.014287000
C	-0.793436000	1.221244000	-1.399596000	C	0.000000000	-4.030634000	-4.014287000
C	-0.446268000	2.546030000	-1.063183000	C	-4.090232000	-3.088465000	-1.184939000
C	-1.176856000	3.635953000	-1.524637000	H	-5.083342000	-0.038010000	2.970549000
C	-2.270513000	3.453146000	-2.370669000	H	-2.165570000	1.727112000	0.377290000
C	0.000000000	0.000000000	-0.845722000	H	-1.140145000	-1.702370000	2.771309000
H	2.305711000	4.620604000	2.726166000	H	2.578508000	1.011882000	0.377290000
H	3.580109000	3.079018000	1.221401000	H	2.508753000	4.421308000	2.970549000
H	2.592070000	1.012755000	0.440650000	H	-0.904223000	1.838579000	2.771309000
H	-0.993940000	1.890026000	2.665372000	H	2.044368000	-0.136210000	2.771309000
H	0.016790000	3.946364000	3.467955000	H	-0.412938000	-2.738995000	0.377290000
H	-0.418963000	-2.751176000	0.440650000	H	2.574589000	-4.383298000	2.970549000
H	0.876453000	-4.639974000	1.221401000	H	5.083342000	0.038010000	-2.970549000
H	2.848705000	-4.307106000	2.726166000	H	1.140145000	1.702370000	-2.771309000
H	3.409257000	-1.987723000	3.467955000	H	2.165570000	-1.727112000	-0.377290000
H	2.133780000	-0.084236000	2.665372000	H	0.412938000	2.738995000	-0.377290000
H	-3.426047000	-1.958642000	3.467955000	H	-2.574589000	4.383298000	-2.970549000
H	-1.139841000	-1.805790000	2.665372000	H	-2.044368000	0.136210000	-2.771309000
H	-2.173106000	1.738421000	0.440650000	H	0.904223000	-1.838579000	-2.771309000
H	-4.456562000	1.560956000	1.221401000	H	-2.578508000	-1.011882000	-0.377290000
H	-5.154416000	-0.313498000	2.726166000	H	-2.508753000	-4.421308000	-2.970549000
H	-2.305711000	-4.620604000	-2.726166000	H	-4.306232000	2.662794000	0.412784000
H	-0.016790000	-3.946364000	-3.467955000	H	-5.030981000	2.622625000	2.040012000
H	0.993940000	-1.890026000	-2.665372000	H	-5.635319000	1.536095000	0.777947000
H	-2.592070000	-1.012755000	-0.440650000	H	-4.530827000	-1.910360000	4.357355000
H	-3.580109000	-3.079018000	-1.221401000	H	-2.834254000	-1.932567000	4.897117000
H	2.173106000	-1.738421000	-0.440650000	H	-3.366388000	-3.037787000	3.619517000
H	4.456562000	-1.560956000	-1.221401000	H	4.459163000	2.397910000	0.412784000
H	5.154416000	0.313498000	-2.726166000	H	4.786750000	3.045645000	2.040012000
H	3.426047000	1.958642000	-3.467955000	H	4.147957000	4.112281000	0.777947000
H	1.139841000	1.805790000	-2.665372000	H	0.610993000	4.878992000	4.357355000
H	-3.409257000	1.987723000	-3.467955000	H	-0.256525000	3.420819000	4.897117000
H	-2.133780000	0.084236000	-2.665372000	H	-0.947607000	4.434271000	3.619517000
H	0.418963000	2.751176000	-0.440650000	H	3.919834000	-2.968631000	4.357355000
H	-0.876453000	4.639974000	-1.221401000	H	3.090779000	-1.488252000	4.897117000
H	-2.848705000	4.307106000	-2.726166000	H	4.313995000	-1.396484000	3.619517000

Me-1₂

B3LYP

C	-4.072567000	-0.030376000	2.550822000	C	-4.161896000	-0.052619000	2.231077000
C	-3.717729000	0.948367000	1.607861000	C	-3.707999000	0.999915000	1.420453000
C	-2.424343000	0.942186000	1.079978000	C	-2.369296000	1.023440000	1.032092000
C	-1.461706000	-0.028315000	1.440499000	C	-1.460329000	0.006453000	1.394620000
C	-1.848413000	-0.957882000	2.415530000	C	-1.935199000	-0.981774000	2.262330000
C	-3.140710000	-0.976962000	2.973349000	C	-3.277037000	-1.032888000	2.677539000
C	0.706332000	1.280032000	1.440499000	C	0.735753000	1.261455000	1.394620000
C	2.028129000	1.628449000	1.079978000	C	2.070973000	1.540150000	1.032092000
C	2.680174000	2.745464000	1.607861000				
C	2.009977000	3.542134000	2.550822000				
C	0.724280000	3.208416000	2.973349000				
C	0.094656000	2.079714000	2.415530000				
C	2.416429000	-2.231453000	2.973349000				
C	1.753757000	-1.121832000	2.415530000				
C	0.755375000	-1.251717000	1.440499000				
C	0.396214000	-2.570636000	1.079978000				
C	1.037555000	-3.693831000	1.607861000				
C	2.062590000	-3.511758000	2.550822000				
C	0.000000000	0.000000000	0.864097000				
C	4.072567000	0.030376000	-2.550822000				
C	3.140710000	0.976962000	-2.973349000				
C	1.848413000	0.957882000	-2.415530000				
C	1.461706000	0.028315000	-1.440499000				
C	2.424343000	-0.942186000	-1.079978000				
C	3.717729000	-0.948367000	-1.607861000				
C	-0.755375000	1.251717000	-1.440499000				
C	-0.396214000	2.570636000	-1.079978000				

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H	0.621276000	5.209857000	3.774729000	C	3.477406000	-1.465311000	4.344258000
H	-0.322593000	3.858899000	4.448909000	C	2.658147000	-1.005160000	5.564625000
H	-0.905991000	4.709632000	3.008658000	C	4.550033000	-0.425836000	3.979414000
H	4.201231000	-3.142970000	3.774729000	C	1.402797000	-4.976091000	1.365016000
H	3.503202000	-1.650076000	4.448909000	C	2.456897000	-5.385892000	0.319308000
H	4.531656000	-1.570205000	3.008658000	C	0.000000000	-5.381736000	0.899388000
H	-0.314830000	-4.984425000	0.238909000	C	-5.010819000	1.273188000	1.365016000
H	0.116682000	-5.650043000	1.835824000	C	-4.660720000	2.690868000	0.899388000
H	1.310042000	-5.656544000	0.525940000	C	-5.892768000	0.565211000	0.319308000
H	3.180608000	2.208824000	-4.448909000	C	-3.007700000	-2.278866000	4.344258000
H	4.822507000	2.066888000	-3.774729000	C	-2.199568000	-1.799443000	5.564625000
H	3.625666000	3.139427000	-3.008658000	C	-2.643801000	-3.727526000	3.979414000
H	5.553731000	-1.693743000	-0.525940000	C	3.007700000	2.278866000	-4.344258000
H	4.951421000	-2.723972000	-1.835824000	C	2.199568000	1.799443000	-5.564625000
H	4.159224000	-2.764863000	-0.238909000	C	2.643801000	3.727526000	-3.979414000
H	-1.310042000	5.656544000	-0.525940000	C	5.010819000	-1.273188000	-1.365016000
H	-0.116682000	5.650043000	-1.835824000	C	5.892768000	-0.565211000	-0.319308000
H	0.314830000	4.984425000	-0.238909000	C	4.660720000	-2.690868000	-0.899388000
H	-3.503202000	1.650076000	-4.448909000	H	-4.896098000	-0.617245000	3.286210000
H	-4.201231000	3.142970000	-3.774729000	H	-2.446034000	1.303472000	0.337024000
H	-4.531656000	1.570205000	-3.008658000	H	-0.797706000	-1.774400000	2.845219000
H	0.322593000	-3.858899000	-4.448909000	H	2.351856000	1.466591000	0.337024000
H	-0.621276000	-5.209857000	-3.774729000	H	1.913499000	4.548767000	3.286210000
H	0.905991000	-4.709632000	-3.008658000	H	-1.137822000	1.578033000	2.845219000
H	-4.243690000	-3.962801000	-0.525940000	H	1.935528000	0.196366000	2.845219000
H	-4.834740000	-2.926071000	-1.835824000	H	0.094177000	-2.770063000	0.337024000
H	-4.474054000	-2.219562000	-0.238909000	H	2.982598000	-3.931523000	3.286210000

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C	-3.935112000	-0.521870000	2.770405000	H	0.797706000	1.774400000	-2.845219000
C	-3.797856000	0.421377000	1.739988000	H	2.446034000	-1.303472000	-0.337024000
C	-2.554958000	0.545727000	1.104413000	H	-0.094177000	2.770063000	-0.337024000
C	-1.440164000	-0.248990000	1.458320000	H	-2.982598000	3.931523000	-3.286210000
C	-1.630718000	-1.167191000	2.504357000	H	-1.935528000	-0.196366000	-2.845219000
C	-2.860859000	-1.316498000	3.169400000	H	1.137822000	-1.578033000	-2.845219000
C	0.504450000	1.371713000	1.458320000	H	-2.351856000	-1.466591000	-0.337024000
C	1.750093000	1.939795000	1.104413000	H	-1.913499000	-4.548767000	-3.286210000
C	2.263851000	3.078351000	1.739988000	H	-3.991556000	-4.178149000	-2.286228000
C	1.515603000	3.668842000	2.770405000	H	-3.053520000	-4.410317000	0.629618000
C	0.290309000	3.135825000	3.169400000	H	-2.727278000	-5.590831000	-0.661577000
C	-0.195458000	1.995839000	2.504357000	H	-4.401489000	-5.312763000	-0.113464000
C	2.570550000	-1.819328000	3.169400000	H	-4.388937000	-2.230174000	0.063304000
C	1.826176000	-0.828647000	2.504357000	H	-5.633153000	-3.190812000	-0.759295000
C	0.935713000	-1.122723000	1.458320000	H	-4.798658000	-1.881973000	-1.632970000
C	0.804865000	-2.485522000	1.104413000	H	-0.072895000	-4.662617000	-4.629939000
C	1.534005000	-3.499728000	1.739988000	H	1.920287000	-4.849365000	-3.125754000
C	2.419509000	-3.146972000	2.770405000	H	2.519358000	-3.277353000	-3.711328000
C	0.000000000	0.000000000	0.853480000	H	2.395963000	-4.651344000	-4.832729000
C	3.935112000	0.521870000	-2.770405000	H	-0.571043000	-2.550139000	-5.863081000
C	2.860859000	1.316498000	-3.169400000	H	0.957479000	-3.277292000	-6.427354000
C	1.630718000	1.167191000	-2.504357000	H	0.987298000	-1.861752000	-5.345775000
C	1.440164000	0.248990000	-1.458320000	H	3.991556000	4.178149000	2.286228000
C	2.554958000	-0.545727000	-1.104413000	H	4.388937000	2.230174000	-0.063304000
C	3.797856000	-0.421377000	-1.739988000	H	4.798658000	1.881973000	1.632970000
C	-0.935713000	1.122723000	-1.458320000	H	5.633153000	3.190812000	0.759295000
C	-0.804865000	2.485522000	-1.104413000	H	3.053520000	4.410317000	-0.629618000
C	-1.534005000	3.499728000	-1.739988000	H	4.401489000	5.312763000	0.113464000
C	-2.419509000	3.146972000	-2.770405000	H	2.727278000	5.590831000	0.661577000
C	-2.570550000	1.819328000	-3.169400000	H	0.072895000	4.662617000	4.629939000
C	-1.826176000	0.828647000	-2.504357000	H	-1.920287000	4.849365000	3.125754000
C	-0.290309000	-3.135825000	-3.169400000	H	-2.395963000	4.651344000	4.832729000
C	0.195458000	-1.995839000	-2.504357000	H	-2.519358000	3.277353000	3.711328000
C	-0.504450000	-1.371713000	-1.458320000	H	0.571043000	2.550139000	5.863081000
C	-1.750093000	-1.939795000	-1.104413000	H	-0.987298000	1.861752000	5.345775000
C	-2.263851000	-3.078351000	-1.739988000	H	-0.957479000	3.277292000	6.427354000
C	-1.515603000	-3.668842000	-2.770405000	H	-1.622605000	5.545863000	-2.286228000
C	0.000000000	0.000000000	-0.853480000	H	0.263081000	4.916018000	0.063304000
C	-3.608023000	-3.702903000	-1.365016000	H	0.053252000	6.473859000	-0.759295000
C	-3.435871000	-4.820681000	-0.319308000	H	0.769492000	5.096746000	-1.632970000
C	-4.660720000	-2.690868000	-0.899388000	H	-2.292686000	4.849584000	0.629618000
C	0.469706000	-3.744178000	-4.344258000	H	-3.478162000	5.157307000	-0.661577000
C	1.906232000	-4.153362000	-3.979414000	H	-2.400243000	6.468183000	-0.113464000
C	0.458579000	-2.804603000	-5.564625000	H	-4.001498000	2.394438000	-4.629939000
C	3.608023000	3.702903000	1.365016000	H	-5.159817000	0.761665000	-3.125754000
C	4.660720000	2.690868000	0.899388000	H	-4.097950000	-0.543152000	-3.711328000
C	3.435871000	4.820681000	0.319308000	H	-5.226164000	0.250708000	-4.832729000
C	-0.469706000	3.744178000	4.344258000	H	-1.922963000	1.769607000	-5.863081000
C	-1.906232000	4.153362000	3.979414000	H	-3.316957000	0.809445000	-6.427354000
C	-0.458579000	2.804603000	5.564625000	H	-2.105973000	0.075851000	-5.345775000
C	-1.402797000	4.976091000	-1.365016000	H	4.001498000	-2.394438000	4.629939000
C	0.000000000	5.381736000	-0.899388000	H	1.922963000	-1.769607000	5.863081000
C	-2.456897000	5.385892000	-0.319308000	H	2.105973000	-0.075851000	5.345775000
C	-3.477406000	1.465311000	-4.344258000	H	3.316957000	-0.809445000	6.427354000
C	-4.550033000	0.425836000	-3.979414000	H	5.159817000	-0.761665000	3.125754000
C	-2.658147000	1.005160000	-5.564625000	H	5.226164000	-0.250708000	4.832729000
				H	4.097950000	0.543152000	3.711328000
				H	1.622605000	-5.545863000	2.286228000
				H	2.292686000	-4.849584000	-0.629618000
				H	2.400243000	-6.468183000	0.113464000

H	3.478162000	-5.157307000	0.661577000	C	-3.538936000	1.417037000	-4.217990000
H	-0.263081000	-4.916018000	-0.063304000	C	-4.621460000	0.427899000	-3.760739000
H	-0.769492000	-5.096746000	1.632970000	C	-2.748110000	0.855274000	-5.411059000
H	-0.053252000	-6.473859000	0.759295000	C	3.538936000	-1.417037000	4.217990000
H	-5.614161000	1.367715000	2.286228000	C	-2.748110000	-0.855274000	5.411059000
H	-4.125856000	2.685844000	-0.063304000	C	4.621460000	-0.427899000	3.760739000
H	-4.029166000	3.214773000	1.632970000	C	1.393588000	-4.936963000	1.275976000
H	-5.579901000	3.283047000	0.759295000	C	2.468360000	-5.323718000	0.246797000
H	-5.346206000	0.439268000	-0.629618000	C	0.000000000	-5.291740000	0.752330000
H	-6.801732000	1.155420000	0.113464000	C	-4.972329000	1.261599000	1.275976000
H	-6.205440000	-0.433523000	0.661577000	C	-4.582781000	2.645870000	0.752330000
H	-4.074393000	-2.268180000	4.629939000	C	-5.844655000	0.524197000	0.246797000
H	-2.494007000	-0.780531000	5.863081000	C	-2.996658000	-2.356290000	4.217990000
H	-1.118675000	-1.785901000	5.345775000	C	-2.114744000	-1.952296000	5.411059000
H	-2.359478000	-2.467847000	6.427354000	C	-2.681301000	-3.788352000	3.760739000
H	-3.239530000	-4.087700000	3.125754000	C	2.996658000	2.356290000	-4.217990000
H	-2.830201000	-4.406637000	4.832729000	C	2.114744000	1.952296000	-5.411059000
H	-1.578592000	-3.820505000	3.711328000	C	2.681301000	3.788352000	-3.760739000
H	4.074393000	2.268180000	-4.629939000	C	4.972329000	-1.261599000	-1.275976000
H	2.494007000	0.780531000	-5.863081000	C	5.844655000	-0.524197000	-0.246797000
H	2.359478000	2.467847000	-6.427354000	C	4.582781000	-2.645870000	-0.752330000
H	1.118675000	1.785901000	-5.345775000	H	-4.903707000	-0.675611000	3.177126000
H	3.239530000	4.087700000	-3.125754000	H	-2.407044000	1.324216000	0.325480000
H	1.578592000	3.820505000	-3.711328000	H	-0.790788000	-1.799793000	2.780570000
H	2.830201000	4.406637000	-4.832729000	H	2.350327000	1.422453000	0.325480000
H	5.614161000	-1.367715000	-2.286228000	H	1.866757000	4.584541000	3.177126000
H	5.346206000	-0.439268000	0.629618000	H	-1.163273000	1.584739000	2.780570000
H	6.205440000	0.433523000	-0.661577000	H	1.954060000	0.215054000	2.780570000
H	6.801732000	-1.155420000	-0.113464000	H	0.056717000	-2.746669000	0.325480000
H	4.125856000	-2.685844000	0.063304000	H	3.036950000	-3.908929000	3.177126000
H	5.579901000	-3.283047000	-0.759295000	H	4.903707000	0.675611000	-3.177126000
H	4.029166000	-3.214773000	-1.632970000	H	0.790788000	1.799793000	-2.780570000

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C	-3.934060000	-0.562145000	2.682856000	H	-3.036950000	3.908929000	-3.177126000
C	-3.778643000	0.405214000	1.677566000	H	-1.954060000	-0.215054000	-2.780570000
C	-2.529643000	0.548793000	1.069212000	H	1.163273000	-1.584739000	-2.780570000
C	-1.425828000	-0.254097000	1.421978000	H	-2.350327000	-1.422453000	-0.325480000
C	-1.622051000	-1.190515000	2.441997000	H	-1.866757000	-4.584541000	-3.177126000
C	-2.861291000	-1.356990000	3.080648000	H	-4.004632000	-4.131487000	-2.187696000
C	0.492860000	1.361852000	1.421978000	H	-2.939374000	-4.392134000	0.677991000
C	1.740090000	1.916339000	1.069212000	H	-2.695046000	-5.576886000	-0.624707000
C	2.240247000	3.069794000	1.677566000	H	-4.337635000	-5.275860000	0.007570000
C	1.480198000	3.688069000	2.682856000	H	-4.258556000	-2.211618000	0.206043000
C	0.255457000	3.156446000	3.080648000	H	-5.563441000	-3.118466000	-0.583418000
C	-0.219990000	1.999995000	2.441997000	H	-4.720678000	-1.819082000	-1.464247000
C	2.605834000	-1.799456000	3.080648000	H	-0.005588000	-4.671818000	-4.550752000
C	1.842042000	-0.809480000	2.441997000	H	1.877010000	-4.932680000	-2.927393000
C	0.932969000	-1.107755000	1.421978000	H	2.536200000	-3.354296000	-3.419052000
C	0.789553000	-2.465132000	1.069212000	H	2.489044000	-4.696175000	-4.587333000
C	1.538396000	-3.475008000	1.677566000	H	-0.368901000	-5.755408000	-5.755408000
C	2.453862000	-3.125924000	2.682856000	H	1.163918000	-3.275991000	-6.256322000
C	0.000000000	0.000000000	0.831860000	H	1.181069000	-1.891192000	-5.135314000
C	3.934060000	0.562145000	-2.682856000	H	4.004632000	4.131487000	2.187696000
C	2.861291000	1.356990000	-3.080648000	H	4.258556000	2.211618000	-0.206043000
C	1.622051000	1.190515000	-2.441997000	H	4.720678000	1.819082000	1.464247000
C	1.425828000	0.254097000	-1.421978000	H	5.563441000	3.118466000	0.583418000
C	2.529643000	-0.548793000	-1.069212000	H	2.939374000	4.392134000	-0.677991000
C	3.778643000	-0.405214000	-1.677566000	H	4.337635000	5.275860000	-0.007570000
C	-0.932969000	1.107755000	-1.421978000	H	2.695046000	5.576886000	0.624707000
C	-0.789553000	2.465132000	-1.069212000	H	0.005588000	4.671818000	4.550752000
C	-1.538396000	3.475008000	-1.677566000	H	-1.877010000	4.932680000	2.927393000
C	-2.453862000	3.125924000	-2.682856000	H	-2.489044000	4.696175000	4.587333000
C	-2.605834000	1.799456000	-3.080648000	H	-2.536200000	3.354296000	3.419052000
C	-1.842042000	0.809480000	-2.441997000	H	0.368901000	2.507365000	5.755408000
C	-0.255457000	-3.156446000	-3.080648000	H	-1.181069000	1.891192000	5.135314000
C	0.219990000	-1.999995000	-2.441997000	H	-1.163918000	3.275991000	6.256322000
C	-0.492860000	-1.361852000	-1.421978000	H	-1.575657000	5.533857000	-2.187696000
C	-1.740090000	-1.916339000	-1.069212000	H	0.213960000	4.793826000	0.206043000
C	-2.240247000	-3.069794000	-1.677566000	H	0.081050000	6.377314000	-0.583418000
C	-1.480198000	-3.688069000	-2.682856000	H	0.784968000	4.997768000	-1.464247000
C	0.000000000	0.000000000	-0.831860000	H	-2.334012000	4.741639000	0.677991000
C	-3.578741000	-3.675364000	-1.275976000	H	-3.482202000	5.122422000	-0.624707000
C	-3.376295000	-4.799521000	-0.246797000	H	-2.400212000	6.394432000	0.007570000
C	-4.582781000	-2.645870000	-0.752330000	H	-4.043119000	2.340749000	-4.550752000
C	0.542278000	-3.773327000	-4.217990000	H	-5.210331000	0.840801000	-2.927393000
C	1.940159000	-4.216251000	-3.760739000	H	-4.173005000	-0.519266000	-3.419052000
C	0.633366000	-2.807570000	-5.411059000	H	-5.311529000	0.192512000	-4.587333000
C	3.578741000	3.675364000	1.275976000	H	-1.986991000	1.573161000	-5.755408000
C	4.582781000	2.645870000	0.752330000	H	-3.419051000	0.630013000	-6.256322000
C	3.376295000	4.799521000	0.246797000	H	-2.228355000	-0.077240000	-5.135314000
C	-0.542278000	3.773327000	4.217990000	H	4.043119000	-2.340749000	4.550752000
C	-1.940159000	4.216251000	3.760739000	H	1.986991000	-1.573161000	5.755408000
C	-0.633366000	2.807570000	5.411059000	H	2.228355000	0.077240000	5.135314000
C	-1.393588000	4.936963000	-1.275976000	H	3.419051000	-0.630013000	6.256322000
C	0.000000000	5.291740000	-0.752330000	H	5.210331000	-0.840801000	2.927393000
C	-2.468360000	5.323718000	-0.246797000	H	5.311529000	-0.192512000	4.587333000
				H	4.173005000	0.519266000	3.419052000

H	1.575657000	-5.533857000	2.187696000	C	-4.021930000	3.164994000	-1.272240000
H	2.334012000	-4.741639000	-0.677991000	C	-3.105614000	4.242839000	-0.699930000
H	2.400212000	-6.394432000	-0.007570000	C	-5.132693000	2.828516000	-0.271700000
H	3.482202000	-5.122422000	0.624707000	C	-3.729499000	-0.956682000	-4.181180000
H	-0.213960000	-4.793826000	-0.206043000	C	-3.904348000	-2.418250000	-3.761250000
H	-0.784968000	-4.997768000	1.464247000	C	-2.820172000	-0.850742000	-5.411130000
H	-0.081050000	-6.377314000	0.583418000	C	3.729499000	0.956682000	4.181180000
H	-5.580289000	1.402369000	2.187696000	C	2.820172000	0.850742000	5.411130000
H	-4.044595000	2.582208000	-0.206043000	C	3.904348000	2.418250000	3.761250000
H	-3.935710000	3.178686000	1.464247000	C	4.021930000	-3.164994000	1.272240000
H	-5.482391000	3.258848000	0.583418000	C	5.132693000	-2.828516000	0.271700000
H	-5.273386000	0.349505000	-0.677991000	C	3.105614000	-4.242839000	0.699930000
H	-6.737846000	1.118571000	-0.007570000	C	-4.751930000	-1.900596000	1.272240000
H	-6.177248000	-0.454465000	0.624707000	C	-5.227214000	-0.568121000	0.699930000
H	-4.048708000	-2.331070000	4.550752000	C	-5.015913000	-3.030784000	0.271700000
H	-2.355893000	-0.934205000	5.755408000	C	-1.036239000	-3.708182000	4.181180000
H	-1.047286000	-1.968432000	5.135314000	C	-0.673322000	-2.867712000	5.411130000
H	-2.255133000	-2.645978000	6.256322000	C	0.142092000	-4.590390000	3.761250000
H	-3.333321000	-4.091878000	2.927393000	C	1.036239000	3.708182000	-4.181180000
H	-2.822485000	-4.503663000	4.587333000	C	0.673322000	2.867712000	-5.411130000
H	-1.636805000	-3.873562000	3.419052000	C	-0.142092000	4.590390000	-3.761250000
H	4.048708000	2.331070000	-4.550752000	C	4.751930000	1.900596000	-1.272240000
H	2.355893000	0.934205000	-5.755408000	C	5.015913000	3.030784000	-0.271700000
H	2.255133000	2.645978000	-6.256322000	C	5.227214000	0.568121000	-0.699930000
H	1.047286000	1.968432000	-5.135314000	H	-3.562470000	-3.466920000	3.138580000
H	3.333321000	4.091878000	-2.927393000	H	-2.735070000	-0.305510000	0.374000000
H	1.636805000	3.873562000	-3.419052000	H	0.421790000	-1.953200000	2.777600000
H	2.822485000	4.503663000	-4.587333000	H	1.102956000	2.521395000	0.374000000
H	5.580289000	-1.402369000	-2.187696000	H	-1.221206000	4.818650000	3.138580000
H	5.273386000	-0.349505000	0.677991000	H	-1.902416000	0.611319000	2.777600000
H	6.177248000	0.454465000	-0.624707000	H	1.480626000	1.341881000	2.777600000
H	6.737846000	-1.118571000	0.007570000	H	1.632114000	-2.215885000	0.374000000
H	4.044595000	-2.582208000	0.206043000	H	4.783676000	-1.351730000	3.138580000
H	5.482391000	-3.258848000	-0.583418000	H	3.562470000	3.466920000	-3.138580000
H	3.935710000	-3.178686000	-1.464247000	H	-0.421790000	1.953200000	-2.777600000

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C	-2.844330000	-2.795010000	2.657900000	H	-4.783676000	1.351730000	-3.138580000
C	-3.286990000	-1.897750000	1.675970000	H	-1.480626000	-1.341881000	-2.777600000
C	-2.365680000	-1.035150000	1.085780000	H	1.902416000	-0.611319000	-2.777600000
C	-0.997560000	-1.048680000	1.425440000	H	-1.102956000	-2.521395000	-0.374000000
C	-0.607490000	-1.939430000	2.427860000	H	1.221206000	-4.818650000	-3.138580000
C	-1.512270000	-2.813490000	3.051350000	H	-0.839000000	-5.675240000	-2.185480000
C	-0.409404000	1.388252000	1.425440000	H	0.248980000	-5.265280000	0.646350000
C	0.286374000	2.566314000	1.085780000	H	1.115730000	-6.085280000	-0.673950000
C	-0.000005000	3.795492000	1.675970000	H	-0.376000000	-6.806990000	-0.005010000
C	-0.998385000	3.860767000	2.657900000	H	-2.066350000	-4.298500000	0.275020000
C	-1.680419000	2.716409000	3.051350000	H	-2.649430000	-5.763500000	-0.543130000
C	-1.375851000	1.495817000	2.427860000	H	-2.726130000	-4.188640000	-1.375800000
C	3.192689000	0.097081000	3.051350000	H	2.842120000	-3.809370000	-4.452790000
C	1.983341000	0.443613000	2.427860000	H	4.457860000	-2.711850000	-2.895730000
C	1.406964000	-0.339572000	1.425440000	H	3.950980000	-1.108580000	-3.488450000
C	2.079306000	-1.531164000	1.085780000	H	4.770200000	-2.241050000	-4.587270000
C	3.286995000	-1.897742000	1.675970000	H	1.190170000	-2.450730000	-5.737010000
C	3.842715000	-1.065757000	2.657900000	H	2.858950000	-2.072390000	-6.248500000
C	0.000000000	0.000000000	0.834410000	H	1.974840000	-0.953450000	-5.179580000
C	2.844330000	2.795010000	-2.657900000	H	0.839000000	5.675240000	2.185480000
C	1.512270000	2.813490000	-3.051350000	H	2.066350000	4.298500000	-0.275020000
C	0.607490000	1.939430000	-2.427860000	H	2.726130000	4.188640000	1.375800000
C	0.997560000	1.048680000	-1.425440000	H	2.649430000	5.763500000	0.543130000
C	2.365680000	1.035150000	-1.085780000	H	-0.248980000	5.265280000	-0.646350000
C	3.286990000	1.897750000	-1.675970000	H	0.376000000	6.806990000	0.005010000
C	-1.406964000	0.339572000	-1.425440000	H	-1.115730000	6.085280000	0.673950000
C	-2.079306000	1.531164000	-1.085780000	H	-2.842120000	3.809370000	4.452790000
C	-3.286995000	1.897742000	-1.675970000	H	-4.457860000	2.711850000	2.895730000
C	-3.842715000	1.065757000	-2.657900000	H	-4.770200000	2.241050000	4.587270000
C	-3.192689000	-0.097081000	-3.051350000	H	-3.950980000	1.108580000	3.488450000
C	-1.983341000	-0.443613000	-2.427860000	H	-1.190170000	2.450730000	5.737010000
C	1.680419000	-2.716409000	-3.051350000	H	-1.974840000	0.953450000	5.179580000
C	1.375851000	-1.495817000	-2.427860000	H	-2.858950000	2.072390000	6.248500000
C	0.409404000	-1.388252000	-1.425440000	H	-4.495402000	3.564215000	-2.185480000
C	-0.286374000	-2.566314000	-1.085780000	H	-2.689435000	3.938762000	0.275020000
C	0.000005000	-3.795492000	-1.675970000	H	-3.666622000	5.176224000	-0.543130000
C	0.998385000	-3.860767000	-2.657900000	H	-2.264404000	4.455218000	-1.375800000
C	0.000000000	0.000000000	-0.834410000	H	-4.684356000	2.417017000	0.646350000
C	-0.730000000	-5.065590000	-1.272240000	H	-5.827872000	2.076389000	-0.673950000
C	0.116780000	-5.859300000	-0.271700000	H	-5.707026000	3.729121000	-0.005010000
C	-2.121600000	-4.810960000	-0.699930000	H	-4.720071000	-0.556663000	-4.452790000
C	2.693260000	-2.751500000	-4.181180000	H	-4.577461000	-2.504695000	-2.895730000
C	4.064400000	-2.172140000	-3.761250000	H	-2.935548000	-2.867359000	-3.488450000
C	2.146850000	-2.016970000	-5.411130000	H	-4.325906000	-3.010589000	-4.587270000
C	0.730000000	5.065590000	1.272240000	H	-2.717479000	0.194648000	-5.737010000
C	2.121600000	4.810960000	0.699930000	H	-3.224217000	-1.439728000	-6.248500000
C	-0.116780000	5.859300000	0.271700000	H	-1.813132000	-1.233537000	-5.179580000
C	-2.693260000	2.751500000	4.181180000	H	4.720071000	0.556663000	4.452790000
C	-4.064400000	2.172140000	3.761250000	H	2.717479000	-0.194648000	5.737010000
C	-2.146850000	2.016970000	5.411130000	H	1.813132000	1.233537000	5.179580000
				H	3.224217000	1.439728000	6.248500000

H	4.577461000	2.504695000	2.895730000	C	0.094720000	5.160000000	-1.302090000
H	4.325906000	3.010589000	4.587270000	C	-4.516051000	-2.497970000	-1.302090000
H	2.935548000	2.867359000	3.488450000	C	-0.663750000	-3.656331000	-4.453210000
H	4.495402000	-3.564215000	2.185480000	C	3.498350000	1.253341000	-4.453210000
H	4.684356000	-2.417017000	-0.646350000	C	4.4211331000	-2.662030000	-1.302090000
H	5.707026000	-3.729121000	0.005010000	C	0.625130000	-6.352660000	1.960990000
H	5.827872000	-2.076389000	0.673950000	C	0.000000000	-5.339920000	-0.227710000
H	2.689435000	-3.938762000	-0.275020000	C	-1.580640000	-5.203160000	1.725970000
H	2.264404000	-4.455218000	1.375800000	C	3.259480000	-0.966230000	4.804760000
H	3.666622000	-5.176224000	0.543130000	C	4.112280000	-3.228940000	4.178350000
H	-5.334402000	-2.111025000	2.185480000	C	2.100970000	-2.996470000	5.679260000
H	-4.755785000	-0.359738000	-0.275020000	C	-5.814130000	2.634952000	1.960990000
H	-4.990534000	0.266578000	1.375800000	C	-4.624506000	2.669960000	-0.227710000
H	-6.316052000	-0.587276000	0.543130000	C	-3.715749000	3.970454000	1.725970000
H	-4.435376000	-2.848263000	-0.646350000	C	-2.466520000	-2.339677000	4.804760000
H	-6.083026000	-3.077869000	0.005010000	C	-4.852484000	-1.946869000	4.178350000
H	-4.712142000	-4.008891000	0.673950000	C	-3.645504000	-0.321258000	5.679260000
H	-1.877951000	-4.366033000	4.452790000	C	-0.792960000	3.305907000	4.804760000
H	-1.527309000	-2.256082000	5.737010000	C	0.740204000	5.175809000	4.178350000
H	0.161708000	-2.186987000	5.179580000	C	1.544534000	3.317728000	5.679260000
H	-0.365267000	-3.512118000	6.248500000	C	5.189000000	3.717708000	1.960990000
H	-0.119601000	-5.216545000	2.895730000	C	4.624506000	2.669960000	-0.227710000
H	0.444294000	-5.251639000	4.587270000	C	5.296389000	1.232706000	1.725970000
H	1.015432000	-3.975939000	3.488450000	C	-2.100970000	2.996470000	-5.679260000
H	1.877951000	4.366033000	-4.452790000	C	-4.112280000	3.228940000	-4.178350000
H	1.527309000	2.256082000	-5.737010000	C	-3.259480000	0.966230000	-4.804760000
H	0.365267000	3.512118000	-6.248500000	C	0.000000000	5.339920000	0.227710000
H	-0.161708000	2.186987000	-5.179580000	C	-0.625130000	6.352660000	-1.960990000
H	0.119601000	5.216545000	-2.895730000	C	1.580640000	5.203160000	-1.725970000
H	-1.015432000	3.975939000	-3.488450000	C	-4.624506000	-2.669960000	0.227710000
H	-0.444294000	5.251639000	-4.587270000	C	-5.189000000	-3.717708000	-1.960990000
H	5.334402000	2.111025000	-2.185480000	C	-5.296389000	-1.232706000	-1.725970000
H	4.435376000	2.848263000	0.646350000	C	-1.544534000	-3.317728000	-5.679260000
H	4.712142000	4.008891000	-0.673950000	C	-0.740204000	-5.175809000	-4.178350000
H	6.083026000	3.077869000	-0.005010000	C	0.792960000	-3.305907000	-4.804760000
H	4.755785000	0.359738000	0.275020000	C	3.645504000	0.321258000	-5.679260000
H	6.316052000	0.587276000	-0.543130000	C	4.852484000	1.946869000	-4.178350000
H	4.990534000	-0.266578000	-1.375800000	C	2.466520000	2.339677000	-4.804760000

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C	1.413190000	-3.701170000	2.788120000	C	5.814130000	-2.634952000	-1.960990000
C	0.504770000	-3.800890000	1.728820000	C	3.715749000	-3.970454000	-1.725970000
C	0.089490000	-2.613660000	1.094900000	H	0.514740000	-6.353260000	3.056530000
C	0.572090000	-1.345770000	1.466190000	H	1.700990000	-6.364830000	1.723870000
C	1.476820000	-1.308020000	2.547810000	H	0.191460000	-7.295140000	1.590380000
C	1.897230000	-2.459810000	3.227310000	H	-0.514410000	-4.538760000	-0.776520000
C	-1.451516000	0.177441000	1.466190000	H	-0.460280000	-6.296340000	-0.526880000
C	-2.308241000	1.229329000	1.094900000	H	1.051170000	-5.355730000	-0.556760000
C	-3.544052000	1.463301000	1.728820000	H	-1.680570000	-5.118510000	2.820150000
C	-3.911902000	0.626727000	2.788120000	H	-2.045060000	-6.154390000	1.414810000
C	-3.078873000	-0.413144000	3.227310000	H	-2.151850000	-4.381020000	1.269950000
C	-1.871189000	-0.624954000	2.547810000	H	3.926560000	-0.980690000	5.681580000
C	1.181643000	2.872954000	3.227310000	H	2.395690000	-0.331050000	5.055600000
C	0.394369000	1.932974000	2.547810000	H	3.804270000	-0.485000000	3.978720000
C	0.879426000	1.168329000	1.466190000	H	4.773390000	-3.217500000	5.061180000
C	2.218751000	1.384331000	1.094900000	H	4.675120000	-2.815320000	3.326720000
C	3.039282000	2.337589000	1.728820000	H	3.881320000	-4.280850000	3.949670000
C	2.498712000	3.074443000	2.788120000	H	2.750620000	-2.961880000	6.569970000
C	0.000000000	0.000000000	0.853720000	H	1.810540000	-4.046150000	5.518430000
C	-1.413190000	3.701170000	-2.788120000	H	1.184960000	-2.426040000	5.903490000
C	-1.897230000	2.459810000	-3.227310000	H	-5.759455000	2.730852000	3.056530000
C	-1.476820000	1.308020000	-2.547810000	H	-6.362599000	1.709314000	1.723870000
C	-0.572090000	1.345770000	-1.466190000	H	-6.413507000	3.481761000	1.590380000
C	-0.089490000	2.613660000	-1.094900000	H	-3.673476000	-2.714872000	-0.776520000
C	-0.504770000	3.800890000	-1.728820000	H	-5.222650000	3.546784000	-0.526880000
C	-0.879426000	-1.168329000	-1.466190000	H	-5.163783000	1.767525000	-0.556760000
C	-2.218751000	-1.384331000	-1.094900000	H	-3.592475000	4.014671000	2.820150000
C	-3.039282000	-2.337589000	-1.728820000	H	-4.307328000	4.848269000	1.414810000
C	-2.498712000	-3.074443000	-2.788120000	H	-2.718150000	4.054067000	1.269950000
C	-1.181643000	-2.872954000	-3.227310000	H	-2.812582000	-2.910156000	5.681580000
C	-0.394369000	-1.932974000	-2.547810000	H	-1.484543000	-1.909203000	5.055600000
C	3.078873000	0.413144000	-3.227310000	H	-2.322157000	-3.052094000	3.978720000
C	1.871189000	0.624954000	-2.547810000	H	-5.173132000	-2.525127000	5.061180000
C	1.451516000	-0.177441000	-1.466190000	H	-4.775699000	-2.641113000	3.326720000
C	2.308241000	-1.229329000	-1.094900000	H	-5.647985000	-1.220897000	3.949670000
C	3.544052000	-1.463301000	-1.728820000	H	-3.940373000	-0.901167000	6.569970000
C	3.911902000	-0.626727000	-2.788120000	H	-4.409339000	0.455101000	5.518430000
C	0.000000000	0.000000000	-0.853720000	H	-2.693492000	0.186815000	5.903490000
C	-0.094720000	-5.160000000	1.302090000	H	-1.113978000	3.890846000	5.681580000
C	2.834600000	-2.402990000	4.453210000	H	-0.911147000	2.240253000	5.055600000
C	-4.421331000	2.662030000	1.302090000	H	-1.482113000	3.537094000	3.978720000
C	-3.498350000	-1.253341000	4.453210000	H	0.399742000	5.742627000	5.061180000
C	0.663750000	3.656331000	4.453210000	H	0.100579000	5.456433000	3.326720000
C	4.516051000	2.497970000	1.302090000	H	1.766665000	5.501747000	3.949670000
C	-2.834600000	2.402990000	-4.453210000	H	1.189753000	3.863047000	6.569970000
				H	2.598799000	3.591049000	5.518430000
				H	1.508532000	2.239225000	5.903490000
				H	5.244715000	3.622408000	3.056530000
				H	4.661609000	4.655516000	1.723870000

H	6.222047000	3.813379000	1.590380000	C	-0.048223000	1.446194000	1.426698000
H	4.187886000	1.823888000	-0.776520000	C	0.877390000	2.431824000	1.060946000
H	5.682930000	2.749556000	-0.526880000	C	0.907381000	3.696864000	1.667202000
H	4.112613000	3.588205000	-0.556760000	C	0.000000000	3.962609000	2.697076000
H	5.273045000	1.103839000	2.820150000	C	-0.911199000	2.989111000	3.132245000
H	6.352388000	1.306121000	1.414810000	C	-0.926150000	1.752759000	2.479281000
H	4.870000000	0.326953000	1.269950000	C	3.044245000	-0.705434000	3.132245000
H	-1.810540000	4.046150000	-5.518430000	C	1.981008000	-0.074310000	2.479281000
H	-2.750620000	2.961880000	-6.569970000	C	1.276552000	-0.681335000	1.426698000
H	-1.184960000	2.426040000	-5.903490000	C	1.667327000	-1.975754000	1.060946000
H	-3.881320000	4.280850000	-3.949670000	C	2.747888000	-2.634247000	1.667202000
H	-4.675120000	2.815320000	-3.326720000	C	3.431720000	-1.981304000	2.697076000
H	-4.773390000	3.217500000	-5.061180000	C	0.000000000	0.000000000	0.830798000
H	-3.804270000	0.485000000	-3.978720000	C	3.431720000	1.981304000	-2.697076000
H	-2.395690000	0.331050000	-5.055600000	C	2.133047000	2.283677000	-3.132245000
H	-3.926560000	0.980690000	-5.681580000	C	1.054859000	1.678449000	-2.479281000
H	0.460280000	6.296340000	0.526880000	C	1.228329000	0.764859000	-1.426698000
H	0.514410000	4.538760000	0.776520000	C	2.544716000	0.456070000	-1.060946000
H	-1.051170000	5.355730000	0.556760000	C	3.655269000	1.062617000	-1.667202000
H	-0.191460000	7.295140000	-1.590380000	C	-1.276552000	0.681335000	-1.426698000
H	-1.700990000	6.364830000	-1.723870000	C	-1.667327000	1.975754000	-1.060946000
H	-0.514740000	6.353260000	-3.056530000	C	-2.747888000	2.634247000	-1.667202000
H	2.045060000	6.154390000	-1.414810000	C	-3.431720000	1.981304000	-2.697076000
H	1.680570000	5.118510000	-2.820150000	C	-3.044245000	0.705434000	-3.132245000
H	2.151850000	4.381020000	-1.269950000	C	-1.981008000	0.074310000	-2.479281000
H	-5.682930000	-2.749556000	0.526880000	C	0.911199000	-2.989111000	-3.132245000
H	-4.187886000	-1.823888000	0.776520000	C	0.926150000	-1.752759000	-2.479281000
H	-4.112613000	-3.588205000	0.556760000	C	0.048223000	-1.446194000	-1.426698000
H	-6.222047000	-3.813379000	-1.590380000	C	-0.877390000	-2.431824000	-1.060946000
H	-4.661609000	-4.655516000	-1.723870000	C	-0.907381000	-3.696864000	-1.667202000
H	-5.244715000	-3.622408000	-3.056530000	C	0.000000000	-3.962609000	-2.697076000
H	-6.352388000	-1.306121000	-1.414810000	C	0.000000000	0.000000000	-0.830798000
H	-5.273045000	-1.103839000	-2.820150000	C	-5.066400000	-0.639149000	1.227183000
H	-4.870000000	-0.326953000	-1.269950000	C	-1.924826000	-3.227427000	4.327199000
H	-2.598799000	-3.591049000	-5.518430000	C	1.979681000	4.707206000	1.227183000
H	-1.189753000	-3.863047000	-6.569970000	C	-1.832621000	3.280661000	4.327199000
H	-1.508532000	-2.239225000	-5.903490000	C	3.757446000	-0.053235000	4.327199000
H	-1.766665000	-5.501747000	-3.949670000	C	3.086719000	-4.068057000	1.227183000
H	-0.100579000	-5.456433000	-3.326720000	C	1.924826000	3.227427000	-4.327199000
H	-0.399742000	-5.742627000	-5.061180000	C	5.066400000	0.639149000	-1.227183000
H	1.482113000	-3.537094000	-3.978720000	C	-3.086719000	4.068057000	-1.227183000
H	0.911147000	-2.240253000	-5.055600000	C	-3.757446000	0.053235000	-4.327199000
H	1.113978000	-3.890846000	-5.681580000	C	1.832621000	-3.280661000	-4.327199000
H	4.409339000	-0.455101000	-5.518430000	C	-1.979681000	-4.707206000	-1.227183000
H	3.940373000	0.901167000	-6.569970000	C	-6.162976000	-1.489779000	1.885289000
H	2.693492000	-0.186815000	-5.903490000	C	-5.205455000	-0.767882000	-0.302204000
H	5.647985000	1.220897000	-3.949670000	C	-5.278026000	0.835485000	1.629182000
H	4.775699000	2.641113000	-3.326720000	C	-0.437121000	-3.425034000	4.659205000
H	5.173132000	2.525127000	-5.061180000	C	-2.538300000	-4.608258000	4.017538000
H	2.322157000	3.052094000	-3.978720000	C	-2.620268000	-2.620205000	5.564489000
H	1.484543000	1.909203000	-5.055600000	C	1.791301000	6.082183000	1.885289000
H	2.812582000	2.910156000	-5.681580000	C	1.937723000	4.891997000	-0.302204000
H	5.222650000	-3.546784000	0.526880000	C	3.362565000	4.153162000	1.629182000
H	3.673476000	-2.714872000	0.776520000	C	-2.747606000	2.091075000	4.659205000
H	5.163783000	-1.767525000	0.556760000	C	-2.721719000	4.502361000	4.017538000
H	6.413507000	-3.481761000	-1.590380000	C	-0.959030000	3.579321000	5.564489000
H	6.362599000	-1.709314000	-1.723870000	C	3.184727000	1.333959000	4.659205000
H	5.759455000	-2.730852000	-3.056530000	C	5.260018000	0.105897000	4.017538000
H	4.307328000	-4.848269000	-1.414810000	C	3.579298000	-0.959116000	5.564489000
H	3.592475000	-4.014671000	-2.820150000	C	4.371674000	-4.592404000	1.885289000
H	2.718150000	-4.054067000	-1.269950000	C	3.267732000	-4.124115000	-0.302204000
H	1.738290000	-4.604030000	3.302290000	C	1.915461000	-4.988647000	1.629182000
H	-0.649070000	-2.687310000	0.304620000	C	2.620268000	2.620205000	-5.564489000
H	1.844340000	-0.348980000	2.891120000	C	2.538300000	4.608258000	-4.017538000
H	-2.002744000	1.905766000	0.304620000	C	0.437121000	3.425034000	-4.659205000
H	-4.856352000	0.796612000	3.302290000	C	5.205455000	0.767882000	0.302204000
H	-1.224396000	-1.422755000	2.891120000	C	6.162976000	1.489779000	-1.885289000
H	-0.619944000	1.771735000	2.891120000	C	5.278026000	-0.835485000	-1.629182000
H	2.651814000	0.781544000	0.304620000	C	-3.267732000	4.124115000	0.302204000
H	3.118062000	3.807418000	3.302290000	C	-4.371674000	4.592404000	-1.885289000
H	-1.738290000	4.604030000	-3.302290000	C	-1.915461000	4.988647000	-1.629182000
H	-1.844340000	0.348980000	-2.891120000	C	-3.579298000	0.959116000	-5.564489000
H	0.649070000	2.687310000	-0.304620000	C	-5.260018000	-0.105897000	-4.017538000
H	-2.651814000	-0.781544000	-0.304620000	C	-3.184727000	-1.333959000	-4.659205000
H	-3.118062000	-3.807418000	-3.302290000	C	0.959030000	-3.579321000	-5.564489000
H	0.619944000	-1.771735000	-2.891120000	C	2.721719000	-4.502361000	-4.017538000
H	1.224396000	1.422755000	-2.891120000	C	2.747606000	-2.091075000	-4.659205000
H	2.002744000	-1.905766000	-0.304620000	C	-1.937723000	4.891997000	0.302204000
H	4.856352000	-0.796612000	-3.302290000	C	-1.791301000	-6.082183000	-1.885289000
H				C	-3.362565000	-4.153162000	-1.629182000
H				H	-6.169111000	-1.378658000	2.980605000
H				H	-6.042429000	-2.558605000	1.648393000
C	-3.431720000	-1.981304000	2.697076000	H	-7.150649000	-1.172897000	1.515703000
C	-3.655269000	-1.062617000	1.667202000	H	-4.452482000	-0.175374000	-0.838706000
C	-2.544716000	-0.456070000	1.060946000	H	-6.198996000	-0.417038000	-0.625639000
C	-1.228329000	-0.764859000	1.426698000	H	-5.097621000	-1.817004000	-0.618214000
C	-1.054859000	-1.678449000	2.479281000	H	-5.218095000	0.955833000	2.722395000
C	-2.133047000	-2.283677000	3.132245000	H	-6.268180000	1.190404000	1.298210000

B3LYP-D3(BJ)

H	-4.514383000	1.482955000	1.175085000	H	3.395604000	-1.827419000	-3.810672000
H	-0.336132000	-4.114899000	5.511542000	H	2.171910000	-1.193914000	-4.934736000
H	0.051996000	-2.477886000	4.934736000	H	3.395541000	-2.348548000	-5.511542000
H	0.115211000	-3.854389000	3.810672000	H	-2.738333000	-5.577007000	0.625639000
H	-2.438419000	-5.276245000	4.888874000	H	-2.074363000	-3.943650000	0.838706000
H	-2.027888000	-5.079477000	3.164109000	H	-0.975238000	-5.323171000	0.618214000
H	-3.608421000	-4.534030000	3.771396000	H	-2.559566000	-6.779092000	-1.515703000
H	-2.472374000	-3.265784000	6.445974000	H	-0.805398000	-6.512199000	-1.648393000
H	-3.703689000	-2.506007000	5.408040000	H	-1.890603000	-6.031936000	-2.980605000
H	-2.207007000	-1.624672000	5.793052000	H	-4.165010000	-4.833201000	-1.298210000
H	1.890603000	6.031936000	2.980605000	H	-3.436823000	-4.041086000	-2.722395000
H	0.805398000	6.512199000	1.648393000	H	-3.541468000	-3.168093000	-1.175085000
H	2.559566000	6.779092000	1.515703000	H	-4.278889000	-2.453561000	3.190599000
H	2.074363000	3.943650000	-0.838706000	H	-2.721075000	0.293996000	0.301476000
H	2.738333000	5.577007000	-0.625639000	H	-0.052859000	-1.906398000	2.815913000
H	0.975238000	5.323171000	-0.618214000	H	1.615146000	2.209522000	0.301476000
H	3.436823000	4.041086000	2.722395000	H	0.014598000	4.932407000	3.190599000
H	4.165010000	4.833201000	1.298210000	H	-1.624560000	0.998976000	2.815913000
H	3.541468000	3.168093000	1.175085000	H	1.677418000	0.907422000	2.815913000
H	-3.395541000	2.348548000	5.511542000	H	1.105929000	-2.503518000	0.301476000
H	-2.171910000	1.193914000	4.934736000	H	4.264291000	-2.478846000	3.190599000
H	-3.395604000	1.827419000	3.810672000	H	4.278889000	2.453561000	-3.190599000
H	-3.350153000	4.749855000	4.888874000	H	0.052859000	1.906398000	-2.815913000
H	-3.385012000	4.295942000	3.164109000	H	2.721075000	-0.293996000	-0.301476000
H	-2.122374000	5.391999000	3.771396000	H	-1.105929000	2.503518000	-0.301476000
H	-1.592065000	3.774031000	6.445974000	H	-4.264291000	2.478846000	-3.190599000
H	-0.318421000	4.460492000	5.408040000	H	-1.677418000	-0.907422000	-2.815913000
H	-0.303503000	2.723660000	5.793052000	H	1.624560000	-0.998976000	-2.815913000
H	3.731673000	1.766351000	5.511542000	H	-1.615146000	-2.209522000	-0.301476000
H	2.119915000	1.283973000	4.934736000	H	-0.014598000	-4.932407000	-3.190599000
H	3.280394000	2.026970000	3.810672000				
H	5.788572000	0.526390000	4.888874000				
H	5.412900000	0.783536000	3.164109000				
H	5.730795000	-0.857969000	3.771396000				
H	4.064439000	-0.508247000	6.445974000	C	1.522580000	-3.663230000	2.698180000
H	4.022110000	-1.954485000	5.408040000	C	0.567670000	-3.757410000	1.684590000
H	2.510510000	-1.098988000	5.793052000	C	0.112340000	-2.576150000	1.082920000
H	4.278508000	-4.653278000	2.980605000	C	0.604320000	-1.313650000	1.433370000
H	5.237031000	-3.953594000	1.648393000	C	1.542700000	-1.268040000	2.477340000
H	4.591083000	-5.606195000	1.515703000	C	1.999740000	-2.418510000	3.126800000
H	2.378120000	-3.768276000	-0.838706000	C	-1.439814000	0.133469000	1.433370000
H	3.460663000	-5.159970000	-0.625639000	C	-2.287181000	1.190786000	1.082920000
H	4.122382000	-3.506167000	-0.618214000	C	-3.537848000	1.387088000	1.684590000
H	1.781272000	-4.996919000	2.722395000	C	-3.933740000	0.513022000	2.698180000
H	2.103170000	-6.023605000	1.298210000	C	-3.094361000	-0.522571000	3.126800000
H	0.972915000	-4.651048000	1.175085000	C	-1.869505000	-0.701997000	2.477340000
H	3.703689000	2.506007000	-5.408040000	C	1.094621000	2.941081000	3.126800000
H	2.472374000	3.265784000	-6.445974000	C	0.326805000	1.970037000	2.477340000
H	2.207007000	1.624672000	-5.793052000	C	0.835494000	1.180181000	1.433370000
H	3.608421000	4.534030000	-3.771396000	C	2.174841000	1.385364000	1.082920000
H	2.027888000	5.079477000	-3.164109000	C	2.970178000	2.370322000	1.684590000
H	2.438419000	5.276245000	-4.888874000	C	2.411160000	3.150208000	2.698180000
H	-0.115211000	3.854389000	-3.810672000	C	0.000000000	0.000000000	0.832810000
H	-0.051996000	2.477886000	-4.934736000	C	-1.522580000	3.663230000	-2.698180000
H	0.336132000	4.114899000	-5.511542000	C	-1.999740000	2.418510000	-3.126800000
H	6.198996000	0.417038000	0.625639000	C	-1.542700000	1.268040000	-2.477340000
H	4.452482000	0.175374000	0.838706000	C	-0.604320000	1.313650000	-1.433370000
H	5.097621000	1.817004000	0.618214000	C	-0.112340000	2.576150000	-1.082920000
H	7.150649000	1.172897000	-1.515703000	C	-0.567670000	3.757410000	-1.684590000
H	6.042429000	2.558605000	-1.648393000	C	-0.835494000	-1.180181000	-1.433370000
H	6.169111000	1.378658000	-2.980605000	C	-2.174841000	-1.385364000	-1.082920000
H	6.268180000	-1.190404000	-1.298210000	C	-2.970178000	-2.370322000	-1.684590000
H	5.218095000	-0.955833000	-2.722395000	C	-2.411160000	-3.150208000	-2.698180000
H	4.514383000	-1.482955000	-1.175085000	C	-1.094621000	-2.941081000	-3.126800000
H	-3.460663000	5.159970000	0.625639000	C	-0.326805000	-1.970037000	-2.477340000
H	-2.378120000	3.768276000	0.838706000	C	3.094361000	0.522571000	-3.126800000
H	-4.122382000	3.506167000	0.618214000	C	1.869505000	0.701997000	-2.477340000
H	-4.591083000	5.606195000	-1.515703000	C	1.439814000	-0.133469000	-1.433370000
H	-5.237031000	3.953594000	-1.648393000	C	2.287181000	-1.190786000	-1.082920000
H	-4.278508000	4.653278000	-2.980605000	C	3.537848000	-1.387088000	-1.684590000
H	-2.103170000	6.023605000	-1.298210000	C	3.933740000	-0.513022000	-2.698180000
H	-1.781272000	4.996919000	-2.722395000	C	0.000000000	0.000000000	-0.832810000
H	-0.972915000	4.651048000	-1.175085000	C	-0.064290000	-5.089930000	1.264800000
H	-4.022110000	1.954485000	-5.408040000	C	2.987290000	-2.345200000	4.297520000
H	-4.064439000	0.508247000	-6.445974000	C	-4.375864000	2.600642000	1.264800000
H	-2.510510000	1.098988000	-5.793052000	C	-3.524648000	-1.414469000	4.297520000
H	-5.730795000	0.857969000	-3.771396000	C	0.537358000	3.759669000	4.297520000
H	-5.412900000	-0.783536000	-3.164109000	C	4.440154000	2.489288000	1.264800000
H	-5.788572000	-0.526390000	-4.888874000	C	-2.987290000	2.345200000	-4.297520000
H	-3.280394000	-2.026970000	-3.810672000	C	0.064290000	5.089930000	-1.264800000
H	-2.119915000	-1.283973000	-4.934736000	C	-4.440154000	-2.489288000	-1.264800000
H	-3.731673000	-1.766351000	-5.511542000	C	-0.537358000	-3.759669000	-4.297520000
H	0.318421000	-4.460492000	-5.408040000	C	3.524648000	1.414469000	-4.297520000
H	1.592065000	-3.774031000	-6.445974000	C	4.375864000	-2.600642000	-1.264800000
H	0.303503000	-2.723660000	-5.793052000	C	0.637110000	-6.290550000	1.905020000
H	2.122374000	-5.391999000	-3.771396000	C	0.000000000	-5.248730000	-0.260990000
H	3.385012000	-4.295942000	-3.164109000	C	-1.536210000	-5.086170000	1.707860000
H	3.350153000	-4.749855000	-4.888874000	C	3.305200000	-0.899990000	4.692290000
				C	4.300090000	-3.041940000	3.906130000

M06-2X

C	2.379250000	-3.053910000	5.519170000	H	-4.127890000	4.085500000	-3.602800000
C	-5.766331000	2.593522000	1.905020000	H	-4.782800000	2.516410000	-3.068290000
C	-4.545534000	2.624365000	-0.260990000	H	-4.996780000	3.044560000	-4.759380000
C	-3.636647000	3.873482000	1.707860000	H	-3.773000000	0.348430000	-3.863560000
C	-2.432014000	-2.412392000	4.692290000	H	-2.397960000	0.355500000	-4.996630000
C	-4.784442000	-2.203017000	3.906130000	H	-4.006000000	0.895630000	-5.540490000
C	-3.834389000	-0.533536000	5.519170000	H	0.497660000	6.183670000	0.564480000
C	-0.873186000	3.312382000	4.692290000	H	0.495810000	4.418210000	0.786460000
C	0.484352000	5.244957000	3.906130000	H	-1.046390000	5.295770000	0.600980000
C	1.455139000	3.587446000	5.519170000	H	-0.170670000	7.221350000	-1.549290000
C	5.129221000	3.697028000	1.905020000	H	-1.704580000	6.321830000	-1.638130000
C	4.545534000	2.624365000	-0.260990000	H	-0.553940000	6.274330000	-3.001840000
C	5.172857000	1.212688000	1.707860000	H	2.043560000	6.002120000	-1.365120000
C	-2.379250000	3.053910000	-5.519170000	H	1.610650000	5.041630000	-2.805320000
C	-4.300090000	3.041940000	-3.906130000	H	2.069530000	4.217640000	-1.291360000
C	-3.305200000	0.899990000	-4.692290000	H	-5.604045000	-2.660849000	0.564480000
C	0.000000000	5.248730000	0.260990000	H	-4.074187000	-1.779721000	0.786460000
C	-0.637110000	6.290550000	-1.905020000	H	-4.063076000	-3.554085000	0.600980000
C	1.536210000	5.086170000	-1.707860000	H	-6.168538000	-3.758480000	-1.549290000
C	-4.545534000	-2.624365000	0.260990000	H	-4.622575000	-4.637125000	-1.638130000
C	-5.129221000	-3.697028000	-1.905020000	H	-5.156759000	-3.616891000	-3.001840000
C	-5.172857000	-1.212688000	-1.707860000	H	-6.219768000	-1.231285000	-1.365120000
C	-1.455139000	-3.587446000	-5.519170000	H	-5.171505000	-1.125951000	-2.805320000
C	-0.484352000	-5.244957000	-3.906130000	H	-4.687348000	-0.316554000	-1.291360000
C	0.873186000	-3.312382000	-4.692290000	H	-2.473572000	-3.950307000	-5.318340000
C	3.834389000	0.533536000	-5.519170000	H	-1.057043000	-4.155908000	-6.374050000
C	4.784442000	2.203017000	-3.906130000	H	-1.521132000	-2.527542000	-5.808750000
C	2.432014000	2.412392000	-4.692290000	H	-1.474202000	-5.617608000	-3.602080000
C	4.545534000	-2.624365000	0.260990000	H	0.212125000	-5.400231000	-3.068290000
C	5.766331000	-2.593522000	-1.905020000	H	-0.138276000	-5.849618000	-4.759380000
C	3.636647000	-3.873482000	-1.707860000	H	1.584751000	-3.441729000	-3.863560000
H	0.553940000	-6.274330000	3.001840000	H	0.891108000	-2.254444000	-4.996630000
H	1.704580000	-6.321830000	1.638130000	H	1.227362000	-3.917113000	-5.540490000
H	0.170670000	-7.221350000	1.549290000	H	4.657852000	-0.167023000	-5.318340000
H	-0.495810000	-4.418210000	-0.786460000	H	4.127643000	1.162528000	-6.374050000
H	-0.497660000	-6.183670000	-0.564480000	H	2.949482000	-0.053568000	-5.808750000
H	1.046390000	-5.295770000	-0.600980000	H	5.602092000	1.532108000	-3.602080000
H	-1.610650000	-5.041630000	2.805320000	H	4.570675000	2.883821000	-3.068290000
H	-2.043560000	-6.002120000	1.365120000	H	5.135056000	2.805058000	-4.759380000
H	-2.069530000	-4.217640000	1.291360000	H	2.188249000	3.093299000	-3.863560000
H	4.006000000	-0.895630000	5.540490000	H	1.506852000	1.898944000	-4.996630000
H	2.397960000	-0.355500000	4.996630000	H	2.778638000	3.021483000	-5.540490000
H	3.773000000	-0.348430000	3.863560000	H	5.106385000	-3.522821000	0.564480000
H	4.996780000	-3.044560000	4.759380000	H	3.578377000	-2.638489000	0.786460000
H	4.782800000	-2.516410000	3.068290000	H	5.109466000	-1.741685000	0.600980000
H	4.127890000	-4.085500000	3.602080000	H	6.339208000	-3.462870000	-1.549290000
H	3.070600000	-2.993380000	6.374050000	H	6.327155000	-1.684705000	-1.638130000
H	2.184280000	-4.117330000	5.318340000	H	5.710699000	-2.657439000	-3.001840000
H	1.428350000	-2.581110000	5.808750000	H	4.176208000	-4.770835000	-1.365120000
H	-5.710699000	2.657439000	3.001840000	H	3.560855000	-3.915679000	-2.805320000
H	-6.327155000	1.684705000	1.638130000	H	2.617818000	-3.901086000	-1.291360000
H	-6.339208000	3.462870000	1.549290000	H	1.887550000	-4.567810000	3.184880000
H	-3.578377000	2.638489000	-0.786460000	H	-0.680110000	-2.657400000	0.346210000
H	-5.106385000	3.522821000	-0.564480000	H	1.910830000	-0.308100000	2.820440000
H	-5.109466000	1.741685000	-0.600980000	H	-1.961321000	1.917693000	0.346210000
H	-3.560855000	3.915679000	2.805320000	H	-4.899614000	0.649239000	3.184880000
H	-4.176208000	4.770835000	1.365120000	H	-1.222237000	-1.500777000	2.820440000
H	-2.617818000	3.901086000	1.291360000	H	-0.688593000	1.808877000	2.820440000
H	-2.778638000	-3.021483000	5.540490000	H	2.641431000	0.739707000	0.346210000
H	-1.506852000	-1.898944000	4.996630000	H	3.012064000	3.918571000	3.184880000
H	-2.188249000	-3.093299000	3.863560000	H	-1.887550000	4.567810000	-3.184880000
H	-5.135056000	-2.805058000	4.759380000	H	-1.910830000	0.308100000	-2.820440000
H	-4.570675000	-2.883821000	3.068290000	H	0.680110000	2.657400000	-0.346210000
H	-5.602092000	-1.532108000	3.602080000	H	-2.641431000	-0.739707000	-0.346210000
H	-4.127643000	-1.162528000	6.374050000	H	-3.012064000	-3.918571000	-3.184880000
H	-4.657852000	0.167023000	5.318340000	H	0.688593000	-1.808877000	-2.820440000
H	-2.949482000	0.053568000	5.808750000	H	1.222237000	1.500777000	-2.820440000
H	-1.227362000	3.917113000	5.540490000	H	1.961321000	-1.917693000	-0.346210000
H	-0.891108000	2.254444000	4.996630000	H	4.899614000	-0.649239000	-3.184880000
H	-1.584751000	3.441729000	3.863560000				
H	0.138276000	5.849618000	4.759380000				
H	-0.212125000	5.400231000	3.068290000				
H	1.474202000	5.617608000	3.602080000				
H	1.057043000	4.155908000	6.374050000				
H	2.473572000	3.950307000	5.318340000				
H	1.521132000	2.527542000	5.808750000	C	0.000000000	0.000000000	0.858503000
H	5.156759000	3.616891000	3.001840000	C	-1.630958000	-1.256154000	2.445661000
H	4.622575000	4.637125000	1.638130000	C	-2.881949000	-1.486548000	3.042706000
H	6.168538000	3.758480000	1.549290000	C	-1.431499000	-0.290552000	1.444848000
H	4.074187000	1.779721000	-0.786460000	C	-3.975753000	-0.718999000	2.630615000
H	5.604045000	2.660849000	-0.564480000	C	-2.557026000	0.480514000	1.089741000
H	4.063076000	3.554085000	-0.600980000	C	-3.822284000	0.278317000	1.655899000
H	5.171505000	1.125951000	2.805320000	C	-4.992060000	1.153244000	1.229519000
H	6.219768000	1.231285000	1.365120000	C	-6.159302000	0.342244000	0.624044000
H	4.687348000	0.316554000	1.291360000	C	-5.505079000	2.048145000	2.381001000
H	-2.184280000	4.117330000	-5.318340000	C	-7.314271000	1.249466000	0.176708000
H	-3.070600000	2.993380000	-6.374050000	C	-6.660585000	2.953641000	1.932741000
H	-1.428350000	2.581110000	-5.808750000	C	-7.810479000	2.140284000	1.323700000
				C	5.888221000	4.291416000	1.932741000

Cy-1₂

B3LYP

C	4.526285000	3.743466000	2.381001000	C	-2.152171000	-3.171037000	-1.655899000
C	5.758780000	5.693931000	1.323700000	C	-3.494768000	-3.746629000	-1.229519000
C	1.365205000	3.802603000	2.630615000	C	-5.888221000	-4.291416000	-1.932741000
C	3.494768000	3.746629000	1.229519000	C	-5.758780000	-5.693931000	-1.323700000
C	0.153586000	3.239115000	3.042706000	C	-4.739204000	-5.709611000	-0.176708000
C	2.152171000	3.171037000	1.655899000	C	-4.526285000	-3.743466000	-2.381001000
C	-0.272382000	2.040529000	2.445661000	C	-3.376043000	-5.162990000	-0.624044000
C	1.694650000	1.974192000	1.089741000	C	-1.694650000	-1.974192000	-1.089741000
C	0.464124000	1.384991000	1.444848000	H	-0.795499000	-1.856219000	2.796670000
C	4.739204000	5.709611000	0.176708000	H	-4.955153000	-0.885000000	3.085628000
C	3.376043000	5.162990000	0.624044000	H	-2.458135000	1.278960000	0.361897000
C	2.575066000	-6.959077000	0.176708000	H	-4.619550000	1.826067000	0.436049000
C	2.783259000	-5.505234000	0.624044000	H	-6.533682000	-0.377692000	1.375220000
C	2.051699000	-7.834215000	1.323700000	H	-5.790319000	-0.257421000	-0.225150000
C	2.610548000	-3.083604000	2.630615000	H	-5.846022000	1.407296000	3.215333000
C	1.497292000	-4.899873000	1.229519000	H	-4.672397000	2.654429000	2.775997000
C	2.728363000	-1.752567000	3.042706000	H	-6.970130000	1.889469000	-0.657486000
C	0.772365000	-7.245057000	1.932741000	H	-8.142514000	0.638565000	-0.221075000
C	1.670113000	-3.449353000	1.655899000	H	-6.286833000	3.673448000	1.180284000
C	0.978794000	-5.791611000	2.381001000	H	-7.023109000	3.553966000	2.784574000
C	1.903341000	-0.784374000	2.445661000	H	-8.610541000	2.812165000	0.969163000
C	0.862375000	-2.454706000	1.089741000	H	-8.261460000	1.504005000	2.109014000
C	0.967375000	-1.094439000	1.444848000	H	6.324715000	3.607833000	1.180284000
C	4.277881000	-1.454763000	6.619368000	H	6.589379000	4.305208000	2.784574000
C	3.314581000	-1.913674000	5.515805000	H	4.141765000	4.359156000	3.215333000
C	3.704959000	-1.339956000	4.134585000	H	4.635002000	2.719200000	2.775997000
C	5.733582000	-1.800400000	6.278316000	H	6.740677000	6.050865000	0.969163000
C	6.133298000	-1.235419000	4.908693000	H	5.433236000	6.402632000	2.109014000
C	5.171094000	-1.695656000	3.804215000	H	1.711144000	4.733788000	3.085628000
C	-4.054028000	-3.630470000	3.804215000	H	3.891196000	3.807614000	0.436049000
C	-3.012916000	-2.538610000	4.134585000	H	-1.209784000	1.617032000	2.796670000
C	-3.314581000	-1.913674000	5.515805000	H	2.336680000	1.489327000	0.361897000
C	-4.136553000	-4.693882000	4.908693000	H	5.121393000	5.091575000	-0.657486000
C	-4.425983000	-4.065228000	6.278316000	H	4.624270000	6.732342000	-0.221075000
C	-3.998802000	-2.977372000	6.619368000	H	2.939750000	5.847181000	1.375220000
C	-0.692043000	3.878566000	4.134585000	H	2.672227000	5.143274000	-0.225150000
C	-1.117065000	5.326127000	3.804215000	H	1.848737000	-6.981044000	-0.657486000
C	0.000000000	3.827349000	5.515805000	H	3.518244000	-7.370907000	-0.221075000
C	-1.996745000	5.929301000	4.908693000	H	3.593932000	-5.469489000	1.375220000
C	-0.879078000	4.432135000	6.619368000	H	3.118093000	-4.885853000	-0.225150000
C	-1.307599000	5.865628000	6.278316000	H	1.869864000	-8.863030000	0.969163000
C	-0.464124000	-1.384991000	-1.444848000	H	2.828224000	-7.906636000	2.109014000
C	0.000000000	0.000000000	-0.858503000	H	3.244009000	-3.848788000	3.085628000
C	-0.967375000	1.094439000	-1.444848000	H	0.728354000	-4.913681000	0.436049000
C	-0.862375000	2.454706000	-1.089741000	H	-0.037883000	-7.281281000	1.180284000
C	-1.670113000	3.449353000	-1.655899000	H	0.433730000	-7.859174000	2.784574000
C	-1.497292000	4.899873000	-1.229519000	H	1.704257000	-5.766451000	3.215333000
C	-0.772365000	7.245057000	-1.932741000	H	0.037396000	-5.373629000	2.775997000
C	-2.051699000	7.834215000	-1.323700000	H	2.005282000	0.239188000	2.796670000
C	-2.575066000	6.959077000	-0.176708000	H	0.121456000	-2.768288000	0.361897000
C	-0.978794000	5.791611000	-2.381001000	H	4.185537000	-0.359795000	6.748893000
C	-2.783259000	5.505234000	-0.624044000	H	3.991177000	-1.906999000	7.584065000
C	-2.610548000	3.083604000	-2.630615000	H	2.280542000	-1.617245000	5.759196000
C	-2.728363000	1.752567000	-3.042706000	H	3.317466000	-3.018470000	5.462849000
C	-3.704959000	1.339956000	-4.134585000	H	3.650102000	-0.238777000	4.215756000
C	-3.314581000	1.913674000	-5.515805000	H	5.852760000	-2.900677000	6.266607000
C	-4.277881000	1.454763000	-6.619368000	H	6.411756000	-1.421970000	7.061975000
C	-5.733582000	1.800400000	-6.278316000	H	7.166125000	-1.531078000	4.657477000
C	-6.133298000	1.235419000	-4.908693000	H	6.128944000	-0.129936000	4.956561000
C	-5.171094000	1.695656000	-3.804215000	H	5.262903000	-2.790228000	3.677417000
C	-1.903341000	0.784374000	-2.445661000	H	5.452242000	-1.245564000	2.837206000
C	1.431499000	0.290552000	-1.444848000	H	-5.047860000	-3.162693000	3.677417000
C	1.630958000	1.256154000	-2.445661000	H	-3.804811000	-4.098998000	2.837206000
C	2.881949000	1.486548000	-3.042706000	H	-2.031837000	-3.041692000	4.215756000
C	3.012916000	2.538610000	-4.134585000	H	-2.540846000	-1.166385000	5.759196000
C	4.136553000	4.693882000	-4.908693000	H	-4.272804000	-1.363775000	5.462849000
C	4.425983000	4.065228000	-6.278316000	H	-4.909015000	-5.440507000	4.657477000
C	3.998802000	2.977372000	-6.619368000	H	-3.177000000	-5.242853000	4.956561000
C	4.054028000	3.630470000	-3.804215000	H	-5.438440000	-3.618300000	6.266607000
C	3.314581000	1.913674000	-5.515805000	H	-4.437340000	-4.841758000	7.061975000
C	3.975753000	0.718999000	-2.630615000	H	-2.404360000	-3.444884000	6.748893000
C	3.822284000	-0.278317000	-1.655899000	H	-3.647098000	-2.502961000	7.584065000
C	4.992060000	-1.153244000	-1.229519000	H	-1.618264000	3.280469000	4.215756000
C	6.159302000	-0.342244000	-0.624044000	H	-0.215043000	5.952922000	3.677417000
C	7.314271000	-1.249466000	-0.176708000	H	-1.647431000	5.344562000	2.837206000
C	6.660585000	-2.953641000	-1.932741000	H	0.260304000	2.783630000	5.759196000
C	7.810479000	-2.140284000	-1.323700000	H	0.955338000	4.382244000	5.462849000
C	5.505079000	-2.048145000	-2.381001000	H	-2.257110000	6.971585000	4.657477000
C	2.557026000	-0.480514000	-1.089741000	H	-2.951944000	5.372789000	4.956561000
C	0.272382000	-2.040529000	-2.445661000	H	-1.781177000	3.804679000	6.748893000
C	-0.153586000	-3.239115000	-3.042706000	H	-0.344079000	4.409960000	7.584065000
C	0.692043000	-3.878566000	-4.134585000	H	-0.414320000	6.518977000	6.266607000
C	1.996745000	-5.929301000	-4.908693000	H	-1.974415000	6.263728000	7.061975000
C	1.307599000	-5.865628000	-6.278316000	H	-0.121456000	2.768288000	-0.361897000
C	0.879078000	-4.432135000	-6.619368000	H	-0.728354000	4.913681000	-0.436049000
C	1.117065000	-5.326127000	-3.804215000	H	0.037883000	7.281281000	-1.180284000
C	0.000000000	-3.827349000	-5.515805000	H	-0.433730000	7.859174000	-2.784574000
C	-1.365205000	-3.802603000	-2.630615000	H	-1.869864000	8.863030000	-0.969163000

H	-2.828224000	7.906636000	-2.109014000	C	6.403893000	-4.533512000	1.565970000
H	-1.848737000	6.981044000	0.657486000	C	4.147416000	-0.032964000	2.279230000
H	-3.518244000	7.370907000	0.221075000	C	4.498893000	-2.299709000	1.114090000
H	-1.704257000	5.766451000	-3.215333000	C	3.282430000	0.989596000	2.685930000
H	-0.037396000	5.373629000	-2.775997000	C	3.671693000	-1.083382000	1.483990000
H	-3.593932000	5.469489000	-1.375220000	C	1.949587000	0.965164000	2.254320000
H	-3.118093000	4.885853000	0.225150000	C	2.342099000	-1.058386000	1.053960000
H	-3.244009000	3.848788000	-3.085628000	C	1.457026000	-0.021077000	1.389730000
H	-3.650102000	0.238777000	-4.215756000	C	6.758345000	-3.348623000	0.658670000
H	-2.280542000	1.617245000	-5.759196000	C	6.016018000	-2.074892000	1.081510000
H	-3.317466000	3.018470000	-5.462849000	C	-6.279165000	-4.178587000	0.658670000
H	-4.185537000	0.359795000	-6.748893000	C	-4.804918000	-4.172578000	1.081510000
H	-3.991177000	1.906999000	-7.584065000	C	-7.128083000	-3.279178000	1.565970000
H	-5.852760000	2.900677000	-6.266607000	C	-2.102256000	-3.575286000	2.279230000
H	-6.411756000	1.421970000	-7.061975000	C	-4.241053000	-2.746301000	1.114090000
H	-7.166125000	1.531078000	-4.657477000	C	-0.784200000	-3.337466000	2.685930000
H	-6.128944000	0.129936000	-4.956561000	C	-6.566063000	-1.853746000	1.623280000
H	-5.262903000	2.790228000	-3.677417000	C	-2.774083000	-2.638088000	1.483990000
H	-5.452242000	1.245564000	-2.837206000	C	-5.093520000	-1.854184000	2.042040000
H	-2.005282000	-0.239188000	-2.796670000	C	-0.138937000	-2.170974000	2.254320000
H	0.795499000	1.856219000	-2.796670000	C	-2.087639000	-1.499124000	1.053960000
H	2.031837000	3.041692000	-4.215756000	C	-0.746766000	-1.251283000	1.389730000
H	4.909015000	5.440507000	-4.657477000	C	0.075560000	-5.924890000	5.490970000
H	3.177000000	5.242853000	-4.956561000	C	-0.799310000	-4.970010000	4.670110000
H	5.438440000	3.618300000	-6.266607000	C	0.000000000	-4.328640000	3.524270000
H	4.437340000	4.841758000	-7.061975000	C	0.702020000	-7.009500000	4.606270000
H	2.404360000	3.444884000	-6.748893000	C	1.490240000	-6.393140000	3.444520000
H	3.647098000	2.502961000	-7.584065000	C	0.623000000	-5.424700000	2.635960000
H	5.047860000	3.162693000	-3.677417000	C	-5.009428000	2.172816000	2.635960000
H	3.804811000	4.098998000	-2.837206000	C	-3.748712000	2.164320000	3.524270000
H	2.540846000	1.166385000	-5.759196000	C	-3.904500000	3.177228000	4.670110000
H	4.272804000	1.363775000	-5.462849000	C	-6.281742000	1.905984000	3.444520000
H	4.955153000	0.885000000	-3.085628000	C	-6.421415000	2.896783000	4.606270000
H	4.619550000	-1.826067000	-0.436049000	C	-5.168885000	2.897008000	5.490970000
H	6.533682000	0.377692000	-1.375220000	C	3.748712000	2.164320000	3.524270000
H	5.790319000	0.257421000	0.225150000	C	4.386428000	3.251884000	2.635960000
H	6.970130000	-1.889469000	0.657486000	C	4.703810000	1.792782000	4.670110000
H	8.142514000	-0.638565000	0.221075000	C	4.791502000	4.487156000	3.444520000
H	6.286833000	-3.673448000	-1.180284000	C	5.093325000	3.027882000	5.490970000
H	7.023109000	-3.553966000	-2.784574000	C	5.719395000	4.112717000	4.606270000
H	8.610541000	-2.812165000	-0.969163000	C	-1.457026000	0.021077000	-1.389730000
H	8.261460000	-1.504005000	-2.109014000	C	0.000000000	0.000000000	-0.854920000
H	5.846022000	-1.407296000	-3.215333000	C	0.746766000	1.251283000	-1.389730000
H	4.672397000	-2.654429000	-2.775997000	C	2.087639000	1.499124000	-1.053960000
H	2.458135000	-1.278960000	-0.361897000	C	2.774083000	2.638088000	-1.483990000
H	1.209784000	-1.617032000	-2.796670000	C	4.241053000	2.746301000	-1.114090000
H	1.618264000	-3.280469000	-4.215756000	C	6.566063000	1.853746000	-1.623280000
H	2.257110000	-6.971585000	-4.657477000	C	7.128083000	3.279178000	-1.565970000
H	2.951944000	-5.372789000	-4.956561000	C	6.279165000	4.178587000	-0.658670000
H	0.414320000	-6.518977000	-6.266607000	C	5.093520000	1.854184000	-2.042040000
H	1.974415000	-6.263728000	-7.061975000	C	4.804918000	4.172578000	-1.081510000
H	1.781177000	-3.804679000	-6.748893000	C	2.102256000	3.575286000	-2.279230000
H	0.344079000	-4.409960000	-7.584065000	C	0.784200000	3.337466000	-2.685930000
H	0.215043000	-5.952922000	-3.677417000	C	0.000000000	4.328640000	-3.524270000
H	1.647431000	-5.344562000	-2.837206000	C	0.799310000	4.970010000	-4.670110000
H	-0.260304000	-2.783630000	-5.759196000	C	-0.075560000	5.924890000	-5.490970000
H	-0.955338000	-4.382244000	-5.462849000	C	-0.702020000	7.009500000	-4.606270000
H	-1.711144000	-4.733788000	-3.085628000	C	-1.490240000	6.393140000	-3.444520000
H	-3.891196000	-3.087614000	-0.436049000	C	-0.623000000	5.424700000	-2.635960000
H	-6.324715000	-3.607833000	-1.180284000	C	0.138937000	2.170974000	-2.254320000
H	-6.589379000	-4.305208000	-2.784574000	C	0.710260000	-1.272360000	-1.389730000
H	-6.740677000	-6.050865000	-0.969163000	C	1.810650000	-1.205810000	-2.254320000
H	-5.433236000	-6.402632000	-2.109014000	C	2.498230000	-2.347870000	-2.685930000
H	-5.121393000	-5.091575000	0.657486000	C	3.748712000	-2.164320000	-3.524270000
H	-4.624270000	-6.732342000	0.221075000	C	6.281742000	-1.905984000	-3.444520000
H	-4.141765000	-4.359156000	-3.215333000	C	6.421415000	-2.896783000	-4.606270000
H	-4.635002000	-2.719200000	-2.775997000	C	5.168885000	-2.897008000	-5.490970000
H	-2.939750000	-5.847181000	-1.375220000	C	5.009428000	-2.172816000	-2.635960000
H	-2.672227000	-5.143274000	0.225150000	C	3.904500000	-3.177228000	-4.670110000
H	-2.336680000	-1.489327000	-0.361897000	C	2.045160000	-3.608250000	-2.279230000

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C	0.000000000	0.000000000	0.854920000	C	0.479180000	-7.527210000	-0.658670000
C	-1.810650000	1.205810000	2.254320000	C	-1.677640000	-6.613250000	-1.623280000
C	-2.498230000	2.347870000	2.685930000	C	-0.724190000	-7.812690000	-1.565970000
C	-0.710260000	1.272360000	1.389730000	C	-0.940990000	-5.338210000	-2.042040000
C	-2.045160000	3.608250000	2.279230000	C	0.254460000	-2.557510000	-1.053960000
C	-0.254460000	2.557510000	1.053960000	C	-1.949587000	-0.965164000	-2.254320000
C	-0.897610000	3.721470000	1.483990000	C	-3.282430000	-0.989596000	-2.685930000
C	-0.257840000	5.046010000	1.114090000	C	-3.748712000	-2.164320000	-3.524270000
C	-1.211100000	6.247470000	1.081510000	C	-4.791502000	-4.487156000	-3.444520000
C	0.940990000	5.338210000	2.042040000	C	-5.719395000	-4.112717000	-4.606270000
C	-0.479180000	7.527210000	0.658670000	C	-5.093325000	-3.027882000	-5.490970000
C	1.677640000	6.613250000	1.623280000	C	-4.386428000	-3.251884000	-2.635960000
C	0.724190000	7.812690000	1.565970000	C	-4.703810000	-1.792782000	-4.670110000
C	4.888423000	-4.759504000	1.623280000	C	-4.147416000	0.032964000	-2.279230000
C	4.152530000	-3.484026000	2.042040000	C	-3.671693000	1.083382000	-1.483990000

C	-4.498893000	2.299709000	-1.114090000	H	6.358442000	3.820235000	0.383330000
C	-4.888423000	4.759504000	-1.623280000	H	6.671497000	5.209049000	-0.665900000
C	-6.403893000	4.533512000	-1.565970000	H	4.994568000	2.222895000	-3.079960000
C	-6.758345000	3.348623000	-0.658670000	H	4.691149000	0.829011000	-2.033650000
C	-4.152530000	3.484026000	-2.042040000	H	4.722402000	4.627579000	-2.085100000
C	-6.016018000	2.074892000	-1.081510000	H	4.204015000	4.798632000	-0.400600000
C	-2.342099000	1.058386000	-1.053960000	H	2.613333000	4.482174000	-2.602570000
H	-2.173090000	0.242590000	2.601540000	H	-0.837990000	3.771100000	-3.981320000
H	-2.575010000	4.504300000	2.602570000	H	1.227870000	4.183360000	-5.312350000
H	0.634820000	2.676470000	0.446370000	H	1.651220000	5.537480000	-4.254220000
H	0.155770000	4.924670000	0.098240000	H	-0.880830000	5.347050000	-5.981630000
H	-1.646400000	6.403510000	2.085100000	H	0.517400000	6.384640000	-6.298900000
H	-2.053730000	6.040100000	0.400600000	H	0.101790000	7.650090000	-4.196980000
H	0.572200000	5.436870000	3.079960000	H	-1.352580000	7.666870000	-5.206740000
H	1.627630000	4.477160000	2.033650000	H	-1.891080000	7.182330000	-2.786430000
H	-0.129200000	7.416690000	-0.383330000	H	-2.362910000	5.844270000	-3.844720000
H	-1.175420000	8.382210000	0.665900000	H	0.194860000	5.979450000	-2.141500000
H	2.126510000	6.455210000	0.624560000	H	-1.211620000	4.956840000	-1.831490000
H	2.513090000	6.815360000	2.314270000	H	-0.876456000	2.003246000	-2.601540000
H	1.258480000	8.713420000	1.220560000	H	2.173090000	-0.242590000	-2.601540000
H	0.361810000	8.033620000	2.587530000	H	3.684863000	-1.159829000	-3.981320000
H	4.527121000	-5.069217000	0.624560000	H	7.165620000	-1.953442000	-2.786430000
H	4.645730000	-5.584080000	2.314270000	H	6.242741000	-0.875795000	-3.844720000
H	4.422368000	-3.213975000	3.079960000	H	6.574277000	-3.913198000	-4.196980000
H	3.063519000	-3.648149000	2.033650000	H	7.315994000	-2.662066000	-5.206740000
H	6.916803000	-5.446586000	1.220560000	H	5.071096000	-1.910704000	-5.981630000
H	6.776414000	-4.330147000	2.587530000	H	5.270560000	-3.640402000	-6.298900000
H	5.188343000	-0.022126000	2.602570000	H	5.080926000	-3.158479000	-2.141500000
H	4.187004000	-2.597236000	0.098240000	H	4.898559000	-1.429126000	-1.831490000
H	1.296634000	1.760656000	2.601540000	H	3.008961000	-3.155047000	-5.312350000
H	2.000481000	-1.888005000	0.446370000	H	3.969988000	-4.198738000	-4.254220000
H	6.487642000	-3.596455000	-0.383330000	H	2.575010000	-4.504300000	-2.602570000
H	7.846917000	-3.173161000	0.665900000	H	-0.155770000	-4.924670000	-0.982400000
H	6.368802000	-1.775931000	2.085100000	H	1.646400000	-6.403510000	-2.085100000
H	6.257745000	-1.241468000	0.400600000	H	2.053730000	-6.040100000	-0.400600000
H	-6.358442000	-3.820235000	-0.383330000	H	0.129200000	-7.416690000	0.383330000
H	-6.671497000	-5.209049000	0.665900000	H	1.175420000	-8.382210000	-0.665900000
H	-4.722402000	-4.627579000	2.085100000	H	-2.126510000	-6.455210000	-0.624560000
H	-4.204015000	-4.798632000	0.400600000	H	-2.513090000	-6.815360000	-2.314270000
H	-8.175283000	-3.266834000	1.220560000	H	-1.258480000	-8.713420000	-1.220560000
H	-7.138224000	-3.703473000	2.587530000	H	-0.361810000	-8.033620000	-2.587530000
H	-2.613333000	-4.482174000	2.602570000	H	-0.572200000	-5.436870000	-3.079960000
H	-4.342774000	-2.327434000	0.098240000	H	-1.627630000	-4.477160000	-2.033650000
H	-6.653631000	-1.385993000	0.624560000	H	-0.634820000	-2.676470000	-0.446370000
H	-7.158820000	-1.231280000	2.314270000	H	-1.296634000	-1.760656000	-2.601540000
H	-4.994568000	-2.222895000	3.079960000	H	-2.846873000	-2.611271000	-3.981320000
H	-4.691149000	-0.829011000	2.033650000	H	-5.274540000	-5.228888000	-2.786430000
H	0.876456000	-2.003246000	2.601540000	H	-3.879831000	-4.968475000	-3.844720000
H	-2.635301000	-0.788465000	0.446370000	H	-6.676067000	-3.736892000	-4.196980000
H	0.880830000	-5.347050000	5.981630000	H	-5.963414000	-5.004804000	-5.206740000
H	-0.517400000	-6.384640000	6.298900000	H	-4.190266000	-3.436346000	-5.981630000
H	-1.227870000	-4.183360000	5.312350000	H	-5.787960000	-2.744238000	-6.298900000
H	-1.651220000	-5.537480000	4.254220000	H	-5.275786000	-2.820971000	-2.141500000
H	0.837990000	-3.771100000	3.981320000	H	-3.686939000	-3.527714000	-1.831490000
H	-0.101790000	-7.650090000	4.196980000	H	-4.236831000	-1.028313000	-5.312350000
H	1.352580000	-7.666870000	5.206740000	H	-5.621208000	-1.338742000	-4.254220000
H	1.891080000	-7.182330000	2.786430000	H	-5.188343000	0.022126000	-2.602570000
H	2.362910000	-5.844270000	3.844720000	H	-4.187004000	2.597236000	-0.098240000
H	-0.194860000	-5.979450000	2.141500000	H	-4.527121000	5.069217000	-0.624560000
H	1.211620000	-4.956840000	1.831490000	H	-4.645730000	5.584080000	-2.314270000
H	-5.080926000	3.158479000	2.141500000	H	-6.916803000	5.446586000	-1.220560000
H	-4.898559000	1.429126000	1.831490000	H	-6.776414000	4.330147000	-2.587530000
H	-3.684863000	1.159829000	3.981320000	H	-6.487642000	3.596455000	0.383330000
H	-3.008961000	3.155047000	5.312350000	H	-7.846917000	3.173161000	-0.665900000
H	-3.969988000	4.198738000	4.254220000	H	-4.422368000	3.213975000	-3.079960000
H	-7.165620000	1.953442000	2.786430000	H	-3.063519000	3.648149000	-2.033650000
H	-6.242741000	0.875795000	3.844720000	H	-6.368802000	1.775931000	-2.085100000
H	-6.574277000	3.913198000	4.196980000	H	-6.257745000	1.241468000	-0.400600000
H	-7.315994000	2.662066000	5.206740000	H	-2.000481000	1.888005000	-0.446370000
H	-5.071096000	1.910704000	5.981630000				
H	-5.270560000	3.640402000	6.298900000				
H	2.846873000	2.611271000	3.981320000				
H	5.275786000	2.820971000	2.141500000				
H	3.686939000	3.527714000	1.831490000	C	0.000000000	0.000000000	0.855220000
H	4.236831000	1.028313000	5.312350000	C	-1.825956000	1.212508000	2.238710000
H	5.621208000	1.338742000	4.254220000	C	-2.519998000	2.356518000	2.647670000
H	5.274540000	5.228888000	2.786430000	C	-0.713930000	1.271647000	1.388710000
H	3.879831000	4.968475000	3.844720000	C	-2.076956000	3.611505000	2.220660000
H	4.190266000	3.436346000	5.981630000	C	-0.254355000	2.554576000	1.057570000
H	5.787960000	2.744238000	6.298900000	C	-0.914719000	3.719441000	1.451730000
H	6.676067000	3.736892000	4.196980000	C	-0.280581000	5.041278000	1.068150000
H	5.963414000	5.004804000	5.206740000	C	-1.235258000	6.236563000	1.070730000
H	2.635301000	0.788465000	-0.446370000	C	0.937289000	5.333335000	1.962050000
H	4.342774000	2.327434000	-0.098240000	C	-0.523106000	7.515770000	0.626880000
H	6.653631000	1.385993000	-0.624560000	C	1.652572000	6.610566000	1.522480000
H	7.158820000	1.231280000	-2.314270000	C	0.695578000	7.802952000	1.504960000
H	8.175283000	3.266834000	-1.220560000	C	4.898633000	-4.736452000	1.522480000
H	7.138224000	3.703473000	-2.587530000	C	4.150159000	-3.478384000	1.962050000
				C	6.409766000	-4.503864000	1.504960000

M06-2X

C	4.166133000	-0.007056000	2.220660000	C	-4.898633000	4.736452000	-1.522480000
C	4.506165000	-2.277649000	1.068150000	C	-6.409766000	4.503864000	-1.504960000
C	3.300803000	1.004123000	2.647670000	C	-6.770401000	3.304862000	-0.626880000
C	3.678490000	-1.067551000	1.451730000	C	-4.150159000	3.478384000	-1.962050000
C	1.963040000	0.975070000	2.238710000	C	-6.018651000	2.048517000	-1.070730000
C	2.339505000	-1.057010000	1.057570000	C	-2.339505000	1.057010000	-1.057570000
C	1.458244000	-0.017542000	1.388710000	H	-2.189765000	0.254966000	2.605410000
C	6.770401000	-3.304862000	0.626880000	H	-2.624005000	4.508911000	2.515850000
C	6.018651000	-2.048517000	1.070730000	H	0.657645000	2.681119000	0.480410000
C	-6.247294000	-4.210908000	0.626880000	H	0.107981000	4.923348000	0.040210000
C	-4.783393000	-4.188047000	1.070730000	H	-1.629991000	6.390171000	2.090970000
C	-7.105344000	-3.299088000	1.504960000	H	-2.101703000	6.027820000	0.421130000
C	-2.089177000	-3.604450000	2.220660000	H	0.593936000	5.430848000	3.008490000
C	-4.225584000	-2.763629000	1.068150000	H	4.474290000	1.931590000	1.931590000
C	-0.780805000	-3.360641000	2.647670000	H	-0.195363000	7.401195000	-0.421180000
C	-6.551204000	-1.874114000	1.522480000	H	-1.221836000	8.365779000	0.649700000
C	-2.763771000	-2.651890000	1.451730000	H	2.657301000	6.456634000	0.505580000
C	-5.087448000	-1.854951000	1.962050000	H	2.511723000	6.814112000	2.180460000
C	-0.137085000	-2.187578000	2.238710000	H	1.215398000	8.708070000	1.155610000
C	-2.085150000	-1.497566000	1.057570000	H	0.356460000	8.008453000	2.535990000
C	-0.744314000	-1.254105000	1.388710000	H	4.562958000	-5.009992000	0.505580000
C	0.000000000	-5.852775000	5.540810000	H	4.645332000	-5.582272000	2.180460000
C	-0.829111000	-4.884680000	4.695910000	H	4.406284000	-3.229788000	3.008490000
C	-0.021600000	-4.352842000	3.504860000	H	3.060591000	-3.647480000	1.931590000
C	0.521305000	-7.014620000	4.694400000	H	6.933711000	-5.406600000	1.155610000
C	1.326258000	-6.503097000	3.499610000	H	6.757293000	-4.312930000	2.535990000
C	0.507139000	-5.523422000	2.660790000	H	5.216834000	0.017999000	2.515850000
C	-5.036993000	2.322515000	2.660790000	H	4.209754000	-2.555189000	0.040210000
C	-3.758872000	2.195127000	3.504860000	H	1.315689000	1.768909000	2.605410000
C	-3.815701000	3.160371000	4.695910000	H	1.993094000	-1.910097000	0.480410000
C	-6.294976000	2.102975000	3.499610000	H	6.507305000	-3.531408000	-0.421180000
C	-6.335492000	3.055846000	4.694400000	H	7.855895000	-3.124748000	0.649700000
C	-5.068652000	2.926387000	5.540810000	H	6.349046000	-1.783472000	2.090970000
C	3.780472000	2.157715000	3.504860000	H	6.271097000	-1.193782000	0.421130000
C	4.529854000	3.200907000	2.660790000	H	-6.311941000	-3.869787000	-0.421180000
C	4.644812000	1.724308000	4.695910000	H	-6.634059000	-5.241031000	0.649700000
C	4.968718000	4.400122000	3.499610000	H	-4.719055000	-4.606699000	2.090970000
C	5.068652000	2.926387000	5.540810000	H	-4.169394000	-4.834038000	0.421130000
C	5.814186000	3.958774000	4.694400000	H	-8.149108000	-3.301470000	1.155610000
C	-1.458244000	0.017542000	-1.388710000	H	-7.113753000	-3.695523000	2.535990000
C	0.000000000	0.000000000	-0.855220000	H	-2.592829000	-4.526910000	2.515850000
C	0.744314000	1.254105000	-1.388710000	H	-4.317735000	-2.368160000	0.040210000
C	2.085150000	1.497566000	-1.057570000	H	-6.620260000	-1.446642000	0.505580000
C	2.763771000	2.651890000	-1.451730000	H	-7.157056000	-1.231840000	2.180460000
C	4.225584000	2.763629000	-1.068150000	H	-5.000220000	-2.201060000	3.008490000
C	6.551204000	1.874114000	-1.522480000	H	-4.689106000	-0.826810000	1.931590000
C	7.105344000	3.299088000	-1.504960000	H	0.874075000	-2.023875000	2.605410000
C	6.247294000	4.210908000	-0.626880000	H	-2.650740000	-0.771022000	0.480410000
C	5.087448000	1.854951000	-1.962050000	H	0.857375000	-5.309960000	5.976540000
C	4.783393000	4.188047000	-1.070730000	H	-0.598671000	-6.229477000	6.383900000
C	2.089177000	3.604450000	-2.220660000	H	-1.189741000	-4.041799000	5.305450000
C	0.780805000	3.360641000	-2.647670000	H	-1.723684000	-5.415031000	4.324220000
C	0.021600000	4.352842000	-3.504860000	H	0.857794000	-3.822175000	3.912910000
C	0.829111000	4.884680000	-4.695910000	H	-0.336539000	-7.604614000	4.324610000
C	0.000000000	5.852775000	-5.540810000	H	1.133089000	-7.693747000	5.307570000
C	-0.521305000	7.014620000	-4.694400000	H	1.670163000	-7.342640000	2.874920000
C	-1.326258000	6.503097000	-3.499610000	H	2.231980000	-5.987782000	3.867300000
C	-0.507139000	5.523422000	-2.660790000	H	-0.359375000	-6.047223000	2.214350000
C	0.137085000	2.187578000	-2.238710000	H	1.108159000	-5.132930000	1.822580000
C	0.713930000	-1.271647000	-1.388710000	H	-5.057362000	3.334840000	2.214350000
C	1.825956000	-1.212508000	-2.238710000	H	-4.999327000	1.606771000	1.822580000
C	2.519998000	-2.356518000	-2.647670000	H	-3.738998000	1.168216000	3.912910000
C	3.758872000	-2.195127000	-3.504860000	H	-2.905430000	3.051246000	5.305450000
C	6.294976000	-2.102975000	-3.499610000	H	-3.827712000	4.200270000	4.324220000
C	6.335492000	-3.055846000	-4.694400000	H	-7.193994000	2.224917000	2.874920000
C	5.068652000	-2.926387000	-5.540810000	H	-6.301561000	1.060940000	3.867300000
C	5.036993000	-2.322515000	-2.660790000	H	-6.417519000	4.093759000	4.324610000
C	3.815701000	-3.160371000	-4.695910000	H	-7.229525000	2.865590000	5.307570000
C	2.076956000	-3.611505000	-2.220660000	H	-5.027248000	1.912471000	5.976540000
C	0.914719000	-3.719441000	-1.451730000	H	-5.095549000	3.633203000	6.383900000
C	0.280581000	-5.041278000	-1.068150000	H	2.881204000	2.653959000	3.912910000
C	1.235258000	-6.236563000	-1.070730000	H	5.416737000	2.712384000	2.214350000
C	0.523106000	-7.515770000	-0.626880000	H	3.891168000	3.526159000	1.822580000
C	-1.652572000	-6.610566000	-1.522480000	H	4.095171000	0.990554000	5.305450000
C	-0.695578000	-7.802952000	-1.504960000	H	5.551396000	1.214761000	4.324220000
C	-0.937289000	-5.333335000	-1.962050000	H	5.523831000	5.117724000	2.874920000
C	0.254355000	-2.554576000	-1.057570000	H	4.069581000	4.926842000	3.867300000
C	-1.963040000	-0.975070000	-2.238710000	H	4.169873000	3.397489000	5.976540000
C	-3.300803000	-1.004123000	-2.647670000	H	5.694221000	2.596274000	6.383900000
C	-3.780472000	-2.157715000	-3.504860000	H	6.754058000	3.510855000	4.324610000
C	-4.968718000	-4.400122000	-3.499610000	H	6.096436000	4.828157000	5.307570000
C	-5.814186000	-3.958774000	-4.694400000	H	2.650740000	0.771022000	-0.480410000
C	-5.068652000	-2.926387000	-5.540810000	H	4.317735000	2.368160000	-0.040210000
C	-4.529854000	-3.200907000	-2.660790000	H	6.620260000	1.446642000	-0.505580000
C	-4.644812000	-1.724308000	-4.695910000	H	7.157056000	1.231840000	-2.180460000
C	-4.166133000	0.007056000	-2.220660000	H	8.149108000	3.301470000	-1.155610000
C	-3.678490000	1.067551000	-1.451730000	H	7.113753000	3.695523000	-2.535990000
C	-4.506165000	2.277649000	-1.068150000	H	6.311941000	3.869787000	0.421180000

H	6.634059000	5.241031000	-0.649700000	C	-7.295820000	-0.087622000	2.272740000
H	5.000220000	2.201060000	-3.008490000	C	-7.980725000	-1.440580000	1.998300000
H	4.689106000	0.826810000	-1.931590000	C	3.572027000	6.362177000	2.272740000
H	4.719055000	4.606699000	-2.090970000	C	2.623280000	5.188458000	2.585370000
H	4.169394000	4.834038000	-0.421130000	C	4.417152000	6.022834000	1.030960000
H	2.592829000	4.526910000	-2.515850000	C	2.742784000	7.631801000	1.998300000
H	-0.857794000	3.822175000	-3.912910000	C	-0.179354000	3.926908000	2.834770000
H	1.189741000	4.041799000	-5.305450000	C	1.660624000	4.908357000	1.393730000
H	1.723684000	5.415031000	-4.324220000	C	-1.035389000	2.904203000	3.255590000
H	-0.857375000	5.309960000	-5.976540000	C	3.481078000	5.774163000	-0.166840000
H	0.598671000	6.229477000	-6.383900000	C	0.706188000	3.757063000	1.759130000
H	0.336539000	7.604614000	-4.324610000	C	2.530669000	4.602465000	0.152440000
H	-1.133089000	7.693747000	-5.307570000	C	-0.997466000	1.685800000	2.555570000
H	-1.670163000	7.342640000	-2.874920000	C	0.715791000	2.519750000	1.096620000
H	-2.231980000	5.987782000	-3.867300000	C	-0.134646000	1.455389000	1.468910000
H	0.359375000	6.047223000	-2.214350000	C	1.815068000	7.388098000	0.791920000
H	-1.108159000	5.132930000	-1.822580000	C	0.864815000	6.213632000	1.099900000
H	-0.874075000	2.023875000	-2.605410000	C	2.662668000	7.048296000	-0.447730000
H	2.189765000	-0.254966000	-2.605410000	C	5.490747000	-5.265944000	0.791920000
H	3.738998000	-1.168216000	-3.912910000	C	4.948756000	-3.855768000	1.099900000
H	7.193994000	-2.224917000	-2.874920000	C	5.237941000	-6.191221000	1.998300000
H	6.301561000	-1.060940000	-3.867300000	C	4.772669000	-5.830086000	-0.447730000
H	6.417519000	-4.093759000	-4.324610000	C	3.490480000	-1.808129000	2.834770000
H	7.229525000	-2.865590000	-5.307570000	C	3.420450000	-3.892321000	1.393730000
H	5.027248000	-1.912471000	-5.976540000	C	3.032808000	-0.555429000	3.255590000
H	5.095549000	-3.633203000	-6.383900000	C	3.723793000	-6.274555000	2.272740000
H	5.057362000	-3.334840000	-2.214350000	C	2.900618000	-2.490108000	1.759130000
H	4.999327000	-1.606771000	-1.822580000	C	3.181696000	-4.866056000	2.585370000
H	2.905430000	-3.051246000	-5.305450000	C	1.958678000	0.020931000	2.555570000
H	3.827712000	-4.200270000	-4.324220000	C	1.822735000	-1.878881000	1.096620000
H	2.624005000	-4.508911000	-2.515850000	C	1.327727000	-0.611087000	1.468910000
H	-0.107981000	-4.923348000	-0.040210000	C	3.260033000	-5.901784000	-0.166840000
H	1.629991000	-6.390171000	-2.090970000	C	2.720517000	-4.492856000	0.152440000
H	2.101703000	-6.027820000	-0.421130000	C	3.007351000	-6.836782000	1.030960000
H	0.195363000	-7.401195000	0.421180000	C	3.595821000	1.195180000	7.266980000
H	1.221836000	-8.365779000	-0.649700000	C	4.292026000	-0.137582000	6.935360000
H	-2.057301000	-6.456634000	-0.505580000	C	3.604288000	-0.789846000	5.719710000
H	-2.511723000	-6.814112000	-2.180460000	C	3.695075000	2.133355000	6.049610000
H	-1.215398000	-8.708070000	-1.155610000	C	3.012888000	1.476286000	4.833230000
H	-0.356460000	-8.008453000	-2.535990000	C	3.687300000	0.130977000	4.466760000
H	-0.593936000	-5.430848000	-3.008490000	C	5.775581000	0.123955000	6.607950000
H	-1.628514000	-4.474290000	-1.931590000	C	5.177374000	2.403308000	5.728800000
H	-0.657645000	-2.681119000	-0.480410000	C	5.874968000	1.071035000	5.396130000
H	-1.315689000	-1.768909000	-2.605410000	C	5.189245000	0.420994000	4.178070000
H	-2.881204000	-2.653959000	-3.912910000	C	-2.230031000	-4.704514000	4.178070000
H	-5.523831000	-5.117724000	-2.874920000	C	-1.730220000	-3.258784000	4.466760000
H	-4.069581000	-4.926842000	-3.867300000	C	-2.486170000	-2.726482000	5.719710000
H	-6.754058000	-3.510855000	-4.324610000	C	-2.009940000	-5.623390000	5.396130000
H	-6.096436000	-4.828157000	-5.307570000	C	-0.227943000	-3.347381000	4.833230000
H	-4.169873000	-3.397489000	-5.976540000	C	-2.780442000	-5.063777000	6.607950000
H	-5.694221000	-2.596274000	-6.383900000	C	-2.265162000	-3.648213000	6.935360000
H	-5.416737000	-2.712384000	-2.214350000	C	-0.507362000	-5.685391000	5.728800000
H	-3.891168000	-3.526159000	-1.822580000	C	0.000003000	-4.266706000	6.049610000
H	-4.095171000	-0.990554000	-5.305450000	C	-0.762855000	-3.711663000	7.266980000
H	-5.551396000	-1.214761000	-4.324220000	C	-2.784945000	1.871095000	4.833230000
H	-5.216834000	-0.017999000	-2.515850000	C	-1.957079000	3.127807000	4.466760000
H	-4.209754000	2.555189000	-0.040210000	C	-2.959213000	4.283521000	4.178070000
H	-4.562958000	5.009992000	-0.505580000	C	-3.695077000	2.133351000	6.049610000
H	-4.645332000	5.582272000	-2.180460000	C	-1.118117000	3.516328000	5.719710000
H	-6.933711000	5.406600000	-1.155610000	C	-4.670012000	3.282084000	5.728800000
H	-6.757293000	4.312930000	-2.535990000	C	-3.865028000	4.552354000	5.396130000
H	-6.507305000	3.531408000	0.421180000	C	-2.832967000	2.516483000	7.266980000
H	-7.855895000	3.124748000	-0.649700000	C	-2.026864000	3.785794000	6.935360000
H	-4.406284000	3.229788000	-3.008490000	C	-2.995139000	4.939822000	6.607950000
H	-3.060591000	3.647480000	-1.931590000	C	0.134646000	-1.455389000	-1.468910000
H	-6.349046000	1.783472000	-2.090970000	C	0.000000000	0.000000000	-0.853240000
H	-6.271097000	1.193782000	-0.421130000	C	-1.327727000	0.611087000	-1.468910000
H	-1.993094000	1.910097000	-0.480410000	C	-1.822735000	1.878881000	-1.096620000

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C	0.000000000	0.000000000	0.853240000	C	-7.295820000	-0.087622000	2.272740000
C	-0.961212000	-1.706731000	2.555570000	C	-7.980725000	-1.440580000	1.998300000
C	-1.997419000	-2.348775000	3.255590000	C	3.572027000	6.362177000	2.272740000
C	-1.193080000	-0.844302000	1.468910000	C	2.623280000	5.188458000	2.585370000
C	-3.311125000	-2.118780000	2.834770000	C	4.417152000	6.022834000	1.030960000
C	-2.538526000	-0.639095000	1.096620000	C	2.742784000	7.631801000	1.998300000
C	-3.606806000	-1.266955000	1.759130000	C	-0.179354000	3.926908000	2.834770000
C	-5.251186000	-0.109608000	0.152440000	C	1.660624000	4.908357000	1.393730000
C	-5.081073000	-1.016036000	1.393730000	C	-1.035389000	2.904203000	3.255590000
C	-5.813571000	-2.357864000	1.099900000	C	3.481078000	5.774163000	-0.166840000
C	-5.804976000	-0.322402000	2.585370000	C	0.706188000	3.757063000	1.759130000
C	-6.741111000	0.127621000	-0.166840000	C	2.530669000	4.602465000	0.152440000
C	-7.435337000	-1.218210000	-0.447730000	C	-0.997466000	1.685800000	2.555570000
C	-7.424503000	0.813949000	1.030960000	C	0.715791000	2.519750000	1.096620000
C	-7.305815000	-2.122154000	0.791920000	C	-0.134646000	1.455389000	1.468910000

C	-3.595821000	-1.195180000	-7.266980000	H	0.187167000	6.041361000	0.246320000
C	-5.189245000	-0.420994000	-4.178070000	H	3.336564000	7.888292000	-0.692160000
C	-3.012888000	-1.476286000	-4.833230000	H	2.009145000	6.895762000	-1.324510000
C	-1.958678000	-0.020931000	-2.555570000	H	6.574826000	-5.199480000	0.596440000
C	1.193080000	0.844302000	-1.468910000	H	5.492486000	-3.433437000	1.960600000
C	0.961212000	1.706731000	-2.555570000	H	5.138388000	-3.182772000	0.246320000
C	1.997419000	2.348775000	-3.255590000	H	5.643375000	-7.198104000	1.796140000
C	1.730220000	3.258784000	-4.466760000	H	5.765457000	-5.807561000	2.889520000
C	0.227943000	3.347381000	-4.833230000	H	5.163179000	-6.833695000	-0.692160000
C	-0.000003000	4.266706000	-6.049610000	H	4.967333000	-5.187851000	-1.324510000
C	0.507362000	5.685391000	-5.728800000	H	4.318503000	-2.277106000	3.368110000
C	2.009940000	5.623390000	-5.396130000	H	3.539393000	-6.932271000	3.139570000
C	2.780442000	5.063777000	-6.607950000	H	3.665933000	-4.475097000	3.495490000
C	2.265162000	3.648213000	-6.935360000	H	2.100087000	-4.916038000	2.800600000
C	0.762855000	3.711663000	-7.266980000	H	1.586590000	0.980178000	2.891380000
C	2.230031000	4.704514000	-4.178070000	H	1.337371000	-2.412467000	0.289430000
C	2.486170000	2.726482000	-5.719710000	H	2.735582000	-6.289270000	-1.056430000
C	3.311125000	2.118780000	-2.834770000	H	2.864170000	-3.832446000	-0.718430000
C	3.606806000	1.266955000	-1.759130000	H	1.633944000	-4.549082000	0.325520000
C	5.081073000	1.016036000	-1.393730000	H	1.923768000	-6.924433000	1.224540000
C	5.813571000	2.357864000	-1.099900000	H	3.375167000	-7.853303000	0.805350000
C	7.305815000	2.122154000	-0.791920000	H	4.065864000	1.663351000	8.149740000
C	7.435337000	1.218210000	0.447730000	H	2.536952000	1.016394000	7.524040000
C	6.741111000	-0.127621000	0.166840000	H	4.218599000	-0.820873000	7.798890000
C	7.424503000	-0.813949000	-1.030960000	H	2.544052000	-0.997086000	5.947480000
C	7.295820000	0.087622000	-2.272740000	H	4.076700000	-1.763039000	5.508210000
C	7.980725000	1.440580000	-1.998300000	H	3.184779000	3.085744000	6.272280000
C	5.251186000	0.109608000	-0.152440000	H	3.054189000	2.164798000	3.973490000
C	5.804976000	0.322402000	-2.585370000	H	1.944760000	1.312200000	5.054040000
C	2.538526000	0.639095000	-1.096620000	H	6.290468000	-0.828418000	6.389320000
C	0.997466000	-1.685800000	-2.555570000	H	6.284683000	0.569066000	7.480790000
C	1.035389000	-2.904203000	-3.255590000	H	5.671861000	2.889703000	6.588050000
C	1.957079000	-3.127807000	-4.466760000	H	5.261133000	3.099047000	4.875390000
C	2.784945000	-1.871095000	-4.833230000	H	6.936014000	1.256278000	5.156080000
C	3.695077000	-2.133351000	-6.049610000	H	5.709206000	-0.514759000	3.913090000
C	4.670012000	-3.282084000	-5.728800000	H	5.267338000	1.084368000	3.299250000
C	3.865028000	-4.552354000	-5.396130000	H	-3.300397000	-4.686937000	3.913090000
C	2.995139000	-4.939822000	-6.607950000	H	-1.694579000	-5.103832000	3.299250000
C	2.026864000	-3.785794000	-6.935360000	H	-2.135528000	-1.704670000	5.947480000
C	2.832967000	-2.516483000	-7.266980000	H	-3.565187000	-2.649006000	5.508210000
C	2.959213000	-4.283521000	-4.178070000	H	-2.380038000	-6.634903000	5.156080000
C	1.118117000	-3.516328000	-3.519710000	H	0.347676000	-3.727404000	3.973490000
C	0.179354000	-3.926908000	-2.834770000	H	0.164019000	-2.340311000	5.054040000
C	-0.706188000	-3.757063000	-1.759130000	H	-3.862664000	-5.033496000	6.389320000
C	-1.660624000	-4.908357000	-1.393730000	H	-2.649516000	-5.727228000	7.480790000
C	-2.530669000	-4.602465000	-0.152440000	H	-2.820196000	-3.242978000	7.798890000
C	-3.481078000	-5.774163000	0.166840000	H	-0.333375000	-6.356827000	6.588050000
C	-4.417152000	-6.022834000	-1.030960000	H	0.053287000	-6.105798000	4.875390000
C	-3.572027000	-6.362177000	-2.272740000	H	1.079943000	-4.300971000	6.272280000
C	-2.742784000	-7.631801000	-1.998300000	H	-0.592428000	-4.352817000	8.149740000
C	-1.815068000	-3.388098000	-0.791920000	H	-0.388253000	-2.705262000	7.524040000
C	-2.662668000	-7.048296000	0.447730000	H	-3.401864000	1.562606000	3.973490000
C	-2.623280000	-5.188458000	-2.585370000	H	-2.108778000	1.028111000	5.054040000
C	-0.864815000	-6.213632000	-1.099900000	H	-2.408808000	5.201697000	3.913090000
C	-0.715791000	-2.517975000	-1.096620000	H	-3.572759000	4.019465000	3.299250000
H	0.055563000	-1.864116000	2.891380000	H	-4.264722000	1.215227000	6.272280000
H	-4.131283000	-2.601380000	3.368110000	H	-0.408524000	2.701757000	5.947480000
H	-2.757943000	0.048036000	0.289430000	H	-0.511513000	4.412045000	5.508210000
H	-4.751080000	-0.564221000	-0.718430000	H	-5.338487000	3.467125000	6.588050000
H	-4.756592000	0.859504000	0.325520000	H	-5.314420000	3.006751000	4.875390000
H	-5.719687000	-3.039914000	1.960600000	H	-4.555976000	5.378625000	5.156080000
H	-5.325555000	-2.858589000	0.246320000	H	-3.473436000	2.689466000	8.149740000
H	-5.708514000	-0.937242000	3.495490000	H	-2.148699000	1.688868000	7.524040000
H	-5.307457000	0.639290000	2.800600000	H	-1.398403000	4.063850000	7.798890000
H	-6.814459000	0.775551000	-1.056430000	H	-2.427803000	5.861914000	6.389320000
H	-8.499743000	-1.054597000	-0.692160000	H	-3.635167000	5.158162000	7.480790000
H	-6.976478000	-1.707911000	-1.324510000	H	-1.337371000	2.412467000	-0.289430000
H	-6.958619000	1.796185000	1.224540000	H	-2.864170000	3.832446000	0.718430000
H	-8.488744000	1.003671000	0.805350000	H	-1.633944000	4.549082000	-0.325520000
H	-7.790295000	-3.094226000	0.596440000	H	-2.735582000	6.289270000	1.056430000
H	-7.773220000	0.400932000	3.139570000	H	-1.923768000	6.924433000	-1.224540000
H	-9.055428000	-1.288254000	1.796140000	H	-3.375167000	7.853303000	-0.805350000
H	-7.912223000	-2.089252000	2.889520000	H	-3.539393000	6.932271000	-3.139570000
H	4.233827000	6.531340000	3.139570000	H	-5.643375000	7.198104000	-1.796140000
H	2.042581000	5.412340000	3.495490000	H	-5.765457000	5.807561000	-2.889520000
H	3.207370000	4.276747000	2.800600000	H	-6.574826000	5.199480000	-0.596440000
H	5.034851000	5.128248000	1.224540000	H	-5.163179000	6.833695000	0.692160000
H	5.113576000	6.849632000	0.805350000	H	-4.967333000	5.187851000	1.324510000
H	3.412053000	8.486358000	1.796140000	H	-3.665933000	4.475097000	-3.495490000
H	2.146767000	7.896812000	2.889520000	H	-2.100087000	4.916038000	-2.800600000
H	-0.187220000	4.878486000	3.368110000	H	-5.492486000	3.433437000	-1.960600000
H	4.078876000	5.513719000	-1.056430000	H	-5.138388000	3.182772000	-0.246320000
H	1.886910000	4.396667000	-0.718430000	H	-4.318503000	2.277106000	-3.368110000
H	3.122649000	3.689578000	0.325520000	H	-2.544052000	0.997086000	-5.947480000
H	-1.642154000	0.883939000	2.891380000	H	-4.076700000	1.763039000	-5.508210000
H	1.420572000	2.364431000	0.289430000	H	-4.218599000	0.820873000	-7.798890000
H	1.215469000	8.293706000	0.596440000	H	-6.290468000	0.828418000	-6.389320000
H	0.227201000	6.473351000	1.960600000	H	-6.284683000	-0.569066000	-7.480790000

H	-6.936014000	-1.256278000	-5.156080000	C	-3.517500000	3.705780000	1.392680000
H	-5.671861000	-2.889703000	-6.588050000	C	-4.989000000	3.678460000	0.906730000
H	-5.261133000	-3.099047000	-4.875390000	C	-3.441710000	4.563070000	2.684220000
H	-3.184779000	-3.085744000	-6.272280000	C	-3.191190000	5.837110000	0.048900000
H	-4.065864000	-1.663351000	-8.149740000	C	-4.656480000	5.786290000	-0.416870000
H	-2.536952000	-1.016394000	-7.524040000	C	-3.099040000	6.658670000	1.345520000
H	-5.709206000	0.514759000	-3.913090000	C	-5.510960000	5.105560000	0.664420000
H	-5.267338000	-1.084368000	-3.299250000	C	-3.957140000	5.988060000	2.432360000
H	-3.054189000	-2.164798000	-3.973490000	C	-5.422770000	5.918250000	1.968020000
H	-1.944760000	-1.312200000	-5.054040000	C	7.164382000	0.432954000	2.432360000
H	-1.586590000	-0.980178000	-2.891380000	C	5.672590000	0.699073000	2.684220000
H	-0.055563000	1.864116000	-2.891380000	C	7.316097000	-0.645488000	1.345520000
H	-0.347676000	3.727404000	-3.973490000	C	7.836740000	1.737132000	1.968020000
H	-0.164019000	2.340311000	-5.054040000	C	3.148837000	2.419065000	2.666510000
H	-1.079943000	4.300971000	-6.272280000	C	4.968050000	1.193354000	1.392680000
H	0.333375000	6.356827000	-6.588050000	C	1.820960000	2.611136000	3.054870000
H	-0.053287000	6.105798000	-4.875390000	C	6.650681000	-0.154903000	0.048900000
H	2.380038000	6.634903000	-5.156080000	C	3.495149000	1.464455000	1.697390000
H	3.862664000	5.033496000	-6.389320000	C	5.159170000	0.109264000	0.310730000
H	2.649516000	5.727228000	-7.480790000	C	0.829527000	1.844803000	2.424790000
H	2.820196000	3.242978000	-7.798890000	C	2.472717000	0.733952000	1.085310000
H	0.592428000	4.352817000	-8.149740000	C	1.119174000	0.917886000	1.418840000
H	0.388253000	2.705262000	-7.524040000	C	7.177025000	2.219851000	0.664420000
H	3.300397000	4.686937000	-3.913090000	C	5.680140000	2.481371000	0.906730000
H	1.694579000	5.103832000	-3.299250000	C	7.339314000	1.139485000	-0.416870000
H	2.135528000	1.704670000	-5.947480000	C	-1.666065000	-7.325411000	0.664420000
H	3.565187000	2.649006000	-5.508210000	C	-0.691140000	-6.159831000	0.906730000
H	4.131283000	2.601380000	-3.368110000	C	-2.413970000	-7.655382000	1.968020000
H	5.719687000	3.039914000	-1.960600000	C	-2.682834000	-6.925775000	-0.416870000
H	5.325555000	2.858589000	-0.246320000	C	0.520553000	-3.936505000	2.666510000
H	7.790295000	3.094226000	-0.596440000	C	-1.450550000	-4.899134000	1.392680000
H	8.499743000	1.054597000	0.692160000	C	1.350830000	-2.882566000	3.054870000
H	6.976478000	1.707911000	1.324510000	C	-3.207242000	-6.421014000	2.432360000
H	6.814459000	-0.775551000	1.056430000	C	-0.479319000	-3.759115000	1.697390000
H	6.958619000	-1.796185000	-1.224540000	C	-2.230880000	-5.262143000	2.684220000
H	8.488744000	-1.003671000	-0.805350000	C	1.182883000	-1.640793000	2.424790000
H	7.773220000	-0.400932000	-3.139570000	C	-0.600737000	-2.508412000	1.085310000
H	9.055428000	1.288254000	-1.796140000	C	0.235326000	-1.428176000	1.418840000
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H	4.751080000	0.564221000	0.718430000	C	-2.484960000	-4.522604000	0.310730000
H	4.756592000	-0.859504000	-0.325520000	C	-4.217057000	-6.013182000	1.345520000
H	5.708514000	0.937242000	-3.495490000	C	3.592000000	-2.768480000	6.843470000
H	5.307457000	-0.639290000	-2.800060000	C	3.021150000	-4.112350000	6.362160000
H	2.757943000	-0.048036000	-0.289430000	C	1.901260000	-3.859900000	5.338000000
H	1.642154000	-1.003671000	-2.891380000	C	4.155750000	-1.998860000	5.638340000
H	3.401864000	-1.562606000	-3.973490000	C	3.038130000	-1.754060000	4.611250000
H	2.108778000	-1.028111000	-5.054040000	C	2.441020000	-3.088130000	4.107680000
H	4.264722000	-1.215227000	-6.272280000	C	4.139260000	-4.940120000	5.702640000
H	5.338487000	-3.467125000	-6.588050000	C	5.279430000	-2.820580000	4.982220000
H	5.314420000	-3.006751000	-4.875390000	C	4.712180000	-4.166990000	4.502060000
H	4.555976000	-5.378625000	-5.156080000	C	3.593230000	-3.913360000	3.480340000
H	2.427803000	-5.861914000	-6.389320000	C	-5.185684000	-1.155148000	3.480340000
H	3.635167000	-5.158162000	-7.480790000	C	-3.894909000	-0.569920000	4.107680000
H	1.398403000	-4.063850000	-7.798890000	C	-4.293401000	0.283411000	5.338000000
H	3.473346000	-2.689466000	-8.149740000	C	-5.964809000	-1.997373000	4.502060000
H	2.148699000	-1.688868000	-7.524040000	C	-3.038126000	-1.754068000	4.611250000
H	2.408808000	-5.201697000	-3.913090000	C	-6.347899000	-1.114644000	5.702640000
H	3.572759000	-4.019465000	-3.299250000	C	-5.071975000	-0.560218000	6.362160000
H	0.408524000	-2.701757000	-5.947480000	C	-5.082409000	-3.161830000	4.982220000
H	0.511513000	-4.412045000	-5.508210000	C	-3.808939000	-2.599555000	5.638340000
H	0.187220000	-4.878486000	-3.368110000	C	-4.193574000	-1.726523000	6.843470000
H	-1.886910000	-4.396667000	0.718430000	C	-0.000004000	3.508128000	4.611250000
H	-3.122649000	-3.689578000	-0.325520000	C	1.453889000	3.658050000	4.107680000
H	-4.078876000	-5.513719000	1.056430000	C	1.592454000	5.068508000	3.480340000
H	-5.034851000	-5.128248000	-1.224540000	C	-0.346811000	4.598415000	5.638340000
H	-5.113576000	-6.849632000	-0.805350000	C	2.392141000	3.576489000	5.338000000
H	-4.233827000	-6.531340000	-3.139570000	C	-0.197021000	5.982410000	4.982220000
H	-3.412053000	-8.486358000	-1.796140000	C	1.252629000	6.164363000	4.502060000
H	-2.146767000	-7.896812000	-2.889520000	C	0.601574000	4.495003000	6.843470000
H	-1.215469000	-8.293706000	-0.596440000	C	2.050825000	4.672568000	6.362160000
H	-3.336564000	-7.888292000	0.692160000	C	2.208639000	6.054764000	5.702640000
H	-2.009145000	-6.895762000	1.324510000	C	-1.119174000	-0.917886000	-1.418840000
H	-2.042581000	-5.412340000	-3.495490000	C	0.000000000	0.000000000	-0.831840000
H	-3.207370000	-4.276747000	-2.800060000	C	-0.235326000	1.428176000	-1.418840000
H	-0.227201000	-6.473351000	-1.960600000	C	0.600737000	2.508412000	-1.085310000
H	-0.187167000	-6.041361000	-0.246320000	C	0.479319000	3.759115000	-1.697390000
H	-1.420572000	-2.364431000	-0.289430000	C	1.450550000	4.899134000	-1.392680000
				C	2.484960000	4.522604000	-0.310730000
				C	3.459491000	5.682207000	-0.048900000
				C	4.217057000	6.013182000	-1.345520000
				C	3.207242000	6.421014000	-2.432360000
				C	2.413970000	7.655382000	-1.968020000
				C	1.666065000	7.325411000	-0.664420000
				C	2.682834000	6.925775000	0.416870000
				C	2.230880000	5.262143000	-2.684220000
				C	0.691140000	6.159831000	-0.906730000
				C	-0.520553000	3.936505000	-2.666510000
				C	-1.350830000	2.882566000	-3.054870000

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C	0.000000000	0.000000000	0.831840000				
C	-2.012410000	-0.204010000	2.424790000				
C	-3.171790000	0.271430000	3.054870000				
C	-1.354500000	0.510290000	1.418840000				
C	-3.669390000	1.517440000	2.666510000				
C	-1.871980000	1.774460000	1.085310000				
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C	-2.441020000	3.088130000	-4.107680000	H	6.741731000	-0.927439000	-0.732350000
C	-1.901260000	3.859900000	-5.338000000	H	4.660976000	0.412947000	-0.621530000
C	-3.021150000	4.112350000	-6.362160000	H	4.674875000	-0.826659000	0.631770000
C	-4.139260000	4.940120000	-5.702640000	H	-0.195321000	1.969735000	2.743160000
C	-4.712180000	4.166990000	-4.502060000	H	2.734743000	-0.025786000	0.363620000
C	-5.279430000	2.820580000	-4.982220000	H	7.657015000	3.154818000	0.330290000
C	-4.155750000	1.998860000	-5.638340000	H	5.558249000	3.284991000	1.650760000
C	-3.592000000	2.768480000	-6.843470000	H	5.198192000	2.832773000	-0.021020000
C	-3.593230000	3.913360000	-3.480340000	H	8.410078000	0.950862000	-0.606960000
C	-3.038130000	1.754060000	-4.611250000	H	6.898990000	1.486602000	-1.363860000
C	-1.182883000	1.640793000	-2.424790000	H	-1.096355000	-8.208578000	0.330290000
C	1.354500000	-0.510290000	-1.418840000	H	0.065761000	-6.456081000	1.650760000
C	2.012410000	0.204010000	-2.424790000	H	-0.145842000	-5.918153000	-0.021020000
C	3.171790000	-0.271430000	-3.054870000	H	-3.096137000	-8.507254000	1.805790000
C	3.894909000	0.569920000	-4.107680000	H	-1.697664000	-7.958799000	2.751120000
C	3.038126000	1.754060000	-4.611250000	H	-3.381568000	-7.758772000	-0.606960000
C	3.808939000	2.599555000	-5.638340000	H	-2.162060000	-6.718002000	-1.363860000
C	5.082409000	3.161830000	-4.982220000	H	0.632909000	-4.911571000	3.140410000
C	5.964809000	1.997373000	-4.502060000	H	-3.742606000	-6.652996000	3.368360000
C	6.347899000	1.114644000	-5.702640000	H	-1.526049000	-5.532926000	3.486640000
C	5.071975000	0.560218000	-6.362160000	H	-2.777904000	-4.371110000	3.031440000
C	4.193574000	1.726523000	-6.843470000	H	1.803501000	-0.815715000	2.743160000
C	5.185684000	1.155148000	-3.480340000	H	-1.389703000	-2.355464000	0.363620000
C	4.293401000	-0.283411000	-5.338000000	H	-4.174051000	-5.374791000	-0.732350000
C	3.669390000	-1.517440000	-2.666510000	H	-1.972866000	-4.242997000	-0.621530000
C	3.015830000	-2.294660000	-1.697390000	H	-3.053345000	-3.635231000	0.631770000
C	3.517500000	-3.705780000	-1.392680000	H	-4.797664000	-5.135522000	1.679410000
C	4.989000000	-3.678460000	-0.906730000	H	-4.937484000	-6.830287000	1.169240000
C	5.510960000	-5.105560000	-0.664420000	H	4.383510000	-2.936830000	7.593850000
C	4.656480000	-5.786290000	-0.416870000	H	2.800790000	-2.176090000	7.334300000
C	3.191190000	-5.837110000	-0.048900000	H	2.606640000	-4.668260000	7.219580000
C	3.099040000	-6.658670000	-1.345520000	H	1.081110000	-3.281780000	5.796350000
C	3.957140000	-5.988060000	-2.432360000	H	1.475210000	-4.825770000	5.025140000
C	5.422770000	-5.918250000	-1.968020000	H	4.554840000	-1.025770000	5.969210000
C	2.674210000	-4.413340000	-0.310730000	H	3.450620000	-1.184120000	3.765890000
C	3.441710000	-4.563070000	-2.684220000	H	2.241770000	-1.132730000	5.053980000
C	1.871980000	-1.774460000	-1.085310000	H	3.742170000	-5.914730000	5.369720000
C	-0.829527000	-1.844803000	-2.424790000	H	4.937730000	-5.149260000	6.434840000
C	-1.820960000	-2.6111136000	-3.054870000	H	6.098410000	-2.987860000	5.702590000
C	-1.453889000	-3.658050000	-4.107680000	H	5.707550000	-2.265050000	4.130040000
C	0.000004000	-3.508128000	-4.611250000	H	5.510740000	-4.759240000	4.024420000
C	0.346811000	-4.598415000	-5.638340000	H	3.196310000	-4.869820000	3.102970000
C	0.197021000	-5.982410000	-4.982220000	H	3.989290000	-3.368010000	2.607510000
C	-1.252629000	-6.164363000	-4.502060000	H	-5.815543000	-0.333176000	3.102970000
C	-2.208639000	-6.054764000	-5.702640000	H	-4.911427000	-1.770821000	2.607510000
C	-2.050825000	-4.672568000	-6.362160000	H	-3.382660000	0.704621000	5.796350000
C	-0.601574000	-4.495003000	-6.843470000	H	-4.916844000	1.135316000	5.025140000
C	-1.592454000	-5.068508000	-3.480340000	H	-6.876993000	-2.392821000	4.024420000
C	-2.392141000	-3.576489000	-5.338000000	H	-2.750788000	-2.396265000	3.765890000
C	-3.148837000	-2.419065000	-2.666510000	H	-2.101858000	-1.375065000	5.053980000
C	-3.495149000	-1.464455000	-1.697390000	H	-6.993391000	-0.283449000	5.369720000
C	-4.968050000	-1.193354000	-1.392680000	H	-6.928255000	-1.701570000	6.434840000
C	-5.159170000	-0.109264000	-0.310730000	H	-5.346152000	0.076714000	7.219580000
C	-6.650681000	0.154903000	-0.048900000	H	-5.636768000	-3.787448000	5.702590000
C	-7.316097000	0.645488000	-1.345520000	H	-4.815366000	-3.810358000	4.130040000
C	-7.164382000	-0.432954000	-2.432360000	H	-3.165763000	-3.431722000	5.969210000
C	-7.836740000	-1.737132000	-1.968020000	H	-4.735124000	-2.327816000	7.593850000
C	-7.177025000	-2.219851000	-0.664420000	H	-3.284944000	-1.337510000	7.334300000
C	-7.339314000	-1.139485000	0.416870000	H	-0.699832000	3.580385000	3.765890000
C	-5.672590000	-0.699073000	-2.684220000	H	-0.139912000	2.507795000	5.053980000
C	-5.680140000	-2.481371000	-0.906730000	H	2.619233000	5.202996000	3.102970000
C	-2.472717000	-0.733952000	-1.085310000	H	0.922137000	5.138831000	2.607510000
H	-1.608180000	-1.154020000	2.743160000	H	-1.389077000	4.457492000	5.969210000
H	-4.570000000	1.907670000	3.140410000	H	2.301550000	2.577159000	5.796350000
H	-1.345040000	2.381250000	0.363620000	H	3.441634000	3.690454000	5.025140000
H	-2.688110000	3.830050000	-0.621530000	H	-0.461642000	6.775308000	5.702590000
H	-1.621530000	4.461890000	0.631770000	H	-0.892184000	6.075408000	4.130040000
H	-5.624010000	3.171090000	1.650760000	H	1.366253000	7.152061000	4.024420000
H	-5.052350000	3.085380000	-0.021020000	H	0.351614000	5.264646000	7.593850000
H	-4.028630000	4.088060000	3.486640000	H	0.484154000	3.513600000	7.334300000
H	-2.396540000	4.591290000	3.031440000	H	2.739512000	4.591546000	7.219580000
H	-2.567680000	6.302230000	-0.732350000	H	3.251221000	6.198179000	5.369720000
H	-5.028510000	6.807910000	-0.606960000	H	1.990525000	6.850830000	6.434840000
H	-4.736930000	5.231400000	-1.363860000	H	1.389703000	2.355464000	-0.363620000
H	-2.048660000	6.722660000	1.679410000	H	1.972866000	4.242997000	0.621530000
H	-3.446460000	7.691130000	1.169240000	H	3.053345000	3.635231000	-0.631770000
H	-6.560660000	5.053760000	0.330290000	H	4.174051000	5.374791000	0.732350000
H	-3.890360000	6.567690000	3.368360000	H	4.797664000	5.135522000	-1.679410000
H	-5.819430000	6.934960000	1.805790000	H	4.937484000	6.830287000	-1.169240000
H	-6.043690000	5.449620000	2.751120000	H	3.742606000	6.652996000	-3.368360000
H	7.632966000	0.085306000	3.368360000	H	3.096137000	8.507254000	-1.805790000
H	5.554679000	1.444866000	3.486640000	H	1.697664000	7.958799000	-2.751120000
H	5.174444000	-0.220180000	3.031440000	H	1.096355000	8.208578000	-0.330290000
H	6.846324000	-1.587138000	1.679410000	H	3.381568000	7.758772000	0.606960000
H	8.383944000	-0.860843000	1.169240000	H	2.162060000	6.718002000	1.363860000
H	8.915567000	1.572294000	1.805790000	H	1.526049000	5.532926000	-3.486640000
H	7.741354000	2.509179000	2.751120000	H	2.777904000	4.371110000	-0.331440000
H	3.937091000	3.003901000	3.140410000	H	-0.065761000	6.456081000	-1.650760000

H	0.145842000	5.918153000	0.021020000				
H	-0.632909000	4.911571000	-3.140410000				
H	-1.081110000	3.281780000	-5.796350000				
H	-1.475210000	4.825770000	-5.025140000	C	0.000000000	0.000000000	0.830200000
H	-2.606640000	4.668260000	-7.219580000	C	-1.625780000	-1.183720000	2.442080000
H	-3.742170000	5.914730000	-5.369720000	C	-2.863480000	-1.361270000	3.075610000
H	-4.937730000	5.149260000	-6.434840000	C	-1.425800000	-0.245830000	1.425810000
H	-5.510740000	4.759240000	-4.024420000	C	-3.928600000	-0.552020000	2.683060000
H	-6.098410000	2.987860000	-5.702590000	C	-2.518670000	0.571590000	1.090010000
H	-5.707550000	2.265050000	-4.130040000	C	-3.766010000	0.438420000	1.704070000
H	-4.554840000	1.025770000	-5.969210000	C	-4.567690000	2.392630000	0.279010000
H	-4.383510000	2.936830000	-7.593850000	C	-4.929350000	1.371670000	1.372830000
H	-2.800790000	2.176090000	-7.334300000	C	-6.151820000	0.562330000	0.883970000
H	-3.196310000	4.869820000	-3.102970000	C	-5.341050000	2.157540000	2.640440000
H	-3.989290000	3.368010000	-2.607510000	C	-5.751990000	3.320910000	-0.020910000
H	-3.450620000	1.184120000	-3.765890000	C	-6.958140000	2.496080000	-0.491200000
H	-2.241770000	1.132730000	-5.053980000	C	-6.130780000	4.088140000	1.252880000
H	-1.803501000	0.815715000	-2.743160000	C	-7.342380000	1.489310000	0.599640000
H	1.608180000	1.154020000	-2.743160000	C	-6.525040000	3.088280000	2.348800000
H	2.750788000	2.396265000	-3.765890000	C	-7.720720000	2.248360000	1.878470000
H	2.101858000	1.375065000	-5.053980000	C	5.937049000	4.106710000	2.348800000
H	3.165763000	3.431722000	-5.969210000	C	4.539009000	3.546715000	2.640440000
H	5.636768000	3.787448000	-5.702590000	C	6.605823000	3.265341000	1.252880000
H	4.815366000	3.810358000	-4.130040000	C	5.807497000	5.562160000	1.878470000
H	6.876993000	2.392821000	-4.024420000	C	1.486237000	3.678277000	2.683060000
H	6.993391000	0.283449000	-5.369720000	C	3.652576000	3.583107000	1.372830000
H	6.928255000	1.701570000	-6.434840000	C	0.252846000	3.160481000	3.075610000
H	5.346152000	-0.076714000	-7.219580000	C	5.751987000	3.320914000	-0.020910000
H	4.735124000	2.327816000	-7.593850000	C	2.262688000	3.042250000	1.704070000
H	3.284944000	1.337510000	-7.334300000	C	4.355923000	2.759421000	0.279010000
H	5.815543000	0.333176000	-3.102970000	C	-0.212242000	1.999827000	2.442080000
H	4.911427000	1.770821000	-2.607510000	C	1.754346000	1.895437000	1.090010000
H	3.382660000	-0.704621000	-5.796350000	C	0.500005000	1.357694000	1.425810000
H	4.916844000	-1.135316000	-5.025140000	C	4.960970000	5.614033000	0.599640000
H	4.570000000	-1.907670000	-3.140410000	C	3.562902000	5.046467000	0.883970000
H	5.624010000	-3.171090000	-1.650760000	C	5.640739000	4.777886000	-0.491200000
H	5.052350000	-3.085380000	0.021020000	C	2.381410000	-7.103343000	0.599640000
H	6.560660000	-5.053760000	-0.330290000	C	2.588918000	-5.608797000	0.883970000
H	5.028510000	-6.807910000	0.606960000	C	1.913223000	-7.810520000	1.878470000
H	4.736930000	-5.231400000	1.363860000	C	1.317401000	-7.273966000	-0.491200000
H	2.567680000	-6.302230000	0.732350000	C	2.442363000	-3.126257000	2.683060000
H	2.048660000	-6.722660000	-1.679410000	C	1.276774000	-4.954777000	1.372830000
H	3.446460000	-7.691130000	-1.169240000	C	2.610634000	-1.799211000	3.075610000
H	3.890360000	-6.567690000	-3.368360000	C	0.587991000	-7.194990000	2.348800000
H	5.819430000	-6.934960000	-1.805790000	C	1.503322000	-3.480670000	1.704070000
H	6.043690000	-5.449620000	-2.751120000	C	0.802041000	-5.704255000	2.640440000
H	2.688110000	-3.830050000	0.621530000	C	1.838022000	-0.816107000	2.442080000
H	1.621530000	-4.461890000	-0.631770000	C	0.764324000	-2.467027000	1.090010000
H	4.028630000	-4.088060000	-3.486640000	C	0.925795000	-1.111864000	1.425810000
H	2.396540000	-4.591290000	-3.031440000	C	0.000003000	-6.641824000	-0.020910000
H	1.345040000	-2.381250000	-0.363620000	C	0.211767000	-5.152051000	0.279010000
H	0.195321000	-1.969735000	-2.743160000	C	-0.475043000	-7.353481000	1.252880000
H	0.699832000	-3.580385000	-3.765890000	C	4.457590000	-0.498530000	6.844150000
H	0.139912000	-2.507795000	-5.053980000	C	4.605050000	-1.964350000	6.418230000
H	1.389077000	-4.457492000	-5.969210000	C	3.519690000	-2.313580000	5.389630000
H	0.461642000	-6.775308000	-5.702590000	C	4.604140000	0.402690000	5.612130000
H	0.892184000	-6.075408000	-4.130040000	C	3.523850000	0.048470000	4.582080000
H	-1.366253000	-7.152061000	-4.024420000	C	3.645280000	-1.421450000	4.134200000
H	-3.251221000	-6.198179000	-5.369720000	C	5.989230000	-2.178680000	5.788850000
H	-1.990525000	-6.850830000	-6.434840000	C	5.991410000	0.195320000	4.988500000
H	-2.739512000	-4.591546000	-7.219580000	C	6.142620000	-1.270360000	4.561160000
H	-0.351614000	-5.264646000	-7.593850000	C	5.055960000	-1.610000000	3.533890000
H	-0.484154000	-3.513600000	-7.334300000	C	-3.922281000	-3.573590000	3.533890000
H	-2.619233000	-5.202996000	-3.102970000	C	-3.053652000	-2.446180000	4.134200000
H	-0.922137000	-5.138831000	-2.607510000	C	-3.763464000	-1.891351000	5.389630000
H	-2.301550000	-2.577159000	-5.796350000	C	-4.171474000	-4.684485000	4.561160000
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H	-4.660976000	-0.412947000	0.621530000	C	-4.003702000	-3.005915000	6.418230000
H	-4.674875000	0.826659000	-0.631770000	C	-2.826553000	-5.286373000	4.988500000
H	-6.741731000	0.927439000	0.732350000	C	-1.953330000	-4.188647000	5.612130000
H	-6.846324000	1.587138000	-1.679410000	C	-2.660535000	-3.611121000	6.844150000
H	-8.383944000	0.860843000	-1.169240000	C	-1.803901000	3.027509000	4.582080000
H	-7.632966000	-0.085306000	-3.368360000	C	-0.591628000	3.867630000	4.134200000
H	-8.915567000	-1.572294000	-1.805790000	C	-1.133679000	5.183590000	3.533890000
H	-7.741354000	-2.509179000	-2.751120000	C	-2.650810000	3.785957000	5.612130000
H	-7.657015000	-3.154818000	-0.330290000	C	0.243774000	4.204931000	5.389630000
H	-8.410078000	-0.950862000	0.606960000	C	-3.164857000	5.091053000	4.988500000
H	-6.898990000	-1.486602000	1.363860000	C	-1.971146000	5.954845000	4.561160000
H	-5.554679000	-1.444866000	-3.486640000	C	-1.797055000	4.109651000	6.844150000
H	-5.174444000	0.220180000	-3.031440000	C	-0.601348000	4.970265000	6.418230000
H	-5.558249000	-3.284991000	-1.650760000	C	-1.107823000	6.276165000	5.788850000
H	-5.198192000	-2.832773000	0.021020000	C	-0.500005000	-1.357694000	-1.425810000
H	-2.734743000	0.025786000	-0.363620000	C	0.000000000	0.000000000	-0.830200000
				C	-0.925795000	1.111864000	-1.425810000
				C	-0.764324000	2.467027000	-1.090010000
				C	-1.503322000	3.480670000	-1.704070000
				C	-1.276774000	4.954777000	-1.372830000
				C	-0.211767000	5.152051000	-0.279010000

C	-0.000003000	6.641824000	0.020910000	H	-8.589500000	2.899550000	1.686490000
C	0.475043000	7.353481000	-1.252880000	H	-8.013480000	1.537170000	2.669140000
C	-0.587991000	7.194990000	-2.348800000	H	6.542008000	4.066770000	3.268410000
C	-1.913223000	7.810520000	-1.878470000	H	4.063469000	4.127714000	3.447920000
C	-2.381410000	7.103343000	-0.599640000	H	4.614205000	2.504797000	2.995000000
C	-1.317401000	7.273966000	0.491200000	H	6.710791000	2.220171000	1.591890000
C	-0.802041000	5.704255000	-2.640440000	H	7.619840000	3.647330000	1.047990000
C	-2.588918000	5.608797000	-0.883970000	H	6.805834000	5.988950000	1.686490000
C	-2.442363000	3.126257000	-2.683060000	H	5.337968000	6.171292000	2.669140000
C	-2.610634000	1.799211000	-3.075610000	H	1.866489000	4.585414000	3.157820000
C	-3.645280000	1.421450000	-4.134200000	H	6.218609000	2.708726000	-0.810040000
C	-3.519690000	2.313580000	-5.389630000	H	3.743273000	2.750859000	-0.638650000
C	-4.605050000	1.964350000	-6.418230000	H	4.444919000	1.709085000	0.608410000
C	-5.989230000	2.178680000	-5.788850000	H	-1.151018000	1.579779000	2.777650000
C	-6.142620000	1.270360000	-4.561160000	H	2.369977000	1.385400000	0.360740000
C	-5.991410000	-0.195320000	-4.988500000	H	4.864644000	6.657551000	0.260920000
C	-4.604140000	-0.402690000	-5.612130000	H	3.058225000	5.666701000	1.643420000
C	-4.457590000	0.498530000	-6.844150000	H	2.943205000	5.084421000	-0.028850000
C	-5.055960000	1.610000000	-3.533890000	H	6.644092000	5.182185000	-0.706750000
C	-3.523850000	-0.048470000	-4.582080000	H	5.058422000	4.832363000	-1.424000000
C	-1.838022000	0.816107000	-2.442080000	H	3.333286000	-7.541681000	0.260920000
C	1.425800000	0.245830000	-1.425810000	H	3.378395000	-5.481851000	1.643420000
C	1.625780000	1.183720000	-2.442080000	H	2.931635000	-5.091101000	-0.028850000
C	2.863480000	1.361270000	-3.075610000	H	1.783666000	-8.888500000	1.686490000
C	3.053652000	2.446180000	-4.134200000	H	2.675512000	-7.708462000	2.669140000
C	1.719949000	3.075979000	-4.582080000	H	1.165858000	-8.345045000	-0.706750000
C	1.953330000	4.188647000	-5.612130000	H	1.655738000	-6.796903000	-1.424000000
C	2.826553000	5.286373000	-4.988500000	H	3.037841000	-3.909134000	3.157820000
C	4.171474000	4.684485000	-4.561160000	H	0.250922000	-7.698930000	3.268410000
C	4.881407000	4.097485000	-5.788850000	H	1.542971000	-5.582924000	3.447920000
C	4.003702000	3.005915000	-6.418230000	H	-0.137885000	-5.248417000	2.995000000
C	2.660535000	3.611121000	-6.844150000	H	1.943638000	0.206921000	2.777650000
C	3.922281000	3.573590000	-3.533890000	H	0.014803000	-2.745160000	0.360740000
C	3.763464000	1.891351000	-5.389630000	H	-0.763479000	-6.739836000	-0.810040000
C	3.928600000	0.552020000	-2.683060000	H	0.510677000	-4.617199000	-0.638650000
C	3.766010000	-0.438420000	-1.704070000	H	-0.742349000	-4.703955000	0.608410000
C	4.929350000	-1.371670000	-1.372830000	H	-1.432671000	-6.921801000	1.591890000
C	6.151820000	-0.562330000	-0.883970000	H	-0.651240000	-8.422640000	1.047990000
C	7.342380000	-1.489310000	-0.599640000	H	5.223490000	-0.243140000	7.595280000
C	6.958140000	-2.496080000	0.491200000	H	3.472310000	-0.339520000	7.313000000
C	5.751990000	-3.320910000	0.020910000	H	4.494180000	-2.619310000	7.296420000
C	6.130780000	-4.088140000	-1.252880000	H	2.516000000	-2.179970000	5.827720000
C	6.525040000	-3.088280000	-2.348800000	H	3.612350000	-3.375550000	5.112330000
C	7.720720000	-2.248360000	-1.878470000	H	4.485100000	1.457730000	5.904690000
C	4.567690000	-2.392630000	-0.279010000	H	3.629150000	0.713730000	3.710110000
C	5.341050000	-2.157540000	-2.640440000	H	2.519620000	0.229090000	5.002780000
C	2.518670000	-0.571590000	-1.090010000	H	6.111030000	-3.234760000	5.495640000
C	0.212242000	-1.999827000	-2.442080000	H	6.777640000	-1.951410000	6.525450000
C	-0.252846000	-3.160481000	-3.075610000	H	6.777020000	0.461420000	5.715030000
C	0.591628000	-3.867630000	-4.134200000	H	6.115540000	0.857620000	4.114410000
C	1.803901000	-3.027509000	-4.582080000	H	7.133930000	-1.425290000	4.105930000
C	2.650810000	-3.785957000	-5.612130000	H	5.172030000	-2.649230000	3.178860000
C	3.164857000	-5.091053000	-4.988500000	H	5.150010000	-0.953820000	2.650400000
C	1.971146000	-5.954845000	-4.561160000	H	-4.880315000	-3.154494000	3.178860000
C	1.107823000	-6.276165000	-5.788850000	H	-3.401037000	-3.983129000	2.650400000
C	0.601348000	-4.970265000	-6.418230000	H	-3.145909000	-1.088935000	5.827720000
C	1.797055000	-4.109651000	-6.844150000	H	-4.729487000	-1.440612000	5.112330000
C	1.133679000	-5.183590000	-3.533890000	H	-4.801302000	-5.465520000	4.105930000
C	-0.243774000	-4.204931000	-5.389630000	H	-1.196467000	-3.499801000	3.710110000
C	-1.486237000	-3.678277000	-2.683060000	H	-1.061412000	-2.296000000	5.002780000
C	-2.262688000	-3.042250000	-1.704070000	H	-5.856899000	-3.674927000	5.495640000
C	-3.652576000	-3.583107000	-1.372830000	H	-5.078791000	-4.893903000	6.525450000
C	-4.355923000	-2.759421000	-0.279010000	H	-4.515479000	-2.582419000	7.296420000
C	-5.751987000	-3.320914000	0.020910000	H	-2.988909000	-6.099781000	5.715030000
C	-6.605823000	-3.265341000	-1.252880000	H	-2.315049000	-5.725023000	4.114410000
C	-5.937049000	-4.106710000	-2.348800000	H	-0.980119000	-4.613076000	5.904690000
C	-5.807497000	-5.562160000	-1.878470000	H	-2.822310000	-4.402105000	7.595280000
C	-4.960970000	-5.614033000	-0.599640000	H	-2.030188000	-2.837349000	7.313000000
C	-5.640739000	-4.777886000	0.491200000	H	-2.432683000	2.786071000	3.710110000
C	-4.539009000	-3.546715000	-2.640440000	H	-1.458208000	2.067510000	5.002780000
C	-3.562902000	-5.046467000	-0.883970000	H	-0.291715000	5.803724000	3.178860000
C	-1.754346000	-1.895437000	-1.090010000	H	-1.748973000	4.936949000	2.650400000
H	-0.792620000	-1.786700000	2.777650000	H	-3.504981000	3.155346000	5.904690000
H	-4.904330000	-0.676280000	3.157820000	H	0.629909000	3.268905000	5.827720000
H	-2.384780000	1.359760000	0.360740000	H	1.117137000	4.816162000	5.112330000
H	-4.253950000	1.866340000	-0.638650000	H	-3.788111000	5.638361000	5.715030000
H	-3.702570000	2.994870000	0.608410000	H	-3.800491000	4.867403000	4.114410000
H	-6.436620000	-0.184850000	1.643420000	H	-2.332628000	6.890810000	4.105930000
H	-5.874840000	0.006680000	-0.028850000	H	-2.401180000	4.645245000	7.595280000
H	-5.606440000	1.455210000	3.447920000	H	-1.442122000	3.176869000	7.313000000
H	-4.476320000	2.743620000	2.995000000	H	0.021299000	5.201729000	7.296420000
H	-5.455130000	4.031110000	-0.810040000	H	-0.254131000	6.909687000	5.495640000
H	-7.809950000	3.162860000	-0.706750000	H	-1.698849000	6.845313000	6.525450000
H	-6.714160000	1.964540000	-1.424000000	H	-0.014803000	2.745160000	-0.360740000
H	-5.278120000	4.701630000	1.591890000	H	-0.510677000	4.617199000	0.638650000
H	-6.988600000	4.775310000	1.047990000	H	0.742349000	4.703955000	-0.608410000
H	-8.197930000	0.884130000	0.260920000	H	0.763479000	6.739836000	0.810040000
H	-6.792930000	3.632160000	3.268410000	H	1.432671000	6.921801000	-1.591890000

H	0.651240000	8.422640000	-1.047990000	H	8.197930000	-0.884130000	-0.260920000
H	-0.250922000	7.698930000	-3.268410000	H	7.809950000	-3.162860000	0.706750000
H	-1.783666000	8.888500000	-1.686490000	H	6.714160000	-1.964540000	1.424000000
H	-2.675512000	7.708462000	-2.669140000	H	5.455130000	-4.031110000	0.810040000
H	-3.333286000	7.541681000	-0.260920000	H	5.278120000	-4.701630000	-1.591890000
H	-1.165858000	8.345045000	0.706750000	H	6.968600000	-4.775310000	-1.047990000
H	-1.655738000	6.796903000	1.424000000	H	6.792930000	-3.632160000	-3.268410000
H	-1.542971000	5.582924000	-3.447920000	H	8.589500000	-2.899550000	-1.686490000
H	0.137885000	5.248417000	-2.995000000	H	8.013480000	-1.537170000	-2.669140000
H	-3.378395000	5.481851000	-1.643420000	H	4.253950000	-1.866340000	0.638650000
H	-2.931635000	5.091101000	0.028850000	H	3.702570000	-2.994870000	-0.608410000
H	-3.037841000	3.909134000	-3.157820000	H	5.606440000	-1.455210000	-3.447920000
H	-2.516000000	2.179970000	-5.827720000	H	4.476320000	-2.743620000	-2.995000000
H	-3.612350000	3.375550000	-5.112330000	H	2.384780000	-1.359760000	-0.360740000
H	-4.494180000	2.619310000	-7.296420000	H	1.151018000	-1.579779000	-2.777650000
H	-6.111030000	3.234760000	-5.495640000	H	2.432683000	-2.786071000	-3.710110000
H	-6.777640000	1.951410000	-6.525450000	H	1.458208000	-2.067510000	-5.002780000
H	-7.133930000	1.425290000	-4.105930000	H	3.504981000	-3.155346000	-5.904690000
H	-6.777020000	-0.461420000	-5.715030000	H	3.788110000	-5.638361000	-5.715030000
H	-6.115540000	-0.857620000	-4.114410000	H	3.800491000	-4.867403000	-4.114410000
H	-4.485100000	-1.457730000	-5.904690000	H	2.332628000	-6.890810000	-4.105930000
H	-5.223490000	0.243140000	-7.595280000	H	0.254131000	-6.909687000	-5.495640000
H	-3.472310000	0.339520000	-7.313000000	H	1.698849000	-6.845313000	-6.525450000
H	-5.172030000	2.649230000	-3.178860000	H	-0.021299000	-5.201729000	-7.296420000
H	-5.150010000	0.953820000	-2.650400000	H	2.401180000	-4.645245000	-7.595280000
H	-3.629150000	-0.713730000	-3.710110000	H	1.442122000	-3.176869000	-7.313000000
H	-2.519620000	-0.229090000	-5.002780000	H	0.291715000	-5.803724000	-3.178860000
H	-1.943638000	-0.206921000	-2.777650000	H	1.748973000	-4.936949000	-2.650400000
H	0.792620000	1.786700000	-2.777650000	H	-0.629909000	-3.268905000	-5.827720000
H	1.196467000	3.499801000	-3.710110000	H	-1.117137000	-4.816162000	-5.112330000
H	1.061412000	2.296600000	-5.002780000	H	-1.866489000	-4.585414000	-3.157820000
H	0.980119000	4.613076000	-5.904690000	H	-3.743273000	-2.750859000	0.638650000
H	2.988909000	6.099781000	-5.715030000	H	-4.444919000	-1.709085000	-0.608410000
H	2.315049000	5.725023000	-4.114410000	H	-6.218609000	-2.708726000	0.810040000
H	4.801302000	5.465520000	-4.105930000	H	-6.710791000	-2.220171000	-1.591890000
H	5.856899000	3.674927000	-5.495640000	H	-7.619840000	-3.647330000	-1.047990000
H	5.078791000	4.893903000	-6.525450000	H	-6.542008000	-4.066770000	-3.268410000
H	4.515479000	2.582419000	-7.296420000	H	-6.805834000	-5.988950000	-1.686490000
H	2.822310000	4.402105000	-7.595280000	H	-5.337968000	-6.171292000	-2.669140000
H	2.030188000	2.837349000	-7.313000000	H	-4.864644000	-6.657551000	-0.260920000
H	4.880315000	3.154494000	-3.178860000	H	-6.644092000	-5.182185000	0.706750000
H	3.401037000	3.983129000	-2.650400000	H	-5.058422000	-4.832363000	1.424000000
H	3.145909000	1.088935000	-5.827720000	H	-4.063469000	-4.127714000	-3.447920000
H	4.729487000	1.440612000	-5.112330000	H	-4.614205000	-2.504797000	-2.995000000
H	4.904330000	0.676280000	-3.157820000	H	-3.058225000	-5.666701000	-1.643420000
H	6.436620000	0.184850000	-1.643420000	H	-2.943205000	-5.084421000	0.028850000
H	5.874840000	-0.006680000	0.028850000	H	-2.369977000	-1.385400000	-0.360740000

Table S17. Dimers R-1₂ with C-PCM:cyclohexane.

H-1 ₂			C		
			0.943037000	-2.423275000	-1.090900000
			1.826088000	-3.366606000	-1.619210000
			0.407782000	1.404316000	-1.436980000
			1.627099000	2.028332000	-1.090900000
			2.002522000	3.264741000	-1.619210000
			1.184978000	3.924612000	-2.541520000
			-0.000040000	3.307193000	-2.936950000
			-0.374897000	2.069538000	-2.398610000
			-2.864111000	-1.653600000	-2.936950000
			-1.604824000	-1.359439000	-2.398610000
			-1.420065000	-0.349008000	-1.436980000
			-2.570136000	0.394943000	-1.090900000
			-3.828610000	0.101865000	-1.619210000
			-3.991303000	-0.936085000	-2.541520000
			0.000000000	0.000000000	-0.865340000
			-3.498647000	3.725560000	2.954680000
			-1.735085000	4.410487000	1.309380000
			-0.180170000	2.775154000	0.404750000
			-2.060934000	-0.314070000	2.752380000
			-3.601024000	1.328353000	3.675320000
			2.493439000	-1.231546000	0.404750000
			4.687136000	-0.702616000	1.309380000
			4.975753000	1.167137000	2.954680000
			2.950900000	2.454402000	3.675320000
			0.758474000	1.941856000	2.752380000
			0.650124000	-3.782755000	3.675320000
			1.302460000	-1.627786000	2.752380000

B3LYP			C		
C	-2.806325000	2.988527000	2.541520000		
C	-1.826088000	3.366606000	1.619210000		
C	-0.943037000	2.423275000	1.090900000		
C	-1.012283000	1.055308000	1.436980000		
C	-1.979721000	0.710098000	2.398610000		
C	-2.864115000	1.653593000	2.936950000		
C	1.420065000	0.349008000	1.436980000		
C	2.570136000	-0.394943000	1.090900000		
C	3.828610000	-0.101865000	1.619210000		
C	3.991303000	0.936085000	2.541520000		
C	2.864111000	1.653600000	2.936950000		
C	1.604824000	1.359439000	2.398610000		
C	0.000040000	-3.307193000	2.936950000		
C	0.374897000	-2.069538000	2.398610000		
C	-0.407782000	-1.404316000	1.436980000		
C	-1.627099000	-2.028332000	1.090900000		
C	-2.002522000	-3.264741000	1.619210000		
C	-1.184978000	-3.924612000	2.541520000		
C	0.000000000	0.000000000	0.865340000		
C	2.806325000	-2.988527000	-2.541520000		
C	2.864115000	-1.653593000	-2.936950000		
C	1.979721000	-0.710098000	-2.398610000		
C	1.012283000	-1.055308000	-1.436980000		

H	-2.313269000	-1.543608000	0.404750000
H	-2.952051000	-3.707871000	1.309380000
H	-1.477106000	-4.892698000	2.954680000
H	3.498647000	-3.725560000	-2.954680000
H	3.601024000	-1.328353000	-3.675320000
H	2.060934000	0.314070000	-2.752380000
H	0.180170000	-2.775154000	-0.404750000
H	1.735085000	-4.410487000	-1.309380000
H	2.313269000	1.543608000	-0.404750000
H	2.952051000	3.707871000	-1.309380000
H	1.477106000	4.892698000	-2.954680000
H	-0.650124000	3.782755000	-3.675320000
H	-1.302460000	1.627786000	-2.752380000
H	-2.950900000	-2.454402000	-3.675320000
H	-0.758474000	-1.941856000	-2.752380000
H	-2.493439000	1.231546000	-0.404750000
H	-4.687136000	0.702616000	-1.309380000
H	-4.975753000	-1.167137000	-2.954680000

B3LYP-D3(BJ)

C	-2.822925000	3.003227000	2.416083000
C	-1.800733000	3.374162000	1.537668000
C	-0.899186000	2.426188000	1.055759000
C	-0.996060000	1.062736000	1.405189000
C	-1.994059000	0.725001000	2.332709000
C	-2.898361000	1.673370000	2.824276000
C	1.418386000	0.331245000	1.405189000
C	2.550734000	-0.434376000	1.055759000
C	3.822476000	-0.127600000	1.537668000
C	4.012333000	0.943111000	2.416083000
C	2.898361000	1.673370000	2.824276000
C	1.624898000	1.364405000	2.332709000
C	0.000000000	-3.346739000	2.824276000
C	0.369160000	-2.089406000	2.332709000
C	-0.422327000	-1.393981000	1.405189000
C	-1.651548000	-1.991812000	1.055759000
C	-2.021743000	-3.246561000	1.537668000
C	-1.189408000	-3.946338000	2.416083000
C	0.000000000	0.000000000	0.850679000
C	2.822925000	-3.003227000	-2.416083000
C	2.898361000	-1.673370000	-2.824276000
C	1.994059000	-0.725001000	-2.332709000
C	0.996060000	-1.062736000	-1.405189000
C	0.899186000	-2.426188000	-1.055759000
C	1.800733000	-3.374162000	-1.537668000
C	0.422327000	1.393981000	-1.405189000
C	1.651548000	1.991812000	-1.055759000
C	2.021743000	3.246561000	-1.537668000
C	1.189408000	3.946338000	-2.416083000
C	0.000000000	3.346739000	-2.824276000
C	-0.369160000	2.089406000	-2.332709000
C	-2.898361000	-1.673370000	-2.824276000
C	-1.624898000	-1.364405000	-2.332709000
C	-1.418386000	-0.331245000	-1.405189000
C	-2.550734000	0.434376000	-1.055759000
C	-3.822476000	0.127600000	-1.537668000
C	-4.012333000	-0.943111000	-2.416083000
C	0.000000000	0.000000000	-0.850679000
H	-3.533315000	3.743624000	2.789579000
H	-1.693640000	4.415045000	1.224743000
H	-0.106057000	2.768182000	0.401947000
H	-2.086811000	-0.296937000	2.688237000
H	-3.665959000	1.357050000	3.533961000
H	2.450344000	-1.292243000	0.401947000
H	4.670361000	-0.740788000	1.224743000
H	5.008731000	1.188129000	2.789579000
H	3.008220000	2.496289000	3.533961000
H	0.786251000	1.955700000	2.688237000
H	0.657740000	-3.853339000	3.533961000
H	1.300560000	-1.658763000	2.688237000
H	-2.344287000	-1.475939000	0.401947000
H	-2.976721000	-3.674257000	1.224743000
H	-1.475415000	-4.931753000	2.789579000
H	3.533315000	-3.743624000	-2.789579000
H	3.665959000	-1.357050000	-3.533961000
H	2.086811000	0.296937000	-2.688237000
H	0.106057000	-2.768182000	-0.401947000
H	1.693640000	-4.415045000	-1.224743000
H	2.344287000	1.475939000	-0.401947000
H	2.976721000	3.674257000	-1.224743000
H	1.475415000	4.931753000	-2.789579000
H	-0.657740000	3.853339000	-3.533961000
H	-1.300560000	1.658763000	-2.688237000
H	-3.008220000	-2.496289000	-3.533961000
H	-0.786251000	-1.955700000	-2.688237000
H	-2.450344000	1.292243000	-0.401947000

H	-4.670361000	0.740788000	-1.224743000
H	-5.008731000	-1.188129000	-2.789579000

M06-2X

C	1.856614000	3.695539000	2.367085000
C	2.562163000	2.837270000	1.523315000
C	1.982680000	1.659069000	1.063478000
C	0.661148000	1.298440000	1.399127000
C	0.000000000	2.142474000	2.301207000
C	0.580544000	3.324444000	2.770645000
C	0.793908000	-1.221791000	1.399127000
C	0.445456000	-2.546586000	1.063478000
C	1.176066000	-3.637533000	1.523315000
C	2.272124000	-3.455645000	2.367085000
C	2.588781000	-2.164988000	2.770645000
C	1.855437000	-1.071237000	2.301207000
C	-3.169325000	-1.159456000	2.770645000
C	-1.855437000	-1.071237000	2.301207000
C	-1.455056000	-0.076649000	1.399127000
C	-2.428136000	0.887517000	1.063478000
C	-3.738229000	0.800263000	1.523315000
C	-4.128738000	-0.239894000	2.367085000
C	0.000000000	0.000000000	0.846113000
C	-1.856614000	-3.695539000	-2.367085000
C	-0.580544000	-3.324444000	-2.770645000
C	0.000000000	-2.142474000	-2.301207000
C	-0.661148000	-1.298440000	-1.399127000
C	-1.982680000	-1.659069000	-1.063478000
C	-2.562163000	-2.837270000	-1.523315000
C	1.455056000	0.076649000	-1.399127000
C	2.428136000	-0.887517000	-1.063478000
C	3.738229000	-0.800263000	-1.523315000
C	4.128738000	0.239894000	-2.367085000
C	3.169325000	1.159456000	-2.770645000
C	1.855437000	1.071237000	-2.301207000
C	-2.588781000	2.164988000	-2.770645000
C	-1.855437000	1.071237000	-2.301207000
C	-0.793908000	1.221791000	-1.399127000
C	-0.445456000	2.546586000	-1.063478000
C	-1.176066000	3.637533000	-1.523315000
C	-2.272124000	3.455645000	-2.367085000
C	0.000000000	0.000000000	-0.846113000
H	2.307410000	4.623610000	2.721097000
H	3.582644000	3.077951000	1.221640000
H	2.592964000	1.010191000	0.443110000
H	-0.994958000	1.896474000	2.661699000
H	0.016484000	3.952615000	3.461571000
H	-0.421631000	-2.750668000	0.443110000
H	0.874262000	-4.641636000	1.221640000
H	2.850459000	-4.310081000	2.721097000
H	3.414823000	-1.990583000	3.461571000
H	2.139874000	-0.086578000	2.661699000
H	-3.431307000	-1.962032000	3.461571000
H	-1.144915000	-1.809896000	2.661699000
H	-2.171333000	1.740477000	0.443110000
H	-4.456905000	1.563685000	1.221640000
H	-5.157869000	-0.313529000	2.721097000
H	-2.307410000	-4.623610000	-2.721097000
H	-0.016484000	-3.952615000	-3.461571000
H	0.994958000	-1.896474000	-2.661699000
H	-2.592964000	-1.010191000	-0.443110000
H	-3.582644000	-3.077951000	-1.221640000
H	2.171333000	-1.740477000	-0.443110000
H	4.456905000	-1.563685000	-1.221640000
H	5.157869000	0.313529000	-2.721097000
H	3.431307000	1.962032000	-3.461571000
H	1.144915000	1.809896000	-2.661699000
H	-3.414823000	1.990583000	-3.461571000
H	-2.139874000	0.086578000	-2.661699000
H	0.421631000	2.750668000	-0.443110000
H	-0.874262000	4.641636000	-1.221640000
H	-2.850459000	4.310081000	-2.721097000

Me-1₂

B3LYP

C	-4.071351000	-0.027826000	2.556695000
C	-3.717117000	0.950589000	1.612496000
C	-2.424522000	0.942694000	1.082093000
C	-1.461897000	-0.028708000	1.440984000
C	-1.848390000	-0.958421000	2.416206000
C	-3.139961000	-0.976255000	2.976979000
C	0.706087000	1.280394000	1.440984000
C	2.028658000	1.628350000	1.082093000
C	2.681793000	2.743823000	1.612496000

C	2.011578000	3.539806000	2.556695000	H	-4.315038000	1.400039000	-3.621376000
C	0.724519000	3.207413000	2.976979000	H	0.261847000	-3.417636000	-4.898073000
C	0.094178000	2.079963000	2.416206000	H	-0.613115000	-4.874324000	-4.365063000
C	2.415442000	-2.231158000	2.976979000	H	0.945050000	-4.436953000	-3.621376000
C	1.754212000	-1.121542000	2.416206000	H	-4.140331000	-4.097630000	-0.746846000
C	0.755810000	-1.251686000	1.440984000	H	-4.779856000	-3.086709000	-2.052792000
C	0.395864000	-2.571045000	1.082093000	H	-4.476936000	-2.375372000	-0.447250000
C	1.035324000	-3.694412000	1.612496000				
C	2.059773000	-3.511980000	2.556695000				
B3LYP-D3(BJ)							
C	0.000000000	0.000000000	0.863813000				
C	4.071351000	0.027826000	-2.556695000	C	-4.162574000	-0.051215000	2.232530000
C	3.139961000	0.976255000	-2.976979000	C	-3.707901000	1.001584000	1.422061000
C	1.848390000	0.958421000	-2.416206000	C	-2.369149000	1.024021000	1.033052000
C	1.461897000	0.028708000	-1.440984000	C	-1.460466000	0.006314000	1.394919000
C	2.424522000	-0.942694000	-1.082093000	C	-1.936305000	-0.982389000	2.261895000
C	3.717117000	-0.950589000	-1.612496000	C	-3.278387000	-1.033055000	2.677682000
C	-0.755810000	1.251686000	-1.440984000	C	0.735701000	1.261644000	1.394919000
C	-0.395864000	2.571045000	-1.082093000	C	2.071402000	1.539732000	1.033052000
C	-1.035324000	3.694412000	-1.612496000	C	2.721348000	2.710345000	1.422061000
C	-2.059773000	3.511980000	-2.556695000	C	2.036933000	3.630502000	2.232530000
C	-2.415442000	2.231158000	-2.976979000	C	0.744541000	3.355694000	2.677682000
C	-1.754212000	1.121542000	-2.416206000	C	0.117378000	2.168084000	2.261895000
C	-0.724519000	-3.207413000	-2.976979000	C	2.533846000	-2.322639000	2.677682000
C	-0.094178000	-2.079963000	-2.416206000	C	1.818926000	-1.185695000	2.261895000
C	-0.706087000	-1.280394000	-1.440984000	C	0.724765000	-1.267958000	1.394919000
C	-2.028658000	-1.628350000	-1.082093000	C	0.297746000	-2.563753000	1.033052000
C	-2.681793000	-2.743823000	-1.612496000	C	0.986553000	-3.711929000	1.422061000
C	-2.011578000	-3.539806000	-2.556695000	C	2.125640000	-3.579287000	2.232530000
C	0.000000000	0.000000000	-0.863813000	C	0.000000000	0.000000000	0.862515000
C	-4.720566000	1.999198000	1.190330000	C	4.162574000	0.051215000	-2.232530000
C	-3.489457000	-2.014639000	4.018114000	C	3.278387000	1.033055000	-2.677682000
C	4.091640000	3.088531000	1.190330000	C	1.936305000	0.982389000	-2.261895000
C	0.000000000	4.029278000	4.018114000	C	1.460466000	-0.006314000	-1.394919000
C	3.489457000	-2.014639000	4.018114000	C	2.369149000	-1.024021000	-1.033052000
C	0.628926000	-5.087729000	1.190330000	C	3.707901000	-1.001584000	-1.422061000
C	3.489457000	2.014639000	-4.018114000	C	-0.724765000	1.267958000	-1.394919000
C	4.720566000	-1.999198000	-1.190330000	C	-0.297746000	2.563753000	-1.033052000
C	-0.628926000	5.087729000	-1.190330000	C	-0.986553000	3.711929000	-1.422061000
C	-3.489457000	2.014639000	-4.018114000	C	-2.125640000	3.579287000	-2.232530000
C	0.000000000	-4.029278000	-4.018114000	C	-2.533846000	2.322639000	-2.677682000
C	-4.091640000	-3.088531000	-1.190330000	C	-1.818926000	1.185695000	-2.261895000
H	-5.081026000	-0.033386000	2.978782000	C	-0.744541000	-3.355694000	-2.677682000
H	-2.165434000	1.727583000	0.379387000	C	-0.117378000	-2.168084000	-2.261895000
H	-1.141136000	-1.704436000	2.770701000	C	-0.735701000	-1.261644000	-1.394919000
H	2.578847000	1.011529000	0.379387000	C	-2.071402000	-1.539732000	-1.033052000
H	2.511600000	4.416990000	2.978782000	C	-2.721348000	-2.710345000	-1.422061000
H	-0.905517000	1.840471000	2.770701000	C	-2.036933000	-3.630502000	-2.232530000
H	2.046653000	-0.136035000	2.770701000	C	0.000000000	0.000000000	-0.862515000
H	-0.413414000	-2.739112000	0.379387000	C	-4.647514000	2.095517000	0.977227000
H	2.569426000	-4.383604000	2.978782000	C	-3.737243000	-2.157698000	3.573461000
H	5.081026000	0.033386000	-2.978782000	C	4.138528000	2.977107000	0.977227000
H	1.141136000	1.704436000	-2.770701000	C	0.000000000	4.315397000	3.573461000
H	2.165434000	-1.727583000	-0.379387000	C	3.737243000	-2.157698000	3.573461000
H	0.413414000	2.739112000	-0.379387000	C	0.508986000	-5.072624000	0.977227000
H	-2.569426000	4.383604000	-2.978782000	C	3.737243000	2.157698000	-3.573461000
H	-2.046653000	0.136035000	-2.770701000	C	4.647514000	-2.095517000	-0.977227000
H	0.905517000	-1.840471000	-2.770701000	C	-0.508986000	5.072624000	-0.977227000
H	-2.578847000	-1.011529000	-0.379387000	C	-3.737243000	2.157698000	-3.573461000
H	-2.511600000	-4.416990000	-2.978782000	C	0.000000000	-4.315397000	-3.573461000
H	-4.295600000	2.689454000	0.447250000	C	-4.138528000	-2.977107000	-0.977227000
H	-5.063097000	2.596122000	2.052792000	C	-5.213660000	-0.090873000	2.532739000
H	-5.618817000	1.536817000	0.746846000	H	-2.038677000	1.857150000	0.425395000
H	-4.527846000	-1.906189000	4.365063000	H	-1.268340000	-1.761504000	2.620013000
H	-2.828836000	-1.935585000	4.898073000	H	2.627678000	0.836971000	0.425395000
H	-3.369989000	-3.036913000	3.621376000	H	2.528132000	4.560599000	2.532739000
H	4.476936000	2.375372000	0.447250000	H	-0.891337000	1.979167000	2.620013000
H	4.779856000	3.086709000	2.052792000	H	2.159678000	-0.217663000	2.620013000
H	4.140331000	4.097630000	0.746846000	H	-0.589000000	-2.694121000	0.425395000
H	0.613115000	4.874324000	4.365063000	H	2.685529000	-4.469726000	2.532739000
H	-0.261847000	3.417636000	4.898073000	H	5.213660000	0.090873000	-2.532739000
H	-0.945050000	4.436953000	3.621376000	H	1.268340000	1.761504000	-2.620013000
H	3.914731000	-2.968135000	4.365063000	H	2.038677000	-1.857150000	-0.425395000
H	3.090684000	-1.482052000	4.898073000	H	0.589000000	2.694121000	-0.425395000
H	4.315038000	-1.400039000	3.621376000	H	-2.685529000	4.469726000	-2.532739000
H	-0.181335000	-5.064826000	0.447250000	H	-2.159678000	0.217663000	-2.620013000
H	0.283241000	-5.682831000	2.052792000	H	0.891337000	-1.979167000	-2.620013000
H	1.478486000	-5.634447000	0.746846000	H	-2.627678000	-0.836971000	-0.425395000
H	2.828836000	1.935585000	-4.898073000	H	-2.528132000	-4.560599000	-2.532739000
H	4.527846000	1.906189000	-4.365063000	H	-4.185964000	2.723007000	0.200839000
H	3.369989000	3.036913000	-3.621376000	H	-4.929679000	2.749002000	1.820788000
H	5.618817000	-1.536817000	-0.746846000	H	-5.581783000	1.676509000	0.569287000
H	5.063097000	-2.596122000	-2.052792000	H	-4.798461000	-2.053049000	3.842590000
H	4.295600000	-2.689454000	-0.447250000	H	-3.149891000	-2.189331000	4.506075000
H	-1.478486000	5.634447000	-0.746846000	H	-3.606890000	-3.135351000	3.079809000
H	-0.283241000	5.682831000	-2.052792000	H	4.451175000	2.263648000	0.200839000
H	0.181335000	5.064826000	-0.447250000	H	4.845545000	2.894726000	1.820788000
H	-3.090684000	1.482052000	-4.898073000	H	4.242790000	3.995711000	0.569287000
H	-3.914731000	2.968135000	-4.365063000	H	0.621238000	5.182113000	3.842590000

H	-0.321071000	3.822551000	4.506075000	H	2.695789000	-4.477346000	-2.487860000
H	-0.911849000	4.691334000	3.079809000	H	2.176939000	-0.233990000	-2.609210000
H	4.177223000	-3.129064000	3.842590000	H	-0.616718000	-2.705173000	-0.452190000
H	3.470962000	-1.633220000	4.506075000	H	2.651108000	0.818493000	-0.452190000
H	4.518739000	-1.555983000	3.079809000	H	2.529601000	4.573295000	-2.487860000
H	-0.265211000	-4.986655000	0.200839000	H	-0.885829000	2.002279000	-2.609210000
H	0.084134000	-5.643728000	1.820788000	H	-1.291110000	-1.768290000	-2.609210000
H	1.338992000	-5.672220000	0.569287000	H	-2.034390000	1.886680000	-0.452190000
H	3.149891000	2.189331000	-4.506075000	H	-5.225390000	-0.095949000	-2.487860000
H	4.798461000	2.053049000	-3.842590000	H	0.321162000	4.987753000	0.250950000
H	3.606890000	3.135351000	-3.079809000	H	-0.127622000	5.654070000	1.842590000
H	5.581783000	-1.676509000	-0.569287000	H	-1.309213000	5.653926000	0.522830000
H	4.929679000	-2.749002000	-1.820788000	H	-4.199670000	3.143205000	3.779400000
H	4.185964000	-2.723007000	-0.200839000	H	-3.503660000	1.647978000	4.451870000
H	-1.338992000	5.672220000	-0.569287000	H	-4.531986000	1.571372000	3.011850000
H	-0.084134000	5.643728000	-1.820788000	H	4.158939000	-2.772011000	0.250950000
H	0.265211000	4.986655000	-0.200839000	H	4.960379000	-2.716511000	1.842590000
H	-3.470962000	1.633220000	-4.506075000	H	5.551050000	-1.693151000	0.522830000
H	-4.177223000	3.129064000	-3.842590000	H	4.821930000	2.065419000	3.779400000
H	-4.518739000	1.555983000	-3.079809000	H	3.179021000	2.210269000	4.451870000
H	0.321071000	-3.822551000	-4.506075000	H	3.626841000	3.139129000	3.011850000
H	-0.621238000	-5.182113000	-3.842590000	H	-0.622260000	-5.208624000	3.779400000
H	0.911849000	-4.691334000	-3.079809000	H	0.324639000	-3.858247000	4.451870000
H	-4.242790000	-3.995711000	-0.569287000	H	0.905145000	-4.710501000	3.011850000
H	-4.845545000	-2.894726000	-1.820788000	H	-4.480102000	-2.215742000	0.250950000
H	-4.451175000	-2.263648000	-0.200839000	H	-4.832757000	-2.937559000	1.842590000
M06-2X							
C	-2.132645000	3.585031000	2.199820000	H	-4.241837000	-3.960774000	0.522830000
C	-0.979618000	3.713529000	1.413210000	H	3.503660000	-1.647978000	-4.451870000
C	-0.287016000	2.566947000	1.038070000	H	4.199670000	-3.143205000	-3.779400000
C	-0.721798000	1.270911000	1.390540000	H	4.531986000	-1.571372000	-3.011850000
C	-1.826362000	1.195772000	2.241080000	H	1.309213000	-5.653926000	-0.522830000
C	-2.545944000	2.333925000	2.641050000	H	0.127622000	-5.654070000	-1.842590000
C	1.461540000	-0.010360000	1.390540000	H	-0.321162000	-4.987753000	-0.250950000
C	2.366550000	-1.034911000	1.038070000	H	4.241837000	3.960774000	-0.522830000
C	3.705820000	-1.008391000	1.413210000	H	4.832757000	2.937559000	-1.842590000
C	4.171050000	0.054409000	2.199820000	H	4.480102000	2.215742000	-0.250950000
C	3.294210000	1.037889000	2.641050000	H	-0.324639000	3.858247000	-4.451870000
C	1.948750000	0.983790000	2.241080000	H	0.622260000	5.208624000	-3.779400000
C	-0.748267000	-3.371814000	2.641050000	H	-0.905145000	4.710501000	-3.011850000
C	-0.122388000	-2.179562000	2.241080000	H	-3.179021000	-2.210269000	-4.451870000
C	-0.739742000	-1.260551000	1.390540000	H	-4.821930000	-2.065419000	-3.779400000
C	-2.079534000	-1.532037000	1.038070000	H	-3.626841000	-3.139129000	-3.011850000
C	-2.726202000	-2.705139000	1.413210000	H	-5.551050000	1.693151000	-0.522830000
C	-2.038405000	-3.639440000	2.199820000	H	-4.960379000	2.716511000	-1.842590000
C	0.000000000	0.000000000	0.856100000	H	-4.158939000	2.772011000	-0.250950000
C	2.132645000	-3.585031000	-2.199820000	Pr-1 ₂			
C	2.545944000	-2.333925000	-2.641050000	B3LYP			
C	1.826362000	-1.195772000	-2.241080000	C	-3.794473000	1.164245000	2.770870000
C	0.721798000	-1.270911000	-1.390540000	C	-3.272895000	1.968600000	1.744580000
C	0.287016000	-2.566947000	-1.038070000	C	-2.091121000	1.563625000	1.109940000
C	0.979618000	-3.713529000	-1.413210000	C	-1.414102000	0.371402000	1.457300000
C	0.739742000	1.260551000	-1.390540000	C	-1.972278000	-0.386854000	2.499430000
C	2.079534000	1.532037000	-1.038070000	C	-3.152248000	-0.008714000	3.165880000
C	2.726202000	2.705139000	-1.413210000	C	1.028695000	1.038947000	1.457300000
C	2.038405000	3.639440000	-2.199820000	C	2.399699000	1.029151000	1.109940000
C	0.748267000	3.371814000	-2.641050000	C	3.341305000	1.850110000	1.744580000
C	0.122388000	2.179562000	-2.241080000	C	2.905502000	2.703988000	2.770870000
C	-3.294210000	-1.037889000	-2.641050000	C	1.568577000	2.734284000	3.165880000
C	-1.948750000	-0.983790000	-2.241080000	C	0.651114000	1.901470000	2.499430000
C	-1.461540000	0.010360000	-1.390540000	C	1.583671000	-2.725570000	3.165880000
C	-2.366550000	1.034911000	-1.038070000	C	1.321164000	-1.514616000	2.499430000
C	-3.705820000	1.008391000	-1.413210000	C	0.385407000	-1.410349000	1.457300000
C	-4.171050000	-0.054409000	-2.199820000	C	-0.308579000	-2.592776000	1.109940000
C	0.000000000	0.000000000	-0.856100000	C	-0.068410000	-3.818710000	1.744580000
C	-0.494813000	5.073943000	0.981800000	C	0.888971000	-3.868232000	2.770870000
C	-3.760698000	2.171243000	3.518770000	C	0.000000000	0.000000000	0.852610000
C	4.641570000	-2.108451000	0.981800000	C	3.794473000	-1.164245000	-2.770870000
C	3.760701000	2.171239000	3.518770000	C	3.152248000	0.008714000	-3.165880000
C	-0.000002000	-4.342482000	3.518770000	C	1.972278000	0.386854000	-2.499430000
C	-4.146757000	-2.965492000	0.981800000	C	1.414102000	-0.371402000	-1.457300000
C	3.760698000	-2.171243000	-3.518770000	C	2.091121000	-1.563625000	-1.109940000
C	0.494813000	-5.073943000	-0.981800000	C	3.272895000	-1.968600000	-1.744580000
C	4.146757000	2.965492000	-0.981800000	C	-0.385407000	1.410349000	-1.457300000
C	0.000002000	4.342482000	-3.518770000	C	0.308579000	2.592776000	-1.109940000
C	-3.760701000	-2.171239000	-3.518770000	C	0.068410000	3.818710000	-1.744580000
C	-4.641570000	2.108451000	-0.981800000	C	-0.888971000	3.868232000	-2.770870000
H	-2.695789000	4.477346000	2.487860000	C	-1.583671000	2.725570000	-3.165880000
H	0.616718000	2.705173000	0.452190000	C	-1.321164000	1.514616000	-2.499430000
H	-2.176939000	0.233990000	2.609210000	C	-1.568577000	-2.734284000	-3.165880000
H	2.034390000	-1.886680000	0.452190000	C	-0.651114000	-1.901470000	-2.499430000
H	5.225390000	0.095949000	2.487860000	C	-1.028695000	-1.038947000	-1.457300000
H	1.291110000	1.768290000	2.609210000	C	-2.399699000	-1.029151000	-1.109940000
H	0.885829000	-2.002279000	2.609210000	C	-3.341305000	-1.850110000	-1.744580000
H	-2.651108000	-0.818493000	0.452190000	C	-2.905502000	-2.703988000	-2.770870000
H	-2.529601000	-4.573295000	2.487860000	C	0.000000000	0.000000000	-0.852610000

C	-4.826235000	-1.846109000	-1.383950000	H	0.518010000	6.913980000	-0.193610000
C	-5.160694000	-2.968068000	-0.382420000	H	-2.649542000	3.844796000	-4.622260000
C	-5.346573000	-0.498313000	-0.873100000	H	-4.379549000	2.863060000	-3.104480000
C	-1.127398000	-3.612201000	-4.333530000	H	-3.967193000	1.226557000	-3.676240000
C	0.000000000	-4.586688000	-3.954830000	H	-4.663872000	2.410123000	-4.805540000
C	-0.732036000	-2.762564000	-5.555900000	H	-1.038785000	2.395265000	-5.862610000
C	4.826235000	1.846109000	1.383950000	H	-2.713392000	2.116527000	-6.412420000
C	5.346573000	0.498313000	0.873100000	H	-1.919970000	0.939602000	-5.335880000
C	5.160694000	2.968068000	0.382420000	H	2.649542000	-3.844796000	4.622260000
C	1.127398000	3.612201000	4.333530000	H	1.038785000	-2.395265000	5.862610000
C	0.000000000	4.586688000	3.954830000	H	1.919970000	-0.939602000	5.335880000
C	0.732036000	2.762564000	5.555900000	H	2.713392000	-2.116527000	6.412420000
C	0.814340000	5.102697000	-1.383950000	H	4.379549000	-2.863060000	3.104480000
C	2.241735000	4.879424000	-0.873100000	H	4.663872000	-2.410123000	4.805540000
C	0.009925000	5.953327000	-0.382420000	H	3.967193000	-1.226557000	3.676240000
C	-2.564558000	2.782456000	-4.333530000	H	-0.886407000	-5.687844000	2.318660000
C	-3.972188000	2.293344000	-3.954830000	H	0.092634000	-5.427025000	-0.580760000
C	-2.026433000	2.015244000	-5.555900000	H	-0.518010000	-6.913980000	0.193610000
C	2.564558000	-2.782456000	4.333530000	H	1.002746000	-6.170859000	0.756290000
C	2.026433000	-2.015244000	5.555900000	H	-2.253354000	-4.364876000	-0.100860000
C	3.972188000	-2.293344000	3.954830000	H	-2.835464000	-4.278410000	1.578760000
C	-0.814340000	-5.102697000	1.383950000	H	-2.752411000	-5.846846000	0.738410000
C	-0.009925000	-5.953327000	0.382420000	H	-4.482613000	3.611573000	2.318660000
C	-2.241735000	-4.879424000	0.873100000	H	-2.653416000	4.133900000	-0.100860000
C	-4.011895000	3.256587000	1.383950000	H	-2.287480000	4.594789000	1.578760000
C	-3.104838000	4.381112000	0.873100000	H	-3.687311000	5.307081000	0.738410000
C	-5.150770000	2.985258000	0.382420000	H	-4.746258000	2.633289000	-0.580760000
C	-3.691957000	-0.829745000	4.333530000	H	-5.728678000	3.905599000	0.193610000
C	-2.758469000	-0.747321000	5.555900000	H	-5.845494000	2.217026000	0.756290000
C	-3.972188000	-2.293344000	3.954830000	H	-4.654462000	-0.372173000	4.622260000
C	3.691957000	0.829745000	-4.333530000	H	-2.593753000	0.298018000	5.862610000
C	2.758469000	0.747321000	-5.555900000	H	-1.773704000	-1.192942000	5.335880000
C	3.972188000	2.293344000	-3.954830000	H	-3.189662000	-1.291603000	6.412420000
C	4.011895000	-3.256587000	-1.383950000	H	-4.669257000	-2.361271000	3.104480000
C	5.150770000	-2.985258000	-0.382420000	H	-4.419164000	-2.833970000	4.805540000
C	3.104838000	-4.381112000	-0.873100000	H	-3.045826000	-2.822411000	3.676240000
H	-4.707135000	1.478533000	3.287510000	H	4.654462000	0.372173000	-4.622260000
H	-1.668068000	2.210747000	0.349750000	H	2.593753000	-0.298018000	-5.862610000
H	-1.472548000	-1.290336000	2.836220000	H	3.189662000	1.291603000	-6.412420000
H	2.748597000	0.339216000	0.349750000	H	1.773704000	1.192942000	-5.335880000
H	3.634015000	3.337233000	3.287510000	H	4.669257000	2.361271000	-3.104480000
H	-0.381189000	1.920432000	2.836220000	H	3.045826000	2.822411000	-3.676240000
H	1.853738000	-0.630096000	2.836220000	H	4.419164000	2.833970000	-4.805540000
H	-1.080529000	-2.549963000	0.349750000	H	4.482613000	-3.611573000	-2.318660000
H	1.073121000	-4.815765000	3.287510000	H	4.746258000	-2.633289000	0.580760000
H	4.707135000	-1.478533000	-3.287510000	H	5.845494000	-2.217026000	-0.756290000
H	1.472548000	1.290336000	-2.836220000	H	5.728678000	-3.905599000	-0.193610000
H	1.668068000	-2.210747000	-0.349750000	H	2.653416000	-4.133900000	0.100860000
H	1.080529000	2.549963000	-0.349750000	H	3.687311000	-5.307081000	-0.738410000
H	-1.073121000	4.815765000	-3.287510000	H	2.287480000	-4.594789000	-1.578760000
H	-1.853738000	0.630096000	-2.836220000				
H	0.381189000	-1.920432000	-2.836220000				
H	-2.748597000	-0.339216000	-0.349750000				
H	-3.634015000	-3.337233000	-3.287510000	C	2.531406000	3.067818000	2.678130000
H	-5.369021000	-2.076271000	-2.318660000	C	3.068767000	2.242586000	1.677500000
H	-4.653624000	-2.793736000	0.580760000	C	2.241400000	1.294074000	1.071590000
H	-4.842748000	-3.953833000	-0.756290000	C	0.883741000	1.147979000	1.421840000
H	-6.246687000	-3.008381000	-0.193610000	C	0.398267000	1.974919000	2.439970000
H	-4.906770000	-0.230976000	0.100860000	C	1.202556000	2.934268000	3.075890000
H	-6.439722000	-0.539765000	-0.738410000	C	0.552309000	-1.339332000	1.421840000
H	-5.122944000	0.316379000	-1.578760000	C	0.000001000	-2.588146000	1.071590000
H	-2.004920000	-4.216969000	-4.622260000	C	0.407753000	-3.778924000	1.677500000
H	-0.289708000	-5.224331000	-3.104480000	C	1.391105000	-3.726171000	2.678130000
H	0.921367000	-4.048968000	-3.676240000	C	1.939872000	-2.508578000	3.075890000
H	0.244708000	-5.244094000	-4.805540000	C	1.511197000	-1.332369000	2.439970000
H	-1.554968000	-2.097247000	-5.862610000	C	-3.142428000	-0.425690000	3.075890000
H	-0.476270000	-3.408130000	-6.412420000	C	-1.909463000	-0.642550000	2.439970000
H	0.146266000	-2.132544000	-5.335880000	C	-1.436050000	0.191353000	1.421840000
H	5.369021000	2.076271000	2.318660000	C	-2.241401000	1.294072000	1.071590000
H	4.906770000	0.230976000	-0.100860000	C	-3.476520000	1.536338000	1.677500000
H	5.122944000	-0.316379000	1.578760000	C	-3.922511000	0.658353000	2.678130000
H	6.439722000	0.539765000	0.738410000	C	0.000000000	0.000000000	0.832580000
H	4.653624000	2.793736000	-0.580760000	C	-2.531406000	-3.067818000	-2.678130000
H	6.246687000	3.008381000	0.193610000	C	-1.202556000	-2.934268000	-3.075890000
H	4.842748000	3.953833000	0.756290000	C	-0.398267000	-1.974919000	-2.439970000
H	2.004920000	4.216969000	4.622260000	C	-0.883741000	-1.147979000	-1.421840000
H	0.289708000	5.224331000	3.104480000	C	-2.241400000	-1.294074000	-1.071590000
H	-0.244708000	-4.048968000	-3.676240000	C	-3.068767000	-2.242586000	-1.677500000
H	1.554968000	-2.097247000	-5.862610000	C	1.436050000	-0.191353000	-1.421840000
H	-0.146266000	2.132544000	5.335880000	C	2.241401000	-1.294072000	-1.071590000
H	0.476270000	3.408130000	6.412420000	C	3.476520000	-1.536338000	-1.677500000
H	0.886407000	5.687844000	-2.318660000	C	3.922511000	-0.658353000	-2.678130000
H	2.253354000	4.364876000	0.100860000	C	3.142428000	0.425690000	-3.075890000
H	2.752411000	5.846846000	-0.738410000	C	1.909463000	0.642550000	-2.439970000
H	2.835464000	4.278410000	-1.578760000	C	-1.939872000	2.508578000	-3.075890000
H	-0.092634000	5.427025000	0.580760000	C	-1.511197000	1.332369000	-2.439970000
H	-1.002746000	6.170859000	-0.756290000	C	-0.552309000	1.339332000	-1.421840000
				C	-0.000001000	2.588146000	-1.071590000

B3LYP-D3(BJ)

C	-0.407753000	3.778924000	-1.677500000	H	2.771801000	-4.219965000	-1.485200000
C	-1.391105000	3.726171000	-2.678130000	H	4.904737000	-1.964550000	0.687240000
C	0.000000000	0.000000000	-0.832580000	H	6.016662000	-1.458764000	-0.605280000
C	0.179576000	5.126522000	-1.277920000	H	6.067984000	-3.135442000	0.007940000
C	-0.713675000	5.823590000	-0.239350000	H	4.593049000	1.025299000	-4.510550000
C	1.620821000	5.037254000	-0.769460000	H	4.289423000	2.958693000	-2.950960000
C	-2.935880000	2.429557000	-4.221260000	H	2.616256000	3.169812000	-3.521610000
C	-4.238448000	1.728829000	-3.808720000	H	3.972792000	3.433391000	-4.641870000
C	-2.301496000	1.738340000	-5.440230000	H	2.644348000	0.068433000	-5.755150000
C	-0.179576000	-5.126522000	1.277920000	H	2.994139000	1.735972000	-6.292660000
C	-1.620821000	-5.037254000	0.769460000	H	1.619107000	1.415462000	-5.204050000
C	0.713675000	-5.823590000	0.239350000	H	-4.593049000	-1.025299000	4.510550000
C	2.935880000	-2.429557000	4.221260000	H	-2.644348000	-0.068433000	5.755150000
C	4.238448000	-1.728829000	3.808720000	H	-1.619107000	-1.415462000	5.204050000
C	2.301496000	-1.738340000	5.440230000	H	-2.994139000	-1.735972000	6.292660000
C	4.349910000	-2.718779000	-1.277920000	H	-4.289423000	-2.958693000	2.950960000
C	3.551979000	-3.922299000	-0.769460000	H	-3.972792000	-3.433391000	4.641870000
C	5.400215000	-2.293735000	-0.239350000	H	-2.616256000	-3.169812000	3.521610000
C	3.571998000	1.327768000	-4.221260000	H	-4.890952000	3.031348000	2.188970000
C	3.616434000	2.806189000	-3.808720000	H	-2.904737000	1.964550000	-0.687240000
C	2.656194000	1.123984000	-5.440230000	H	-6.067984000	3.135442000	-0.007940000
C	-3.571998000	-1.327768000	4.221260000	H	-6.016662000	1.458764000	0.605280000
C	-2.656194000	-1.123984000	5.440230000	H	-3.060478000	3.706949000	-0.192020000
C	-3.616434000	-2.806189000	3.808720000	H	-2.771801000	4.219965000	1.485200000
C	-4.349910000	2.718779000	1.277920000	H	-4.218858000	4.784588000	0.610760000
C	-5.400215000	2.293735000	0.239350000	H	5.070700000	2.720014000	2.188970000
C	-3.551979000	3.922299000	0.769460000	H	4.740551000	0.796977000	-0.192020000
C	4.529486000	2.407743000	1.277920000	H	5.040497000	0.290468000	1.485200000
C	5.172800000	1.114955000	0.769460000	H	6.253003000	1.261344000	0.610760000
C	4.686540000	3.529855000	0.239350000	H	4.153719000	3.265352000	-0.687240000
C	0.636118000	3.757325000	4.221260000	H	5.749364000	3.687307000	-0.007940000
C	0.354699000	2.862324000	5.440230000	H	4.271658000	4.481200000	0.605280000
C	-0.622014000	4.535018000	3.808720000	H	1.408590000	4.490347000	4.510550000
C	-0.636118000	-3.757325000	-4.221260000	H	1.262909000	2.324290000	5.755150000
C	-0.354699000	-2.862324000	-5.440230000	H	-0.416273000	2.109919000	5.204050000
C	0.622014000	-4.535018000	-3.808720000	H	-0.006326000	3.460986000	6.292660000
C	-4.529486000	-2.407743000	-1.277920000	H	-0.417592000	5.194096000	2.950960000
C	-4.686540000	-3.529855000	-0.239350000	H	-0.987008000	5.157234000	4.641870000
C	-5.172800000	-1.114955000	-0.769460000	H	-1.437010000	3.850650000	3.521610000
H	3.172171000	3.806337000	3.169180000	H	-1.408590000	-4.490347000	-4.510550000
H	2.671832000	0.633234000	0.331600000	H	-1.262909000	-2.324290000	-5.755150000
H	-0.626409000	1.868622000	2.780140000	H	0.006326000	-3.460986000	-6.292660000
H	-0.787519000	-2.630491000	0.331600000	H	0.416273000	-2.109919000	-5.204050000
H	1.710298000	-4.650349000	3.169180000	H	0.417592000	-5.194096000	-2.950960000
H	1.931479000	-0.391825000	2.780140000	H	1.437010000	-3.850650000	-3.521610000
H	-1.305069000	-1.476797000	2.780140000	H	0.987008000	-5.157234000	-4.641870000
H	-1.884313000	1.997257000	0.331600000	H	-5.070700000	-2.720014000	-2.188970000
H	-4.882470000	0.844013000	3.169180000	H	-4.153719000	-3.265352000	0.687240000
H	-3.172171000	-3.806337000	-3.169180000	H	-4.271658000	-4.481200000	-0.605280000
H	0.626409000	-1.868622000	-2.780140000	H	-5.749364000	-3.687307000	0.007940000
H	-2.671832000	-0.633234000	-0.331600000	H	-4.740551000	-0.796977000	0.192020000
H	1.884313000	-1.997257000	-0.331600000	H	-6.253003000	-1.261344000	-0.610760000
H	4.882470000	-0.844013000	-3.169180000	H	-5.040497000	-0.290468000	-1.485200000
H	1.305069000	1.476797000	-2.780140000				
H	-1.931479000	0.391825000	-2.780140000				
H	0.787519000	2.630491000	-0.331600000				
H	-1.710298000	4.650349000	-3.169180000				
H	0.179749000	5.751362000	-2.188970000				
H	-0.751019000	5.229902000	0.687240000				
H	-1.745004000	5.939964000	-0.605280000	C	2.514355000	3.099590000	2.654270000
H	-0.318620000	6.822749000	0.007940000	C	3.055809000	2.250675000	1.679380000
H	1.680073000	4.503926000	0.192020000	C	2.235521000	1.290676000	1.089600000
H	2.034146000	6.045932000	-0.610760000	C	0.874001000	1.154709000	1.424910000
H	2.268696000	4.510433000	-1.485200000	C	0.385484000	2.001510000	2.423330000
H	-3.184459000	3.465048000	-4.510550000	C	1.186384000	2.972499000	3.044890000
H	-4.707015000	2.235403000	-2.950960000	C	0.563007000	-1.334261000	1.424910000
H	-4.053266000	0.680838000	-3.521610000	C	-0.000002000	-2.581356000	1.089600000
H	-4.959799000	1.723843000	-4.641870000	C	0.421237000	-3.771746000	1.679380000
H	-1.381439000	2.255856000	-5.755150000	C	1.427146000	-3.727290000	2.654270000
H	-3.000465000	1.725014000	-6.292660000	C	1.981067000	-2.513688000	3.044890000
H	-2.035380000	0.694457000	-5.204050000	C	1.540616000	-1.334594000	2.423330000
H	-0.179749000	-5.751362000	2.188970000	C	-3.167452000	-0.458810000	3.044890000
H	-1.680073000	-4.503926000	-0.192020000	C	-1.926101000	-0.666916000	2.423330000
H	-2.268696000	-4.510433000	1.485200000	C	-1.437007000	0.179553000	1.424910000
H	-2.034146000	-6.045932000	0.610760000	C	-2.235519000	1.290680000	1.089600000
H	0.751019000	-5.229902000	-0.687240000	C	-3.477046000	1.521071000	1.679380000
H	0.318620000	-6.822749000	-0.007940000	C	-3.941501000	0.627700000	2.654270000
H	1.745004000	-5.939964000	0.605280000	C	0.000000000	0.000000000	0.834600000
H	3.184459000	-3.465048000	4.510550000	C	-2.514355000	-3.099590000	-2.654270000
H	4.707015000	-2.235403000	2.950960000	C	-1.186384000	-2.972499000	-3.044890000
H	4.959799000	-1.723843000	4.641870000	C	-0.385484000	-2.001510000	-2.423330000
H	4.053266000	-0.680838000	3.521610000	C	-0.874001000	-1.154709000	-1.424910000
H	1.381439000	-2.255856000	5.755150000	C	-2.235521000	-1.290676000	-1.089600000
H	2.035380000	-0.694457000	5.204050000	C	-3.055809000	-2.250675000	-1.679380000
H	3.000465000	-1.725014000	6.292660000	C	1.437007000	-0.179553000	-1.424910000
H	4.890952000	-3.031348000	-2.188970000	C	2.235519000	-1.290680000	-1.089600000
H	3.060478000	-3.706949000	0.192020000	C	3.477046000	-1.521071000	-1.679380000
H	4.218858000	-4.784588000	-0.610760000	C	3.941501000	-0.627700000	-2.654270000
				C	3.167452000	0.458810000	-3.044890000
				C	1.926101000	0.666916000	-2.423330000
				C	-1.981067000	2.513688000	-3.044890000

M06-2X

C	-1.540616000	1.334594000	-2.423330000	H	4.909958000	-3.003061000	-2.170290000
C	-0.563007000	1.334261000	-1.424910000	H	3.039152000	-3.689992000	0.172670000
C	0.000002000	2.581356000	-1.089600000	H	4.203423000	-4.765749000	-0.627320000
C	-0.421237000	3.771746000	-1.679380000	H	2.766577000	-4.191793000	-1.515190000
C	-1.427146000	3.727290000	-2.654270000	H	4.804692000	-1.934805000	0.695970000
C	0.000000000	0.000000000	-0.834600000	H	5.977096000	-1.433395000	-0.547590000
C	0.166651000	5.112214000	-1.273220000	H	6.005502000	-3.106396000	0.080790000
C	-0.710464000	5.767355000	-0.201640000	H	4.651819000	1.115694000	-4.414650000
C	1.610759000	5.016592000	-0.786940000	H	4.125934000	3.074358000	-2.939020000
C	-2.977939000	2.438950000	-4.188210000	H	2.484008000	3.151040000	-3.631450000
C	-4.226402000	1.629299000	-3.830860000	H	3.896204000	3.460837000	-4.663730000
C	-2.302641000	1.861989000	-5.438220000	H	2.842312000	0.004122000	-5.725200000
C	-0.166651000	-5.112214000	1.273220000	H	3.095153000	1.680817000	-6.286770000
C	-1.610759000	-5.016592000	0.786940000	H	1.701253000	1.285189000	-5.247810000
C	0.710464000	-5.767355000	0.201640000	H	-4.651819000	-1.115694000	4.414650000
C	2.977939000	-2.438950000	4.188210000	H	-2.842312000	-0.004122000	5.725200000
C	4.226402000	-1.629299000	3.830860000	H	-1.701253000	-1.285189000	5.247810000
C	2.302641000	-1.861989000	5.438220000	H	-3.095153000	-1.680817000	6.286770000
C	4.343982000	-2.700431000	-1.273220000	H	-4.125934000	-3.074358000	2.939020000
C	3.539116000	-3.903254000	-0.786940000	H	-3.896204000	-3.460837000	4.663730000
C	5.349908000	-2.268397000	-0.201640000	H	-2.484008000	-3.151040000	3.631450000
C	3.601162000	1.359496000	-4.188210000	H	-4.909958000	3.003061000	2.170290000
C	3.524215000	2.845522000	-3.830860000	H	-4.804692000	1.934805000	-0.695970000
C	2.763850000	1.063151000	-5.438220000	H	-6.005502000	3.106396000	-0.080790000
C	-3.601162000	-1.359496000	4.188210000	H	-5.977096000	1.433395000	0.547590000
C	-2.763850000	-1.063151000	5.438220000	H	-3.039152000	3.689992000	-0.172670000
C	-3.524215000	-2.845522000	3.830860000	H	-2.766577000	4.191793000	1.515190000
C	-4.343982000	2.700431000	1.273220000	H	-4.203423000	4.765749000	0.627320000
C	-5.349908000	2.268397000	0.201640000	H	5.055706000	2.750618000	2.170290000
C	-3.539116000	3.903254000	0.786940000	H	4.715203000	0.786987000	-0.172670000
C	4.510633000	2.411783000	1.273220000	H	5.013488000	0.300029000	1.515190000
C	5.149876000	1.113337000	0.786940000	H	6.228971000	1.257397000	0.627320000
C	4.639444000	3.498957000	0.201640000	H	4.077937000	3.193583000	-0.695970000
C	0.623223000	3.798446000	4.188210000	H	5.692969000	3.647719000	-0.080790000
C	0.461209000	2.925140000	5.438220000	H	4.229904000	4.459619000	0.547590000
C	-0.702187000	4.474820000	3.830860000	H	1.359690000	4.586440000	4.414650000
C	-0.623223000	-3.798446000	-4.188210000	H	1.417586000	2.463575000	5.725200000
C	-0.461209000	-2.925140000	-5.438220000	H	-0.262380000	2.115923000	5.247810000
C	0.702187000	-4.474820000	-3.830860000	H	0.091946000	3.520890000	6.286770000
C	-4.510633000	-2.411783000	-1.273220000	H	-0.599505000	5.110343000	2.939020000
C	-4.639444000	-3.498957000	-0.201640000	H	-1.049071000	5.104630000	4.663730000
C	-5.149876000	-1.113337000	-0.786940000	H	-1.486877000	3.726734000	3.631450000
H	3.152822000	3.848853000	3.133090000	H	-1.359690000	-4.586440000	-4.414650000
H	2.684879000	0.605665000	0.379750000	H	-1.417586000	-2.463575000	-5.725200000
H	-0.638663000	1.902996000	2.773320000	H	-0.091946000	-3.520890000	-6.286770000
H	-0.817918000	-2.628006000	0.379750000	H	0.262380000	-2.115923000	-5.247810000
H	1.756794000	-4.654850000	3.133090000	H	0.599505000	-5.110343000	-2.939020000
H	1.967374000	-0.398399000	2.773320000	H	1.486877000	-3.726734000	-3.631450000
H	-1.328711000	-1.504597000	2.773320000	H	1.049071000	-5.104630000	-4.663730000
H	-1.866961000	2.022341000	0.379750000	H	-5.055706000	-2.750618000	-2.170290000
H	-4.909616000	0.805997000	3.133090000	H	-4.077937000	-3.193583000	0.695970000
H	-3.152822000	-3.848853000	-3.133090000	H	-4.229904000	-4.459619000	-0.547590000
H	0.638663000	-1.902996000	-2.773320000	H	-5.692969000	-3.647719000	0.080790000
H	-2.684879000	-0.605665000	-0.379750000	H	-4.715203000	-0.786987000	0.172670000
H	1.866961000	-2.022341000	-0.379750000	H	-6.228971000	-1.257397000	-0.627320000
H	4.909616000	-0.805997000	-3.133090000	H	-5.013488000	-0.300029000	-1.515190000
H	1.328711000	1.504597000	-2.773320000				
H	-1.967374000	0.398399000	-2.773320000			^t Bu-1 ₂	
H	0.817918000	2.628006000	-0.379750000				
H	-1.756794000	4.654850000	-3.133090000			B3LYP	
H	0.145748000	5.753679000	-2.170290000				
H	-0.726756000	5.128388000	0.695970000				
H	-1.747191000	5.893014000	-0.547590000	C	1.413840000	-3.700720000	2.790040000
H	-0.312533000	6.754115000	0.080790000	C	0.507010000	-3.800810000	1.729050000
H	1.676051000	4.476979000	0.172670000	C	0.091910000	-2.613480000	1.094730000
H	2.025548000	6.023145000	-0.627320000	C	0.572880000	-1.345140000	1.467000000
H	2.246911000	4.491823000	-1.515190000	C	1.476160000	-1.307230000	2.550030000
H	-3.292128000	3.470746000	-4.414650000	C	1.896520000	-2.458900000	3.230190000
H	-4.725439000	2.035985000	-2.939020000	C	-1.451365000	0.176441000	1.467000000
H	-3.970884000	0.575694000	-3.631450000	C	-2.309295000	1.227144000	1.094730000
H	-4.945275000	1.643793000	-4.663730000	C	-3.545103000	1.461321000	1.729050000
H	-1.424725000	2.459453000	-5.725200000	C	-3.911838000	0.625939000	2.790040000
H	-3.003207000	1.840073000	-6.286770000	C	-3.077730000	-0.412984000	3.230190000
H	-1.963633000	0.830734000	-5.247810000	C	-1.870174000	-0.624777000	2.550030000
H	-0.145748000	-5.753679000	2.170290000	C	1.181210000	2.871884000	3.230190000
H	-1.676051000	-4.476979000	-0.172670000	C	0.394014000	1.932007000	2.550030000
H	-2.246911000	-4.491823000	1.515190000	C	0.878485000	1.168699000	1.467000000
H	-2.025548000	-6.023145000	0.627320000	C	2.217385000	1.386336000	1.094730000
H	0.726756000	-5.128388000	-0.695970000	C	3.038093000	2.339489000	1.729050000
H	0.312533000	-6.754115000	-0.080790000	C	2.497998000	3.074781000	2.790040000
H	1.747191000	-5.893014000	0.547590000	C	0.000000000	0.000000000	0.854250000
H	3.292128000	-3.470746000	4.414650000	C	-1.413840000	3.700720000	-2.790040000
H	4.725439000	-2.035985000	2.939020000	C	-1.896520000	2.458900000	-3.230190000
H	4.945275000	-1.643793000	4.663730000	C	-1.476160000	1.307230000	-2.550030000
H	3.970884000	-0.575694000	3.631450000	C	-0.572880000	1.345140000	-1.467000000
H	1.424725000	-2.459453000	5.725200000	C	-0.091910000	2.613480000	-1.094730000
H	1.963633000	-0.830734000	5.247810000	C	-0.507010000	3.800810000	-1.729050000
H	3.003207000	-1.840073000	6.286770000	C	-0.878485000	-1.168699000	-1.467000000
				C	-2.217385000	-1.386336000	-1.094730000

C	-3.038093000	-2.339489000	-1.729050000	H	-2.317823000	-3.050347000	3.987040000
C	-2.497998000	-3.074781000	-2.790040000	H	-5.169206000	-2.524207000	5.067410000
C	-1.181210000	-2.871884000	-3.230190000	H	-4.771312000	-2.643715000	3.333290000
C	-0.394014000	-1.932007000	-2.550030000	H	-5.645554000	-1.222427000	3.953370000
C	3.077730000	0.412984000	-3.230190000	H	-3.940125000	-0.897257000	6.572790000
C	1.870174000	0.624777000	-2.550030000	H	-4.410273000	0.457084000	5.519140000
C	1.451365000	-0.176441000	-1.467000000	H	-2.693556000	0.190985000	5.906320000
C	2.309295000	-1.227144000	-1.094730000	H	-1.111215000	3.885801000	5.689050000
C	3.545103000	-1.461321000	-1.729050000	H	-0.907329000	2.235380000	5.063090000
C	3.911838000	-0.625939000	-2.790040000	H	-1.482767000	3.532467000	3.987040000
C	0.000000000	0.000000000	-0.854250000	H	0.398576000	5.738767000	5.067410000
C	-0.090610000	-5.160740000	1.301970000	H	0.096132000	5.453935000	3.333290000
C	2.832240000	-2.401940000	4.457470000	H	1.764124000	5.500407000	3.953370000
C	-4.424027000	2.658841000	1.301970000	H	1.193015000	3.860877000	6.572790000
C	-3.496261000	-1.251822000	4.457470000	H	2.600983000	3.590866000	5.519140000
C	0.664021000	3.653762000	4.457470000	H	1.512176000	2.237195000	5.906320000
C	4.514637000	2.501899000	1.301970000	H	5.240071000	3.633572000	3.052970000
C	-2.832240000	2.401940000	-4.457470000	H	4.653881000	4.660961000	1.717340000
C	0.090610000	5.160740000	-1.301970000	H	6.216851000	3.822319000	1.585810000
C	-4.514637000	-2.501899000	-1.301970000	H	4.190177000	1.820060000	-0.775000000
C	-0.664021000	-3.653762000	-4.457470000	H	5.681865000	2.751562000	-0.526480000
C	3.496261000	1.251822000	-4.457470000	H	4.108841000	3.584919000	-0.560780000
C	4.424027000	-2.658841000	-1.301970000	H	5.274331000	1.114350000	2.824930000
C	0.634270000	-6.352450000	1.957220000	H	6.353874000	1.315708000	1.419590000
C	0.000000000	-5.338700000	-0.228330000	H	4.874889000	0.331265000	1.276620000
C	-1.575270000	-5.208150000	1.730330000	H	-1.809290000	4.047950000	-5.519140000
C	3.254780000	-0.965050000	4.811560000	H	-2.747110000	2.963620000	-6.572790000
C	4.111340000	-3.226120000	4.183310000	H	-1.181380000	2.428180000	-5.906320000
C	2.097820000	-2.998030000	5.681910000	H	-3.881430000	4.277980000	-3.953370000
C	-5.818518000	2.626931000	1.957220000	H	-4.675180000	2.810220000	-3.333290000
C	-4.623450000	2.669350000	-0.228330000	H	-4.770630000	3.214560000	-5.067410000
C	-3.722755000	3.968299000	1.730330000	H	-3.800590000	0.482120000	-3.987040000
C	-2.463148000	-2.336197000	4.811560000	H	-2.389560000	0.331920000	-5.063090000
C	-4.849572000	-1.947465000	4.183310000	H	-3.920810000	0.980560000	-5.689050000
C	-3.645280000	-0.317750000	5.681910000	H	0.458010000	6.296420000	0.526480000
C	-0.791632000	3.301247000	4.811560000	H	0.518870000	4.538830000	0.775000000
C	0.738232000	5.173585000	4.183310000	H	-1.050210000	5.350820000	0.560780000
C	1.547460000	3.315780000	5.681910000	H	-0.201800000	7.295110000	-1.585810000
C	5.184248000	3.725519000	1.957220000	H	-1.709570000	6.360860000	-1.717340000
C	4.623450000	2.669350000	-0.228330000	H	-0.526730000	6.354820000	-3.052970000
C	5.298025000	1.239851000	1.730330000	H	2.037500000	6.160470000	-1.419590000
C	-2.097820000	2.998030000	-5.681910000	H	1.672110000	5.124880000	-5.906320000
C	-4.111340000	3.226120000	-4.183310000	H	2.150560000	4.387410000	-1.276620000
C	-3.254780000	0.965050000	-4.811560000	H	-5.681865000	-2.751562000	0.526480000
C	0.000000000	5.338700000	0.228330000	H	-4.190177000	-1.820060000	0.775000000
C	-0.634270000	6.352450000	-1.957220000	H	-4.108841000	-3.584919000	0.560780000
C	1.575270000	5.208150000	-1.730330000	H	-6.216851000	-3.822319000	-1.585810000
C	-4.623450000	-2.669350000	0.228330000	H	-4.663881000	-4.660961000	-1.717340000
C	-5.184248000	-3.725519000	-1.957220000	H	-5.240071000	-3.633572000	-3.052970000
C	-5.298025000	-1.239851000	-1.730330000	H	-6.353874000	-1.315708000	-1.419590000
C	-1.547460000	-3.315780000	-5.681910000	H	-5.274331000	-1.114350000	-2.824930000
C	-0.738232000	-5.173585000	-4.183310000	H	-4.874889000	-0.331265000	-1.276620000
C	0.791632000	-3.301247000	-4.811560000	H	-2.600983000	-3.590866000	-5.519140000
C	3.645280000	0.317750000	-5.681910000	H	-1.193015000	-3.860877000	-6.572790000
C	4.849572000	1.947465000	-4.183310000	H	-1.512176000	-2.237195000	-5.906320000
C	2.463148000	2.336197000	-4.811560000	H	-1.764124000	-5.500407000	-3.953370000
C	4.623450000	-2.669350000	0.228330000	H	-0.096132000	-5.453935000	-3.333290000
C	5.818518000	-2.626931000	-1.957220000	H	-0.398576000	-5.738767000	-5.067410000
C	3.722755000	-3.968299000	-1.730330000	H	1.482767000	-3.532467000	-3.987040000
H	0.526730000	-6.354820000	3.052970000	H	0.907329000	-2.235380000	-5.063090000
H	1.709570000	-6.360860000	1.717340000	H	1.111215000	-3.885801000	-5.689050000
H	0.201800000	-7.295110000	1.585810000	H	4.410273000	-0.457084000	-5.519140000
H	-0.518870000	-4.538830000	-0.775000000	H	3.940125000	0.897257000	-6.572790000
H	-0.458010000	-6.296420000	-0.526480000	H	2.693556000	-0.190985000	-5.906320000
H	1.050210000	-5.350820000	-0.560780000	H	5.645554000	1.222427000	-3.953370000
H	-1.672110000	-5.124880000	2.824930000	H	4.771312000	2.643715000	-3.333290000
H	-2.037500000	-6.160470000	1.419590000	H	5.169206000	2.524207000	-5.067410000
H	-2.150560000	-4.387410000	1.276620000	H	2.317823000	3.050347000	-3.987040000
H	3.920810000	-0.980560000	5.689050000	H	1.482231000	1.903460000	-5.063090000
H	2.389560000	-0.331920000	5.063090000	H	2.809595000	2.905241000	-5.689050000
H	3.800590000	-0.482120000	3.987040000	H	5.223855000	-3.544858000	0.526480000
H	4.770630000	-3.214560000	5.067410000	H	3.671307000	-2.718770000	0.775000000
H	4.675180000	-2.810220000	3.333290000	H	5.159051000	-1.765901000	0.560780000
H	3.881430000	-4.277980000	3.953370000	H	6.418651000	-3.472791000	-1.585810000
H	2.747110000	-2.963620000	6.572790000	H	6.363451000	-1.699899000	-1.717340000
H	1.809290000	-4.047950000	5.519140000	H	5.766801000	-2.721248000	-3.052970000
H	1.181380000	-2.428180000	5.906320000	H	4.316374000	-4.844762000	-1.419590000
H	-5.766801000	2.721248000	3.052970000	H	3.602221000	-4.010530000	-2.824930000
H	-6.363451000	1.699899000	1.717340000	H	2.724329000	-4.056145000	-1.276620000
H	-6.418651000	3.472791000	1.585810000	H	1.738610000	-4.603420000	3.304700000
H	-3.671307000	2.718770000	-0.775000000	H	-0.645640000	-2.687570000	0.303490000
H	-5.223855000	3.544858000	-0.526480000	H	1.843040000	-0.348110000	2.893940000
H	-5.159051000	1.765901000	-0.560780000	H	-2.004684000	1.902926000	0.303490000
H	-3.602221000	4.010530000	2.824930000	H	-4.855984000	0.796030000	3.304700000
H	-4.316374000	4.844762000	1.419590000	H	-1.222992000	-1.422064000	2.893940000
H	-2.724329000	4.056145000	1.276620000	H	-0.620048000	1.770174000	2.893940000
H	-2.809595000	-2.905241000	5.689050000	H	2.650324000	0.784644000	0.303490000
H	-1.482231000	-1.903460000	5.063090000	H	3.117374000	3.807390000	3.304700000

H	-1.738610000	4.603420000	-3.304700000	C	-5.028202000	-1.812731000	-1.625360000
H	-1.843040000	0.348110000	-2.893940000	C	-1.027719000	-3.561777000	-5.564200000
H	0.645640000	2.687570000	-0.303490000	C	0.000006000	-5.263990000	-4.015880000
H	-2.650324000	-0.784644000	-0.303490000	C	1.271866000	-3.214450000	-4.656760000
H	-3.117374000	-3.807390000	-3.304700000	C	3.598449000	0.890858000	-5.564200000
H	0.620048000	-1.770174000	-2.893940000	C	4.558746000	2.632000000	-4.015880000
H	1.222992000	1.422064000	-2.893940000	C	2.147862000	2.708693000	-4.656760000
H	2.004684000	-1.902926000	-0.303490000	C	4.856070000	-2.031299000	0.299340000
H	4.855984000	-0.796030000	-3.304700000	C	6.043678000	-1.918534000	-1.891930000
				C	4.083972000	-3.448185000	-1.625360000
				H	1.244975000	-6.195168000	2.986770000
				H	2.432434000	-6.096712000	1.658870000
				H	1.022202000	-7.173643000	1.521880000
				H	0.098757000	-4.452471000	-0.838000000
				H	0.294738000	-6.205387000	-0.624830000
				H	1.721935000	-5.139586000	-0.610170000
				H	-1.067307000	-5.202074000	2.718390000
				H	-1.317893000	-6.242667000	1.290290000
				H	-1.575105000	-4.483138000	1.171750000
				H	4.113164000	-0.419537000	5.507700000
				H	2.483104000	0.002076000	4.934840000
				H	3.859202000	0.038064000	3.807760000
				H	5.229127000	-2.542830000	4.886470000
				H	5.039292000	-2.133758000	3.160380000
				H	4.461671000	-3.701215000	3.773710000
				H	3.219500000	-2.533117000	6.444930000
				H	2.437096000	-3.752362000	5.409400000
				H	1.583405000	-2.237874000	5.792320000
				H	-5.987661000	2.019404000	2.986770000
				H	-6.496124000	0.941807000	1.658870000
				H	-6.723658000	2.701569000	1.521880000
				H	-3.905332000	2.140709000	-0.838000000
				H	-5.521392000	2.847443000	-0.624830000
				H	-5.311980000	1.078553000	-0.610170000
				H	-3.971475000	3.525352000	2.718390000
				H	-4.747361000	4.262663000	1.290290000
				H	-3.094959000	3.605650000	1.171750000
				H	-2.419911000	-3.352336000	5.507700000
				H	-1.239754000	-2.151469000	4.934840000
				H	-1.896636000	-3.361199000	3.807760000
				H	-4.816719000	-3.257142000	4.886470000
				H	-4.367535000	-3.297276000	3.160380000
				H	-5.436182000	-2.013313000	3.773710000
				H	-3.803494000	-1.521610000	6.444930000
				H	-4.468189000	-0.234406000	5.409400000
				H	-2.729758000	-0.252332000	5.792320000
				H	-1.693253000	3.771873000	5.507700000
				H	-1.243349000	2.149393000	4.934840000
				H	-1.962565000	3.323135000	3.807760000
				H	-0.412408000	5.799972000	4.886470000
				H	-0.671757000	5.431034000	3.160380000
				H	0.974511000	5.714528000	3.773710000
				H	0.583994000	4.054727000	6.444930000
				H	2.031093000	3.986768000	5.409400000
				H	1.146353000	2.490206000	5.792320000
				H	4.742685000	4.175764000	2.986770000
				H	4.063691000	5.154905000	1.658870000
				H	5.701456000	4.472075000	1.521880000
				H	3.806575000	2.311762000	-0.838000000
				H	5.226654000	3.357944000	-0.624830000
				H	3.590044000	4.061033000	-0.610170000
				H	5.038782000	1.676722000	2.718390000
				H	6.065255000	1.980004000	1.290290000
				H	4.670064000	0.877488000	1.171750000
				H	-2.437096000	3.752362000	-5.409400000
				H	-3.219500000	2.533117000	-6.444930000
				H	-1.583405000	2.237874000	-5.792320000
				H	-4.461671000	3.701215000	-3.773710000
				H	-5.039292000	2.133758000	-3.160380000
				H	-5.229127000	2.542830000	-4.886470000
				H	-3.859202000	-0.038064000	-3.807760000
				H	-2.483104000	-0.002076000	-4.934840000
				H	-4.113164000	0.419537000	-5.507700000
				H	-0.294738000	6.205387000	0.624830000
				H	-0.098757000	4.452471000	0.838000000
				H	-1.721935000	5.139586000	0.610170000
				H	-1.022202000	7.173643000	-1.521880000
				H	-2.432434000	6.096712000	-1.658870000
				H	-1.244975000	6.195168000	-2.986770000
				H	1.317893000	6.242667000	-1.290290000
				H	1.067307000	5.202074000	-2.718390000
				H	1.575105000	4.483138000	-1.171750000
				H	-5.226654000	-3.357944000	0.624830000
				H	-3.806575000	-2.311762000	0.838000000
				H	-3.590044000	-4.061033000	0.610170000
				H	-5.701456000	-4.472075000	-1.521880000
				H	-4.063691000	-5.154905000	-1.658870000
				H	-4.742685000	-4.175764000	-2.986770000

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H	-6.065255000	-1.980004000	-1.290290000	C	0.000000000	0.000000000	-0.832810000
H	-5.038782000	-1.676722000	-2.718390000	C	-0.064290000	-5.089930000	1.264800000
H	-4.670064000	-0.877488000	-1.171750000	C	2.987290000	-2.345200000	4.297520000
H	-2.031093000	-3.986768000	-5.409400000	C	-4.375864000	2.600642000	1.264800000
H	-0.583994000	-4.054727000	-6.444930000	C	-3.524648000	-1.414469000	4.297520000
H	-1.146353000	-2.490206000	-5.792320000	C	0.537358000	3.759669000	4.297520000
H	-0.974511000	-5.714528000	-3.773710000	C	4.440154000	2.489288000	1.264800000
H	0.671757000	-5.431034000	-3.160380000	C	-2.987290000	2.345200000	-4.297520000
H	0.412408000	-5.799972000	-4.886470000	C	0.064290000	5.089930000	-1.264800000
H	1.962565000	-3.323135000	-3.807760000	C	-4.440154000	-2.489288000	-1.264800000
H	1.243349000	-2.149393000	-4.934840000	C	-0.537358000	-3.759669000	-4.297520000
H	1.693253000	-3.771873000	-5.507700000	C	3.524648000	1.414469000	-4.297520000
H	4.468189000	0.234406000	-5.409400000	C	4.375864000	-2.600642000	-1.264800000
H	3.803494000	1.521610000	-6.444930000	C	0.637110000	-6.290550000	1.905020000
H	2.729758000	0.252332000	-5.792320000	C	0.000000000	-5.248730000	-0.260990000
H	5.436182000	2.013313000	-3.773710000	C	-1.536210000	-5.086170000	1.707860000
H	4.367535000	3.297276000	-3.160380000	C	3.305200000	-0.899990000	4.692290000
H	4.816719000	3.257142000	-4.886470000	C	4.300090000	-3.041940000	3.906130000
H	1.896363000	3.361199000	-3.807760000	C	2.379250000	-3.053910000	5.519170000
H	1.239754000	2.151469000	-4.934840000	C	-5.766331000	2.593522000	1.905020000
H	2.419911000	3.352336000	-5.507700000	C	-4.545534000	2.624365000	-0.260990000
H	5.521392000	-2.847443000	0.624830000	C	-3.636647000	3.873482000	1.707860000
H	3.905332000	-2.140709000	0.838000000	C	-2.432014000	-2.412392000	4.692290000
H	5.311980000	-1.078553000	0.610170000	C	-4.784442000	-2.203017000	3.906130000
H	6.723658000	-2.701569000	-1.521880000	C	-3.834389000	-0.533536000	5.519170000
H	6.496124000	-0.941807000	-1.658870000	C	-0.873186000	3.312382000	4.692290000
H	5.987661000	-2.019404000	-2.986770000	C	0.484352000	5.244957000	3.906130000
H	4.747361000	-4.262663000	-1.290290000	C	1.455139000	3.587446000	5.519170000
H	3.971475000	-3.525352000	-2.718390000	C	5.129221000	3.697028000	1.905020000
H	3.094959000	-3.605650000	-1.171750000	C	4.545534000	2.624365000	-0.260990000
H	2.365756000	-4.328560000	3.192610000	C	5.172857000	1.212688000	1.707860000
H	-0.351453000	-2.715799000	0.304750000	C	-2.379250000	3.053910000	-5.519170000
H	1.913196000	-0.092396000	2.810390000	C	-4.300090000	3.041940000	-3.906130000
H	-2.176224000	1.662267000	0.304750000	C	-3.305200000	0.899990000	-4.692290000
H	-4.931521000	0.115476000	3.192610000	C	0.000000000	5.248730000	0.260990000
H	-1.036615000	-1.610678000	2.810390000	C	-0.637110000	6.290550000	-1.905020000
H	-0.876581000	1.703074000	2.810390000	C	1.536210000	5.086170000	-1.707860000
H	2.527677000	1.053532000	0.304750000	C	-4.545534000	-2.624365000	0.260990000
H	2.565766000	4.213085000	3.192610000	C	-5.129221000	-3.697028000	-1.905020000
H	-2.365756000	4.328560000	-3.192610000	C	-5.172857000	-1.212688000	-1.707860000
H	-1.913196000	0.092396000	-2.810390000	C	-1.455139000	-3.587446000	-5.519170000
H	0.351453000	2.715799000	-0.304750000	C	-0.484352000	-5.244957000	-3.906130000
H	-2.527677000	-1.053532000	-0.304750000	C	0.873186000	-3.312382000	-4.692290000
H	-2.565766000	-4.213085000	-3.192610000	C	3.834389000	0.533536000	-5.519170000
H	0.876581000	-1.703074000	-2.810390000	C	4.784442000	2.203017000	-3.906130000
H	1.036615000	1.610678000	-2.810390000	C	2.432014000	2.412392000	-4.692290000
H	2.176224000	-1.662267000	-0.304750000	C	4.545534000	-2.624365000	0.260990000
H	4.931521000	-0.115476000	-3.192610000	C	5.766331000	-2.593522000	-1.905020000

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C	1.522580000	-3.663230000	2.698180000	H	0.553940000	-6.274330000	3.001840000
C	0.567670000	-3.757410000	1.684590000	H	1.704580000	-6.321830000	1.638130000
C	0.112340000	-2.576150000	1.082920000	H	0.170670000	-7.221350000	1.549290000
C	0.604320000	-1.313650000	1.433370000	H	-0.495810000	-4.418210000	-0.786460000
C	1.542700000	-1.268040000	2.477340000	H	-0.497660000	-6.183670000	-0.564480000
C	1.999740000	-2.418510000	3.126800000	H	1.046390000	-5.295770000	-0.600980000
C	-1.439814000	0.133469000	1.433370000	H	-1.610650000	-5.041630000	2.805320000
C	-2.287181000	1.190786000	1.082920000	H	-2.043560000	-6.002120000	1.365120000
C	-3.537848000	1.387088000	1.684590000	H	-2.069530000	-4.217640000	1.291360000
C	-3.933740000	0.513022000	2.698180000	H	4.006000000	-0.895630000	5.540490000
C	-3.094361000	-0.522571000	3.126800000	H	2.397960000	-0.355500000	4.996630000
C	-1.869505000	-0.701997000	2.477340000	H	3.773000000	-0.348430000	3.863560000
C	1.094621000	2.941081000	3.126800000	H	4.996780000	-3.044560000	4.759380000
C	0.326805000	1.970037000	2.477340000	H	4.782800000	-2.516410000	3.068290000
C	0.835494000	1.180181000	1.433370000	H	4.127890000	-4.085500000	3.602080000
C	2.174841000	1.385364000	1.082920000	H	3.070600000	-2.993380000	6.374050000
C	2.970178000	2.370322000	1.684590000	H	2.184280000	-4.117330000	5.318340000
C	2.411160000	3.150208000	2.698180000	H	1.428350000	-2.581110000	5.808750000
C	0.000000000	0.000000000	0.832810000	H	-5.710699000	2.657439000	3.001840000
C	-1.522580000	3.663230000	-2.698180000	H	-6.327155000	1.684705000	1.638130000
C	-1.999740000	2.418510000	-3.126800000	H	-6.339208000	3.462870000	1.549290000
C	-1.542700000	1.268040000	-2.477340000	H	-3.578377000	2.638489000	-0.786460000
C	-0.604320000	1.313650000	-1.433370000	H	-5.106385000	3.522821000	-0.564480000
C	-0.112340000	2.576150000	-1.082920000	H	-5.109466000	1.741685000	-0.600980000
C	-0.567670000	3.757410000	-1.684590000	H	-3.560855000	3.915679000	2.805320000
C	-0.835494000	-1.180181000	-1.433370000	H	-4.176208000	4.770835000	1.365120000
C	-2.174841000	-1.385364000	-1.082920000	H	-2.617818000	3.901086000	1.291360000
C	-2.970178000	-2.370322000	-1.684590000	H	-2.778638000	-3.021483000	5.540490000
C	-2.411160000	-3.150208000	-2.698180000	H	-1.506852000	-1.898944000	4.996630000
C	-1.094621000	-2.941081000	-3.126800000	H	-2.188249000	-3.093299000	3.863560000
C	-0.326805000	-1.970037000	-2.477340000	H	-5.135056000	-2.805058000	4.759380000
C	3.094361000	0.522571000	-3.126800000	H	-4.570675000	-2.883821000	3.068290000
C	1.869505000	0.701997000	-2.477340000	H	-5.602092000	-1.532108000	3.602080000
C	1.439814000	-0.133469000	-1.433370000	H	-4.127643000	-1.162528000	6.374050000
C	2.287181000	-1.190786000	-1.082920000	H	-4.657852000	0.167023000	5.318340000
C	3.537848000	-1.387088000	-1.684590000	H	-2.949482000	0.053568000	5.808750000
C	3.933740000	-0.513022000	-2.698180000	H	-1.227362000	3.917113000	5.540490000
				H	-0.891108000	2.254444000	4.996630000
				H	-1.584751000	3.441729000	3.863560000

H	0.138276000	5.849618000	4.759380000			
H	-0.212125000	5.400231000	3.068290000		Cy-1 ₂	
H	1.474202000	5.617608000	3.602080000			
H	1.057043000	4.155908000	6.374050000		B3LYP	
H	2.473572000	3.950307000	5.318340000			
H	1.521132000	2.527542000	5.808750000	C	0.000000000	0.859260000
H	5.156759000	3.616891000	3.001840000	C	-1.510872000	1.397900000
H	4.622575000	4.637125000	1.638130000	C	-1.946663000	2.592628000
H	6.168538000	3.758480000	1.549290000	C	-0.526429000	1.363075000
H	4.074187000	1.779721000	-0.786460000	C	-1.373457000	3.799907000
H	5.604045000	2.660849000	-0.564480000	C	0.044194000	2.602243000
H	4.063076000	3.554085000	-0.600980000	C	-0.366243000	3.815848000
H	5.171505000	1.125951000	2.805320000	C	0.298387000	5.116294000
H	6.219768000	1.231285000	1.365120000	C	-0.698614000	6.127464000
H	4.687348000	0.316554000	1.291360000	C	1.091440000	5.775870000
H	-2.184280000	4.117330000	-5.318340000	C	0.000000000	7.418708000
H	-3.070600000	2.993380000	-6.374050000	C	1.787861000	7.067542000
H	-1.428350000	2.581110000	-5.808750000	C	0.791588000	8.061196000
H	-4.127890000	4.085500000	-3.602080000	C	5.226741000	-5.082104000
H	-4.782800000	2.516410000	-3.068290000	C	4.456331000	-3.833150000
H	-4.996780000	3.044560000	-4.759380000	C	6.585407000	-4.716133000
H	-3.773000000	0.348430000	-3.863560000	C	3.977545000	-0.710505000
H	-2.397960000	0.355500000	-4.996630000	C	4.281648000	-2.816558000
H	-4.006000000	0.895630000	-5.540490000	C	3.218613000	0.389546000
H	0.497660000	6.183670000	0.564480000	C	3.487743000	-1.590748000
H	0.495810000	4.418210000	0.786460000	C	1.966053000	0.609503000
H	-1.046390000	5.295770000	0.600980000	C	2.231511000	-1.339395000
H	-0.170670000	7.221350000	-1.549290000	C	1.443672000	-0.225637000
H	-1.704580000	6.321830000	-1.638130000	C	6.424789000	-3.709354000
H	-0.553940000	6.274330000	-3.001840000	C	5.655846000	-2.458715000
H	2.043560000	6.002120000	-1.365120000	C	-6.424789000	-3.709354000
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H	2.069530000	4.217640000	-1.291360000	C	-7.376994000	-3.345063000
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H	-5.171505000	-1.125951000	-2.805320000	C	-2.275705000	-1.262848000
H	-4.687348000	-0.316554000	-1.291360000	C	-0.917243000	-1.137438000
H	-2.473572000	-3.950307000	-5.318340000	C	-0.717282000	-4.474886000
H	-1.057043000	-4.155908000	-6.374050000	C	-1.334756000	-3.598961000
H	-1.521132000	-2.527542000	-5.808750000	C	-0.698398000	-3.875902000
H	-1.474202000	-5.617608000	-3.602080000	C	-0.806891000	-5.966330000
H	0.212125000	-5.400231000	-3.068290000	C	-0.178788000	-6.255092000
H	-0.138276000	-5.849618000	-4.759380000	C	-0.795180000	-5.379744000
H	1.584751000	-3.441729000	-3.863560000	C	-4.261405000	3.378518000
H	0.891108000	-2.254444000	-4.996630000	C	-3.007430000	2.542781000
H	1.227362000	-3.917113000	-5.540490000	C	-2.449414000	2.955413000
H	4.657852000	-0.167023000	-5.318340000	C	-5.327675000	3.282381000
H	4.127643000	1.162528000	-6.374050000	C	-4.763548000	3.681953000
H	2.949482000	-0.053568000	-5.808750000	C	-3.516724000	2.858627000
H	5.602092000	1.532108000	-3.602080000	C	3.705828000	1.333121000
H	4.570675000	2.883821000	-3.068290000	C	5.056585000	2.001226000
H	5.135056000	2.805058000	-4.759380000	C	3.784169000	0.643548000
H	2.188249000	3.093299000	-3.863560000	C	5.506462000	2.972711000
H	1.506852000	1.898944000	-4.996630000	C	4.234006000	1.616259000
H	2.778638000	3.021483000	-5.540490000	C	5.570439000	2.284377000
H	5.106385000	-3.522821000	0.564480000	C	-1.443672000	0.225637000
H	3.578377000	-2.638489000	0.786460000	C	0.000000000	0.000000000
H	5.109466000	-1.741685000	0.600980000	C	0.917243000	1.137438000
H	6.339208000	-3.462870000	-1.549290000	C	2.275705000	1.262848000
H	6.327155000	-1.684705000	-1.638130000	C	3.121500000	2.225100000
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H	3.560855000	-3.915679000	-2.805320000	C	7.376994000	3.345063000
H	2.617818000	-3.901086000	-1.291360000	C	6.424789000	3.709354000
H	1.887550000	-4.567810000	3.184880000	C	5.547771000	1.942720000
H	-0.680110000	-2.657400000	0.346210000	C	4.957233000	3.668749000
H	1.910830000	-0.308100000	2.820440000	C	2.604088000	3.089403000
H	-1.961321000	1.917693000	0.346210000	C	1.271950000	2.982174000
H	-4.899614000	0.649239000	3.184880000	C	0.698398000	3.875902000
H	-1.222237000	-1.500777000	2.820440000	C	1.334756000	3.598961000
H	-0.688593000	1.808877000	2.820440000	C	0.717282000	4.474886000
H	2.641431000	0.739707000	0.346210000	C	8.066891000	5.966330000
H	3.012064000	3.918571000	3.184880000	C	0.178788000	6.255092000
H	-1.887550000	4.567810000	-3.184880000	C	0.795180000	5.379744000
H	-1.910830000	0.308100000	-2.820440000	C	4.455181000	2.007403000
H	0.680110000	2.657400000	-0.346210000	C	0.526429000	-1.363075000
H	-2.641431000	-0.739707000	-0.346210000	C	1.510872000	-1.397900000
H	-3.012064000	-3.918571000	-3.184880000	C	1.946663000	-2.592628000
H	0.688593000	-1.808877000	-2.820440000	C	3.007430000	-2.542781000
H	1.222237000	1.500777000	-2.820440000	C	5.327675000	-3.282381000
H	1.961321000	-1.917693000	-0.346210000	C	4.763548000	-3.681953000
H	4.899614000	-0.649239000	-3.184880000	C	3.516724000	-2.858627000
				C	4.261405000	-3.378518000
				C	2.449414000	-2.955413000

C	1.373457000	-3.799907000	-2.634090000	H	-3.806387000	1.798931000	6.748980000
C	0.366243000	-3.815848000	-1.657090000	H	-3.096218000	3.188725000	7.582630000
C	-0.298387000	-5.116294000	-1.229690000	H	2.956714000	2.141441000	4.222660000
C	0.698614000	-6.127464000	-0.620920000	H	5.827850000	1.219837000	3.666540000
C	0.000000000	-7.418708000	-0.172050000	H	4.976720000	2.526601000	2.830740000
C	-1.787861000	-7.067542000	-1.931050000	H	2.802714000	0.207094000	5.769430000
C	-0.791588000	-8.061196000	-1.319080000	H	4.496610000	-0.200570000	5.462740000
C	-1.091440000	-5.775870000	-2.381180000	H	6.487256000	3.407331000	4.640120000
C	-0.044194000	-2.602243000	-1.089830000	H	4.794281000	3.818005000	4.948910000
C	-1.966053000	-0.609503000	-2.447540000	H	3.461114000	2.396962000	6.748980000
C	-3.218613000	-0.389546000	-3.046180000	H	4.309626000	1.087041000	7.582630000
C	-3.705828000	-1.333121000	-4.137690000	H	6.367393000	1.516655000	6.252300000
C	-5.506462000	-2.972711000	-4.897920000	H	5.851887000	3.011002000	7.048940000
C	-5.570439000	-2.284377000	-6.267860000	H	2.708539000	0.585988000	-0.360640000
C	-4.234006000	-1.616259000	-6.617460000	H	4.723888000	1.542386000	-0.437930000
C	-5.056585000	-2.001226000	-3.797410000	H	7.187040000	1.191591000	-1.180020000
C	-3.784169000	-0.643548000	-5.518400000	H	7.677843000	1.758089000	-2.783010000
C	-3.977545000	0.710505000	-2.634090000	H	8.421357000	3.339694000	-0.963360000
C	-3.487743000	1.590748000	-1.657090000	H	7.316583000	4.124125000	-2.102790000
C	-4.281648000	2.816558000	-1.229690000	H	6.568891000	2.995316000	0.660580000
C	-5.226741000	5.082104000	-1.931050000	H	6.669613000	4.708090000	0.227920000
C	-6.585407000	4.716133000	-1.319080000	H	5.400831000	2.655653000	-3.213680000
C	-6.424789000	3.709354000	-0.172050000	H	5.296965000	0.944417000	-2.778190000
C	-4.456331000	3.833150000	-2.381180000	H	4.785274000	4.462644000	-1.371070000
C	-5.655846000	2.458715000	-0.620920000	H	4.289643000	3.891754000	0.228620000
C	-2.231511000	1.339395000	-1.089830000	H	3.252689000	3.840999000	-3.090350000
H	-1.963198000	0.474068000	2.798440000	H	-0.376185000	3.631309000	-4.222660000
H	-1.700058000	4.737411000	3.090350000	H	1.222009000	2.530769000	-5.769430000
H	0.846789000	2.638658000	0.360640000	H	2.422003000	3.793894000	-5.462740000
H	1.026199000	4.862200000	0.437930000	H	-0.345273000	4.195893000	-6.748980000
H	-1.472126000	6.375491000	1.371070000	H	1.213408000	4.275766000	-7.582630000
H	-1.225536000	5.660817000	-0.228620000	H	1.870235000	6.272652000	-6.252300000
H	0.400552000	6.005083000	3.213680000	H	0.318339000	6.573384000	-7.048940000
H	1.830594000	5.059514000	2.778190000	H	0.292792000	7.321794000	-4.640120000
H	0.690426000	7.186485000	-0.660580000	H	-0.909349000	6.060972000	-4.948910000
H	-0.742519000	8.130099000	-0.227920000	H	1.857515000	5.656985000	-3.666540000
H	2.561572000	6.819955000	1.180020000	H	0.300259000	5.573267000	-2.830740000
H	2.316371000	7.528251000	2.783010000	H	-0.571044000	1.937214000	-2.798440000
H	1.318419000	8.962956000	0.963360000	H	1.963198000	-0.474068000	-2.798440000
H	0.086694000	8.398409000	2.102790000	H	3.332899000	-1.489869000	-4.222660000
H	4.625468000	-5.628364000	1.180020000	H	6.194464000	-3.914463000	-4.640120000
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H	5.000279000	-3.349430000	3.213680000	H	4.497158000	-4.755997000	-6.252300000
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H	7.102938000	-5.623263000	0.963360000	H	3.806387000	-1.798931000	-6.748980000
H	7.229889000	-4.274284000	2.102790000	H	3.096218000	-3.188725000	-7.582630000
H	4.952747000	-0.896412000	3.090350000	H	3.970335000	-4.437148000	-3.666540000
H	3.697689000	-3.319814000	0.437930000	H	4.676461000	-3.046665000	-2.830740000
H	1.392154000	1.463145000	2.798440000	H	1.580706000	-2.323675000	-5.769430000
H	1.861750000	-2.052670000	0.360640000	H	2.074606000	-3.994463000	-5.462740000
H	5.878465000	-4.191169000	-0.660580000	H	1.700058000	-4.737411000	-3.090350000
H	7.412132000	-3.422009000	-0.227920000	H	-1.026199000	-4.862200000	-0.437930000
H	6.257400000	-1.912847000	1.371070000	H	1.472126000	-6.375491000	-1.371070000
H	5.515180000	-1.769063000	-0.228620000	H	1.225536000	5.660817000	0.228620000
H	-6.568891000	-2.995316000	-0.660580000	H	-0.690426000	-7.186485000	0.660580000
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H	-4.785274000	-4.462644000	1.371070000	H	-2.561572000	-6.819955000	-1.180020000
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H	-3.252689000	-3.840999000	3.090350000	H	-0.400552000	-6.005083000	-3.213680000
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H	-7.187040000	-1.191591000	1.180020000	H	-0.846789000	-2.638658000	-0.360640000
H	-7.677843000	-1.758089000	2.783010000	H	-1.392154000	-1.463145000	-2.798440000
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H	0.571044000	-1.937214000	2.798440000	H	-4.794281000	-3.818005000	-4.948910000
H	-2.708539000	-0.585988000	0.360640000	H	-6.367393000	-1.516655000	-6.252300000
H	0.345273000	-4.195893000	6.748980000	H	-5.851887000	-3.011002000	-7.048940000
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H	-2.422003000	-3.793894000	5.462740000	H	-5.827850000	-1.219837000	-3.666540000
H	0.376185000	-3.631309000	4.222660000	H	-4.976720000	-2.526601000	-2.830740000
H	-1.870235000	-6.272652000	6.252300000	H	-2.802714000	-0.207094000	-5.769430000
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H	-3.970335000	4.437148000	3.666540000	H	-7.102938000	5.623263000	-0.963360000
H	-4.676461000	3.046665000	2.830740000	H	-7.229889000	4.274284000	-2.102790000
H	-3.332899000	1.489869000	4.222660000	H	-5.878465000	4.191169000	0.660580000
H	-1.580706000	2.323675000	5.769430000	H	-7.412132000	3.422009000	0.227920000
H	-2.074606000	3.994463000	5.462740000	H	-5.000279000	3.349430000	-3.213680000
H	-6.194464000	3.914463000	4.640120000	H	-3.466371000	4.115098000	-2.778190000
H	-5.703630000	2.242967000	4.948910000	H	-6.257400000	1.912847000	-1.371070000
H	-4.497158000	4.755997000	6.252300000	H	-5.515180000	1.769063000	0.228620000
H	-5.533548000	3.562382000	7.048940000	H	-1.861750000	2.052670000	-0.360640000

B3LYP-D3(BJ)

C	0.00000000	0.00000000	0.85926000	C	0.36624300	-3.81584800	-1.65709000
C	-1.51087200	1.39790000	2.44754000	C	-0.29838700	-5.11629400	-1.22969000
C	-1.94666300	2.59262800	3.04618000	C	0.69861400	-6.12746400	-0.62092000
C	-0.52642900	1.36307500	1.44545000	C	0.00000000	-7.41870800	-0.17205000
C	-1.37345700	3.79990700	2.63409000	C	-1.78786100	-7.06754200	-1.93105000
C	0.04419400	2.60224300	1.08983000	C	-0.79158800	-8.06119600	-1.31908000
C	-0.36624300	3.81584800	1.65709000	C	-1.09144000	-5.77587000	-2.38118000
C	0.29838700	5.11629400	1.22969000	C	-0.04419400	-2.60224300	-1.08983000
C	-0.69861400	6.12746400	0.62092000	C	-1.96605300	-0.60950300	-2.44754000
C	1.09144000	5.77587000	2.38118000	C	-3.21861300	-0.38954600	-3.04618000
C	0.00000000	7.41870800	0.17205000	C	-3.70582800	-1.33312100	-4.13769000
C	1.78786100	7.06754200	1.93105000	C	-5.50646200	-2.97271100	-4.89792000
C	0.79158800	8.06119600	1.31908000	C	-5.70439000	-2.28437700	-6.26786000
C	5.22674100	-5.08210400	1.93105000	C	-4.23400600	-1.61625900	-6.61746000
C	4.45633100	-3.83315000	2.38118000	C	-5.05658500	-2.00122600	-3.79741000
C	6.58540700	-4.71613300	1.31908000	C	-3.78416900	-0.64354800	-5.51840000
C	3.97754500	-0.71050500	2.63409000	C	-3.97754500	0.71050500	-2.63409000
C	4.28164800	-2.81655800	1.22969000	C	-3.48774300	1.59074800	-1.65709000
C	3.21861300	0.38954600	3.04618000	C	-4.28164800	2.81655800	-1.22969000
C	3.48774300	-1.59074800	1.65709000	C	-5.22674100	5.08210400	-1.93105000
C	1.96605300	0.60950300	2.44754000	C	-6.58540700	4.71613300	-1.31908000
C	2.23151100	-1.33939500	1.08983000	C	-6.42478900	3.70935400	-0.17205000
C	1.44367200	-0.22563700	1.44545000	C	-4.56331000	3.83315000	-2.38118000
C	6.42478900	-3.70935400	0.17205000	C	-5.65584600	2.45871500	-0.62092000
C	5.65584600	-2.45871500	0.62092000	C	-2.23151100	1.33939500	-1.08983000
C	-6.42478900	-3.70935400	0.17205000	H	-1.96319800	0.47406800	2.79844000
C	-4.95723300	-3.66874900	0.62092000	H	-1.70005800	4.73741100	3.09035000
C	-7.37699400	-3.34506300	1.31908000	H	0.84678900	2.63865800	0.36064000
C	-2.60408800	-3.08940300	2.63409000	H	1.02619900	4.86220000	0.43793000
C	-4.58003400	-2.29973700	1.22969000	H	-1.470212600	6.37549100	1.37107000
C	-1.27195000	-2.98217400	3.04618000	H	-1.22553600	5.66081700	-0.22862000
C	-7.01460200	-1.98543800	1.93105000	H	0.40055200	6.00508300	3.21368000
C	-3.12150000	-2.22510000	1.65709000	H	1.83059400	5.05951400	2.77819000
C	-5.54777100	-1.94272000	2.38118000	H	0.69042600	7.18648500	-0.66058000
C	-0.45518100	-2.00740300	2.44754000	H	-0.74251900	8.13009900	-0.22792000
C	-2.27570500	-1.26284800	1.08983000	H	2.56157200	6.81995500	1.18002000
C	-0.91724300	-1.13743800	1.44545000	H	2.31637100	7.52825100	2.78301000
C	-0.71728200	-4.47488600	6.61746000	H	1.31841900	8.96295600	0.96336000
C	-1.33475600	-3.59896100	5.51840000	H	0.08669400	8.39840900	2.10279000
C	-0.69839800	-3.87590200	4.13769000	H	4.62546800	-5.62836400	1.18002000
C	-0.80689100	-5.96633000	6.26786000	H	5.36147100	-5.77016200	2.78301000
C	-0.17878800	-6.25509200	4.89792000	H	5.00027900	-3.34943000	3.21368000
C	-0.79518000	-5.37974400	3.79741000	H	3.46637100	-4.11509800	2.77819000
C	-4.26140500	3.37851800	3.79741000	H	7.10293800	-5.62326300	0.96336000
C	-3.00743000	2.54278100	4.13769000	H	7.22988900	-4.27428400	2.10279000
C	-2.44941400	2.95541300	5.51840000	H	4.95274700	-0.89641200	3.09035000
C	-5.32767500	3.28238100	4.89792000	H	3.69768900	-3.31981400	0.43793000
C	-4.76354800	3.68195300	6.26786000	H	1.39215400	1.46314500	2.79844000
C	-3.51672400	2.85862700	6.61746000	H	1.86175000	-2.05267000	0.36064000
C	3.70582800	1.33312100	4.13769000	H	5.87846500	-4.19116900	-0.66058000
C	5.05658500	2.00122600	3.79741000	H	7.41213200	-3.42200900	-0.22792000
C	3.78416900	0.64354800	5.51840000	H	6.25740000	-1.91284700	1.37107000
C	5.50646200	2.97271100	4.89792000	H	5.51518000	-1.76906300	-0.22862000
C	4.23400600	1.61625900	6.61746000	H	-6.56889100	-2.99531600	-0.66058000
C	5.70439000	2.28437700	6.26786000	H	-6.66961300	-4.70809000	-0.22792000
C	-1.44367200	0.22563700	-1.44545000	H	-4.78527400	-4.46264400	1.37107000
C	0.00000000	0.00000000	-0.85926000	H	-4.28964300	-3.89175400	-0.22862000
C	0.91724300	1.13743800	-1.44545000	H	-8.42135700	-3.33969400	0.96336000
C	2.27570500	1.26284800	-1.08983000	H	-7.31658300	-4.12412500	2.10279000
C	3.12150000	2.22510000	-1.65709000	H	-3.25268900	-3.84099900	3.09035000
C	4.58003400	2.29973700	-1.22969000	H	-4.72388800	-1.54238600	0.43793000
C	7.01460200	1.98543800	-1.93105000	H	-7.18704000	-1.19159100	1.18002000
C	7.37699400	3.34506300	-1.31908000	H	-7.67784300	-1.75808900	2.78301000
C	6.42478900	3.70935400	-0.17205000	H	-5.40083100	-2.65565300	3.21368000
C	5.54777100	1.94272000	-2.38118000	H	-5.29696500	-0.94441700	2.77819000
C	4.95723300	3.66874900	-0.62092000	H	0.57104400	-1.93721400	2.79844000
C	2.60408800	3.08940300	-2.63409000	H	-2.70853900	-0.58598800	0.36064000
C	1.27195000	2.98217400	-3.04618000	H	0.34527300	-4.19589300	6.74898000
C	0.69839800	3.87590200	-4.13769000	H	-1.21340800	-4.27576600	7.58263000
C	1.33475600	3.59896100	-5.51840000	H	-1.22200900	-2.53076900	5.76943000
C	0.71728200	4.47488600	-6.61746000	H	-2.42200300	-3.79389400	5.46274000
C	0.80689100	5.96633000	-6.26786000	H	0.37618500	-3.63130900	4.22266000
C	0.17878800	6.25509200	-4.89792000	H	-1.87023500	-6.27265200	6.25230000
C	0.79518000	5.37974400	-3.79741000	H	-0.31833900	-6.57338400	7.04894000
C	0.45518100	2.00740300	-2.44754000	H	-0.29279200	-7.32179400	4.64012000
C	0.52642900	-1.36307500	-1.44545000	H	0.90934900	-6.06097200	4.94891000
C	1.51087200	-1.39790000	-2.44754000	H	-1.85751500	-5.65698500	3.66654000
C	1.94666300	-2.59262800	-3.04618000	H	-0.30025900	-5.57326700	2.83074000
C	3.00743000	-2.54278100	-4.13769000	H	-3.97033500	4.43714800	3.66654000
C	5.32767500	-3.28238100	-4.89792000	H	-4.67646100	3.04666500	2.83074000
C	4.76354800	-3.68195300	-6.26786000	H	-3.33289900	1.48986900	4.22266000
C	3.51672400	-2.85862700	-6.61746000	H	-1.58070600	2.32367500	5.76943000
C	4.26140500	-3.37851800	-3.79741000	H	-2.07460600	3.99446300	5.46274000
C	2.44941400	-2.95541300	-5.51840000	H	-6.19446400	3.91446300	4.64012000
C	1.37345700	-3.79990700	-2.63409000	H	-5.70363000	2.24296700	4.94891000
				H	-4.49715800	4.75599700	6.25230000
				H	-5.53354800	3.56238200	7.04894000
				H	-3.80638700	1.79893100	6.74898000

H	-3.096218000	3.188725000	7.582630000			
H	2.956714000	2.141441000	4.222660000			
H	5.827850000	1.219837000	3.666540000			
H	4.976720000	2.526601000	2.830740000	C	0.000000000	0.850080000
H	2.802714000	0.207094000	5.769430000	C	-1.826830000	1.214070000
H	4.496610000	-0.200570000	5.462740000	C	-2.521350000	2.356810000
H	6.487256000	3.407331000	4.640120000	C	-0.711101000	1.274040000
H	4.794281000	3.818005000	4.948910000	C	-2.063950000	3.614290000
H	3.461114000	2.396962000	6.748980000	C	-0.247010000	2.559060000
H	4.309626000	1.087041000	7.582630000	C	-0.896940000	3.723140000
H	6.367393000	1.516655000	6.252300000	C	-0.246020000	5.046610000
H	5.851887000	3.011002000	7.048940000	C	-1.180360000	6.257440000
H	2.708539000	0.585988000	-0.360640000	C	0.980370000	5.294040000
H	4.723888000	1.542386000	-0.437930000	C	-0.447570000	7.535550000
H	7.187040000	1.191591000	-1.180020000	C	1.718250000	6.566340000
H	7.677843000	1.758089000	-2.783010000	C	0.782820000	7.775800000
H	8.421357000	3.339694000	-0.963360000	C	4.827492000	-4.771218000
H	7.316583000	4.124125000	-2.102790000	C	4.094588000	-3.496045000
H	6.568891000	2.995316000	0.660580000	C	6.342630000	-4.565842000
H	6.669613000	4.708090000	0.227920000	C	4.162042000	-0.019712000
H	5.400831000	2.655653000	-3.213680000	C	4.493502000	-2.310245000
H	5.296965000	0.944417000	-2.778190000	C	3.301732000	1.005148000
H	4.785274000	4.462644000	-1.371070000	C	3.672804000	-1.084797000
H	4.289643000	3.891754000	0.228620000	C	1.964830000	0.975046000
H	3.252689000	3.840999000	-3.090350000	C	2.339716000	-1.065613000
H	-0.376185000	3.631309000	-4.222660000	C	1.458856000	-0.021267000
H	1.222009000	2.530769000	-5.769430000	C	6.749763000	-3.380168000
H	2.422003000	3.793894000	-5.462740000	C	6.009282000	-2.106498000
H	-0.345273000	4.195893000	-6.748980000	C	-6.302193000	-4.155382000
H	1.213408000	4.275766000	-7.582630000	C	-4.828922000	-4.150942000
H	1.870235000	6.272652000	-6.252300000	C	-7.125450000	-3.209958000
H	0.318339000	6.573384000	-7.048940000	C	-2.098092000	-3.594578000
H	0.292792000	7.321794000	-4.640120000	C	-4.247482000	-2.736365000
H	-0.909349000	6.060972000	-4.948910000	C	-0.780382000	-3.361958000
H	1.857515000	5.656985000	-3.666540000	C	-6.545742000	-1.795122000
H	0.300259000	5.573267000	-2.830740000	C	-2.775864000	-2.638343000
H	-0.571044000	1.937214000	-2.798440000	C	-5.074958000	-1.797995000
H	1.963198000	-0.474068000	-2.798440000	C	-0.138000000	-2.189116000
H	3.332899000	-1.489869000	-4.222660000	C	-2.092706000	-1.493447000
H	6.194464000	-3.914463000	-4.640120000	C	-0.747846000	-1.252773000
H	5.703630000	-2.242967000	-4.948910000	C	0.074190000	-5.969520000
H	4.497158000	-4.755997000	-6.252300000	C	-0.797970000	-5.006590000
H	5.533548000	-3.562382000	-7.048940000	C	0.000000000	-4.367440000
H	3.806387000	-1.798931000	-6.748980000	C	0.673900000	-7.054320000
H	3.096218000	-3.188725000	-7.582630000	C	1.460860000	-6.437460000
H	3.970335000	-4.437148000	-3.666540000	C	0.594260000	-5.463750000
H	4.676461000	-3.046665000	-2.830740000	C	-5.028876000	2.217231000
H	1.580706000	-2.323675000	-5.769430000	C	-3.782314000	2.183720000
H	2.074606000	-3.994463000	-5.462740000	C	-3.936849000	3.194357000
H	1.700058000	-4.737411000	-3.090350000	C	-6.305434000	1.953588000
H	-1.026199000	-4.862200000	-0.437930000	C	-6.446170000	2.943545000
H	1.472126000	-6.375491000	-1.371070000	C	-5.206851000	2.920510000
H	1.225536000	-5.660817000	0.228620000	C	3.782314000	2.183720000
H	-0.690426000	-7.186485000	0.660580000	C	4.434616000	3.246519000
H	0.742519000	-8.130099000	0.227920000	C	4.734819000	1.812233000
H	-2.561572000	-6.819955000	-1.180020000	C	4.844574000	4.483872000
H	-2.316371000	-7.528251000	-2.783010000	C	5.132661000	3.049010000
H	-1.318419000	-8.962956000	-0.963360000	C	5.772270000	4.110775000
H	-0.086694000	-8.398409000	-2.102790000	C	-1.458856000	0.021267000
H	-0.400552000	-6.005083000	-3.213680000	C	0.000000000	0.000000000
H	-1.830594000	-5.059514000	-2.778190000	C	0.747846000	1.252773000
H	-0.846789000	-2.638658000	-0.360640000	C	2.092706000	1.493447000
H	-1.392154000	-1.463145000	-2.798440000	C	2.775864000	2.638343000
H	-2.956714000	-2.141441000	-4.222660000	C	4.247482000	2.736365000
H	-6.487256000	-3.407331000	-4.640120000	C	6.545742000	1.795122000
H	-4.794281000	-3.818005000	-4.948910000	C	7.125450000	3.209958000
H	-6.367393000	-1.516655000	-6.252300000	C	6.302193000	4.155382000
H	-5.851887000	-3.011002000	-7.048940000	C	5.074958000	1.797995000
H	-3.461114000	-2.396962000	-6.748980000	C	4.828922000	4.150942000
H	-4.309626000	-1.087041000	-7.582630000	C	2.098092000	3.594578000
H	-5.827850000	-1.219837000	-3.666540000	C	0.780382000	3.361958000
H	-4.976720000	0.200570000	5.462740000	C	0.000000000	4.367440000
H	-4.794281000	3.818005000	4.948910000	C	0.797970000	5.006590000
H	-4.496610000	0.200570000	5.462740000	C	-0.074190000	5.969520000
H	-4.952747000	0.896412000	-3.090350000	C	-0.673900000	7.054320000
H	-3.697689000	3.319814000	-0.437930000	C	-1.460860000	6.437460000
H	-4.625468000	5.628364000	-1.180020000	C	-0.594260000	5.463750000
H	-5.361471000	5.770162000	-2.783010000	C	0.138000000	2.189116000
H	-7.102938000	5.623263000	-0.963360000	C	0.711101000	-1.274040000
H	-7.229889000	4.274284000	-2.102790000	C	1.826830000	-1.214070000
H	-5.878465000	4.191169000	0.660580000	C	2.521350000	-2.356810000
H	-7.412132000	3.422009000	0.227920000	C	3.782314000	-2.183720000
H	-5.000279000	3.349430000	-3.213680000	C	6.305434000	-1.953588000
H	-3.466371000	4.115098000	-2.778190000	C	6.446170000	-2.943545000
H	-6.257400000	1.912847000	-1.371070000	C	5.206851000	-2.920510000
H	-5.515180000	1.769063000	0.228620000	C	5.028876000	-2.217231000
H	-1.861750000	2.052670000	-0.360640000	C	3.936849000	-3.194357000
				C	2.063950000	-3.614290000
				C	0.896940000	-3.723140000

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C	0.246020000	-5.046610000	-1.127550000	H	2.886819000	2.647323000	3.918010000
C	1.180360000	-6.257440000	-1.169860000	H	5.325273000	2.794856000	2.090120000
C	0.447570000	-7.535550000	-0.757050000	H	3.743243000	3.518732000	1.750960000
C	-1.718250000	-6.566340000	-1.609460000	H	4.264427000	1.057075000	5.256750000
C	-0.782820000	-7.775800000	-1.633290000	H	5.648637000	1.353873000	4.190940000
C	-0.980370000	-5.294040000	-2.024110000	H	5.326274000	5.219982000	2.700230000
C	0.247010000	-2.559060000	-1.064000000	H	3.934954000	4.964020000	3.767360000
C	-1.964830000	-0.975046000	-2.230150000	H	4.231526000	3.473643000	5.892540000
C	-3.301732000	-1.005148000	-2.643850000	H	5.819331000	2.766923000	6.228240000
C	-3.782314000	-2.183720000	-3.464800000	H	6.717533000	3.713212000	4.109330000
C	-4.844574000	-4.483872000	-3.363150000	H	6.031778000	5.003894000	5.108450000
C	-5.772270000	-4.110775000	-4.520080000	H	2.659474000	0.767595000	-0.485900000
C	-5.132661000	-3.049010000	-5.415740000	H	4.356777000	2.358821000	-0.094920000
C	-4.434616000	-3.246519000	-2.566210000	H	6.624709000	1.389387000	-0.584250000
C	-4.734819000	-1.812233000	-4.608030000	H	7.127454000	1.127007000	-2.263220000
C	-4.162042000	0.019712000	-2.240700000	H	8.176118000	3.201348000	-1.305540000
C	-3.672804000	1.084797000	-1.478060000	H	7.117898000	3.583820000	-2.672830000
C	-4.493502000	2.310245000	-1.127550000	H	6.383022000	3.833861000	0.296150000
C	-4.827492000	4.771218000	-1.609460000	H	6.707277000	5.177375000	-0.809200000
C	-6.342630000	4.565842000	-1.633290000	H	4.978827000	2.133059000	-3.073400000
C	-6.749763000	3.380168000	-0.757050000	H	4.656216000	0.779017000	-1.974760000
C	-4.094588000	3.496045000	-2.024110000	H	4.750325000	4.548576000	-2.197380000
C	-6.009282000	2.106498000	-1.169860000	H	4.241458000	4.821740000	-0.521210000
C	-2.339716000	1.065613000	-1.064000000	H	2.605655000	4.511054000	-2.546030000
H	-2.198240000	0.256320000	2.587810000	H	-0.849240000	3.823720000	-3.918010000
H	-2.603860000	4.512090000	2.546030000	H	1.216760000	4.221640000	-5.256750000
H	0.664980000	2.686970000	0.485900000	H	1.651830000	5.568900000	-4.190940000
H	0.135590000	4.952490000	0.094920000	H	-0.892500000	5.401430000	-5.892540000
H	-1.564020000	6.388190000	2.197380000	H	0.513440000	6.423150000	-6.228240000
H	-2.055020000	6.084080000	0.521210000	H	0.143030000	7.674160000	-4.109330000
H	0.642130000	5.378320000	3.073400000	H	-1.317610000	7.725620000	-5.108450000
H	1.653460000	4.421910000	1.974760000	H	-1.857500000	7.222680000	-2.700230000
H	-0.128710000	7.444790000	-0.296150000	H	-2.331490000	5.889780000	-3.767360000
H	-1.130100000	8.397360000	0.809200000	H	0.242220000	6.009250000	-2.090120000
H	2.109110000	6.431860000	0.584250000	H	-1.175690000	5.001110000	-1.750960000
H	2.587710000	6.736060000	2.263220000	H	-0.877140000	2.031892000	-2.587810000
H	1.315610000	8.681400000	1.305540000	H	2.198240000	-0.256320000	-2.587810000
H	0.455270000	7.956190000	2.672830000	H	3.736059000	-1.176397000	-3.918010000
H	4.515599000	-5.042473000	0.584250000	H	7.183774000	-2.002698000	-2.700230000
H	4.539744000	-5.609053000	2.263220000	H	6.266444000	-0.925760000	-3.767360000
H	4.336697000	-3.245261000	3.073400000	H	6.574503000	-3.960948000	-4.109330000
H	3.002756000	-3.642893000	1.974760000	H	7.349388000	-2.71726000	-5.108450000
H	6.860508000	-5.480052000	1.305540000	H	5.124026000	-1.927787000	-5.892540000
H	6.662628000	-4.372370000	2.672830000	H	5.305891000	-3.656227000	-6.228240000
H	5.209515000	-0.001036000	2.546030000	H	5.083053000	-3.214394000	-2.090120000
H	4.221187000	-2.593669000	0.094920000	H	4.918933000	-1.482378000	-1.750960000
H	1.321100000	1.775572000	2.587810000	H	3.047667000	-3.164565000	-5.256750000
H	1.994494000	-1.919375000	0.485900000	H	3.996807000	-4.214927000	-4.190940000
H	6.511732000	-3.610929000	-0.296150000	H	2.603860000	-4.512090000	-2.546030000
H	7.837377000	-3.219985000	0.809200000	H	-0.135590000	-4.952490000	-0.094920000
H	6.314345000	-1.839614000	2.197380000	H	1.564020000	-6.388190000	-2.197380000
H	6.296478000	-1.262340000	0.521210000	H	2.055020000	-6.084080000	-0.521210000
H	-6.383022000	-3.833861000	-0.296150000	H	0.128710000	-7.444790000	0.296150000
H	-6.707277000	-5.177375000	0.809200000	H	1.130100000	-8.397360000	-0.809200000
H	-4.750325000	-4.548576000	2.197380000	H	-2.109110000	-6.431860000	-0.584250000
H	-4.241458000	-4.821740000	0.521210000	H	-2.587710000	-6.736060000	-2.263220000
H	-8.176118000	-3.201348000	1.305540000	H	-1.315610000	-8.681400000	-1.305540000
H	-7.117898000	-3.583820000	2.672830000	H	-0.455270000	-7.956190000	-2.672830000
H	-2.605655000	-4.511054000	2.546030000	H	-0.642130000	-5.378320000	-3.073400000
H	-4.356777000	-2.358821000	0.094920000	H	-1.653460000	-4.421910000	-1.974760000
H	-6.624709000	-1.389387000	0.584250000	H	-0.664980000	-2.686970000	-0.485900000
H	-7.127454000	-1.127007000	2.263220000	H	-1.321100000	-1.775572000	-2.587810000
H	-4.978827000	-2.133059000	3.073400000	H	-2.886819000	-2.647323000	-3.918010000
H	-4.656216000	-0.779017000	1.974760000	H	-5.326274000	-5.219982000	-2.700230000
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H	-2.659474000	-0.767595000	0.485900000	H	-6.717533000	-3.713212000	-4.109330000
H	0.892500000	-5.401430000	5.892540000	H	-6.031778000	-5.003894000	-5.108450000
H	-0.513440000	-6.423150000	6.228240000	H	-4.231526000	-3.473643000	-5.892540000
H	-1.216760000	-4.221640000	5.256750000	H	-5.819331000	-2.766923000	-6.228240000
H	-1.651830000	-5.568800000	4.190940000	H	-5.325273000	-2.794856000	-2.090120000
H	0.849240000	-3.823720000	3.918010000	H	-3.743243000	-3.518732000	-1.750960000
H	-0.143030000	-7.674160000	4.109330000	H	-4.264427000	-1.057075000	-5.256750000
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H	1.857500000	-7.222680000	2.700230000	H	-5.209515000	0.001036000	-2.546030000
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H	-0.242220000	-6.009250000	2.090120000	H	-4.515599000	5.042473000	-0.584250000
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			C	3.012134000	1.739056000	-4.755520000
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			H	-1.731113000	-6.885059000	-1.367630000
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H	-2.739200000	-8.747698000	1.755970000	H	-8.585463000	0.415698000	-0.984240000
H	-1.448440000	-8.095026000	2.782850000	H	-7.822929000	-0.333978000	-3.259800000
H	-4.200698000	6.607866000	3.259800000	H	-8.945329000	-2.001632000	-1.755970000
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H	-2.441331000	6.826009000	1.490400000	H	-8.406833000	-1.490673000	0.696660000
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H	-2.938169000	3.755462000	-0.640460000	H	-3.948034000	-2.897039000	-3.348380000
H	-1.863944000	4.525643000	0.530600000	H	-1.929790000	-1.905378000	-5.934630000
H	-1.551015000	-1.105265000	2.865860000	H	-3.340511000	-2.885939000	-5.508880000
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H	-5.494377000	6.535195000	-0.696660000	H	0.012749000	-6.516338000	-6.464530000
H	-5.097079000	4.941717000	-1.367630000	H	0.353949000	-6.230081000	-4.746750000
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H	5.087136000	3.083287000	0.109180000	H	-0.117377000	-2.884650000	-7.460410000
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H	6.828192000	1.943342000	-1.367630000	H	0.368687000	-2.464771000	-4.987990000
H	3.948034000	2.897039000	3.348380000	H	0.181680000	-1.895851000	-2.865860000
H	7.822929000	0.333978000	3.259800000	H	-1.732695000	0.790586000	-2.865860000
H	5.650189000	1.507706000	3.513580000	H	-3.598203000	1.423185000	-3.876690000
H	5.388600000	-0.155440000	2.969210000	H	-2.318898000	0.913093000	-4.987990000
H	-0.181680000	1.895851000	2.865860000	H	-4.508918000	1.029843000	-6.150860000
H	2.764522000	0.098815000	0.324100000	H	-5.649689000	3.247128000	-6.464530000
H	6.895031000	-0.510066000	-0.874150000	H	-5.572383000	2.808511000	-4.746750000
H	4.721410000	0.666798000	-0.640460000	H	-4.884084000	5.196382000	-5.073290000
H	4.851294000	-0.648599000	0.530600000	H	-2.799822000	5.720720000	-6.362620000
H	7.132163000	-1.298750000	1.490400000	H	-4.014246000	4.972818000	-7.417160000
H	8.585463000	-0.415698000	0.984240000	H	-1.756438000	3.934869000	-7.777580000
H	0.266600000	4.547563000	8.061040000	H	-3.805005000	2.504664000	-8.061040000
H	0.117377000	2.884650000	7.460410000	H	-2.439492000	1.543977000	-7.460410000
H	2.529478000	3.488554000	7.777580000	H	-2.708209000	5.089013000	-3.879700000
H	1.929790000	1.905378000	5.934630000	H	-3.825198000	3.882022000	-3.227750000
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H	-1.362589000	4.419759000	6.150860000	H	-0.829041000	4.335937000	-5.508880000
H	-0.566587000	3.827728000	3.876690000	H	-0.534892000	4.867617000	-3.348380000
H	-0.368687000	2.464771000	4.987990000	H	-0.256583000	6.457891000	-1.798440000
H	3.554378000	5.285078000	6.362620000	H	-0.126637000	5.947232000	-0.109180000
H	2.299464000	5.962849000	7.417160000	H	0.670176000	8.296037000	-0.408460000
H	-0.012749000	6.516338000	6.464530000	H	2.912456000	8.025867000	0.696660000
H	-0.353949000	6.230081000	4.746750000	H	1.731113000	6.885059000	1.367630000
H	2.058157000	6.827932000	5.073290000	H	3.889246000	5.716239000	0.874150000
H	3.053110000	4.889885000	3.879700000	H	4.690832000	5.527259000	-1.490400000
H	1.449330000	5.253730000	3.227750000	H	4.652737000	7.227380000	-0.984240000
H	2.708209000	-5.089013000	3.879700000	H	3.622231000	6.941844000	-3.259800000
H	3.825198000	-3.882022000	3.227750000	H	2.739200000	8.747698000	-1.755970000
H	0.685211000	-2.623936000	5.934630000	H	1.448440000	8.095026000	-2.782850000
H	0.829041000	-4.335937000	5.508880000	H	1.783241000	4.422260000	0.640460000
H	4.884084000	-5.196382000	5.073290000	H	2.987350000	3.877044000	-0.530600000
H	3.598203000	-1.423185000	3.876690000	H	1.519383000	5.647061000	-3.513580000
H	2.318898000	-0.913093000	4.987990000	H	2.828915000	4.588945000	-2.969210000
H	2.799822000	-5.720720000	6.362620000	H	1.296685000	2.443554000	-0.324100000
H	4.014246000	-4.972818000	7.417160000	H	1.551015000	1.105265000	-2.865860000
H	1.756438000	-3.934869000	7.777580000	H	3.031616000	2.404543000	-3.876690000
H	5.649689000	-3.247128000	6.464530000	H	1.950211000	1.551678000	-4.987990000
H	5.572383000	-2.808511000	4.746750000	H	3.146329000	3.389916000	-6.150860000
H	4.508918000	-1.029843000	6.150860000	H	5.636940000	3.269210000	-6.464530000
H	3.805005000	-2.504664000	8.061040000	H	5.218434000	3.421569000	-4.746750000
H	2.439492000	-1.543977000	7.460410000	H	6.942241000	1.631550000	-5.073290000
H	-3.031616000	-2.404543000	3.876690000	H	6.354200000	-0.435643000	-6.362620000
H	-1.950211000	-1.551678000	4.987990000	H	6.313710000	0.990030000	-7.417160000
H	-5.761319000	0.199129000	3.879700000	H	4.285915000	-0.446315000	-7.777580000
H	-5.274529000	-1.371708000	3.227750000	H	4.071605000	2.042899000	-8.061040000
H	-3.146329000	-3.389916000	6.150860000	H	2.556869000	1.340674000	-7.460410000
H	-2.615001000	0.718558000	5.934630000	H	5.761319000	-0.199129000	-3.879700000
H	-4.169552000	1.449998000	5.508880000	H	5.274529000	1.371708000	-3.227750000
H	-5.636940000	-3.269210000	6.464530000	H	5.215001000	-0.718558000	-5.934630000
H	-5.218434000	-3.421569000	4.746750000	H	4.169552000	-1.449998000	-5.508880000
H	-6.942241000	-1.631550000	5.073290000	H	4.482926000	-1.970579000	-3.348380000
H	-4.071605000	-2.042899000	8.061040000	H	2.938169000	-3.755462000	0.640460000
H	-2.556869000	-1.340674000	7.460410000	H	1.863944000	-4.525643000	-0.530600000
H	-4.285915000	0.446315000	7.777580000	H	3.005786000	-6.226305000	0.874150000
H	-6.354200000	0.435643000	6.362620000	H	2.441331000	-6.826009000	-1.490400000
H	-6.313710000	-0.990030000	7.417160000	H	3.932726000	-7.643078000	-0.984240000
H	-2.764522000	-0.098815000	-0.324100000	H	4.200698000	-6.607866000	-3.259800000
H	-4.721410000	-0.666798000	0.640460000	H	6.206129000	-6.746066000	-1.755970000
H	-4.851294000	0.648599000	-0.530600000	H	6.286278000	-5.301899000	-2.782850000

H	6.849490000	-4.728408000	-0.408460000	C	4.764245000	1.514598000	6.447870000
H	5.494377000	-6.535195000	0.696660000	C	5.921408000	2.313136000	5.821150000
H	5.097079000	-4.941717000	1.367630000	C	-1.428833000	0.219068000	-1.423370000
H	4.130807000	-4.139354000	-3.513580000	C	0.000000000	0.000000000	-0.830910000
H	2.559685000	-4.744385000	-2.969210000	C	0.904135000	1.127871000	-1.423370000
H	5.720989000	-3.006738000	-1.798440000	C	2.261710000	1.236442000	-1.078910000
H	5.213772000	-2.863945000	-0.109180000	C	3.116666000	2.151309000	-1.699960000
H	1.467837000	-2.344739000	-0.324100000	C	4.606242000	2.203718000	-1.363560000
B3LYP-D3(BJ)							
C	0.000000000	0.000000000	0.830910000	C	6.934942000	1.826195000	-2.316070000
C	-1.480055000	1.356254000	2.444990000	C	7.322253000	3.268366000	-1.943770000
C	-1.883299000	2.534573000	3.090440000	C	6.545188000	3.702158000	-0.688020000
C	-0.524698000	1.346940000	1.423370000	C	6.886984000	2.758837000	0.476960000
C	-1.291324000	3.738262000	2.697740000	C	5.427022000	1.767022000	-2.605860000
C	0.060065000	2.576919000	1.078910000	C	5.034203000	3.640452000	-0.969700000
C	-0.304756000	3.774766000	1.699960000	C	2.591768000	2.987451000	-2.697740000
C	1.397028000	4.943890000	0.199250000	C	1.253355000	2.898271000	-3.090440000
C	0.394646000	5.090982000	1.363560000	C	0.685884000	3.824711000	-4.166740000
C	-0.635622000	6.179973000	0.969700000	C	1.619798000	3.899105000	-5.400650000
C	1.183225000	5.583449000	2.605860000	C	1.070442000	4.883256000	-6.447870000
C	2.097544000	6.277906000	-0.101220000	C	0.957469000	6.284657000	-5.821150000
C	1.054269000	7.343721000	-0.476960000	C	0.000000000	6.234803000	-4.617900000
C	2.870068000	6.736468000	1.147320000	C	-1.387664000	5.763205000	-5.084530000
C	0.066431000	7.519378000	0.688020000	C	-1.265373000	4.361290000	-5.707550000
C	1.885939000	6.918933000	2.316070000	C	-0.317723000	4.416821000	-6.916200000
C	0.830638000	7.975440000	1.943770000	C	0.545460000	5.250092000	-3.571840000
C	5.049002000	-5.092738000	2.316070000	C	-0.711835000	3.382067000	-4.658910000
C	4.243796000	-3.816428000	2.605860000	C	0.434523000	1.959892000	-2.444990000
C	4.398918000	-5.853786000	1.147320000	C	0.524698000	-1.346940000	-1.423370000
C	6.491614000	-4.707074000	1.943770000	C	1.480055000	-1.356254000	-2.444990000
C	3.883092000	-0.750812000	2.697740000	C	1.883299000	-2.534573000	-3.090440000
C	4.211596000	-2.887264000	1.363560000	C	2.969354000	-2.506349000	-4.166740000
C	3.136654000	0.363698000	3.090440000	C	3.284873000	-1.074567000	-4.658910000
C	4.388054000	-4.955479000	-0.101220000	C	4.409675000	-1.084800000	-5.707550000
C	3.421421000	-1.623457000	1.699960000	C	5.684914000	-1.679850000	-5.084530000
C	3.583020000	-3.681807000	0.199250000	C	5.399498000	-3.117401000	-4.617900000
C	1.914578000	0.603638000	2.444990000	C	4.963938000	-3.971521000	-5.821150000
C	2.201645000	-1.340477000	1.078910000	C	3.693802000	-3.368658000	-6.447870000
C	1.428833000	-0.219068000	1.423370000	C	3.983941000	-1.933254000	-6.916200000
C	6.478757000	-3.817220000	0.688020000	C	4.273983000	-3.097428000	-3.571840000
C	5.669825000	-2.539522000	0.969700000	C	2.566825000	-3.352339000	-5.400650000
C	5.832715000	-4.584884000	-0.476960000	C	1.291324000	-3.738262000	-2.697740000
C	-6.545188000	-3.702158000	0.688020000	C	0.304756000	-3.774766000	-1.699960000
C	-5.034203000	-3.640452000	0.969700000	C	-0.394646000	-5.090982000	-1.363560000
C	-7.322253000	-3.268366000	1.943770000	C	0.635622000	-6.179973000	-0.969700000
C	-6.886984000	-2.758837000	-0.476960000	C	-0.066431000	-7.519378000	-0.688020000
C	-2.591768000	-2.987451000	2.697740000	C	-1.054269000	-7.343721000	0.476960000
C	-4.606242000	-2.203718000	1.363560000	C	-2.097544000	-6.277906000	0.101220000
C	-1.253355000	-2.898271000	3.090440000	C	-2.870068000	-6.736468000	-1.147320000
C	-6.934942000	-1.826195000	2.316070000	C	-1.885939000	-6.918933000	-2.316070000
C	-3.116666000	-2.151309000	1.699960000	C	-0.830638000	-7.975440000	-1.943770000
C	-5.427022000	-1.767022000	2.605860000	C	-1.397028000	-4.943890000	-0.199250000
C	-0.434523000	-1.959892000	2.444990000	C	-1.183225000	-5.583449000	-2.605860000
C	-2.261710000	-1.236442000	1.078910000	C	-0.060065000	-2.576919000	-1.078910000
C	-0.904135000	-1.127871000	1.423370000	C	-1.914578000	-0.603638000	-2.444990000
C	-6.485598000	-1.322427000	-0.101220000	C	-3.136654000	-0.363698000	-3.090440000
C	-4.980049000	-1.262083000	0.199250000	C	-3.655239000	-1.318362000	-4.166740000
C	-7.268986000	-0.882682000	1.147320000	C	-2.573039000	-2.307500000	-4.658910000
C	0.317723000	-4.416821000	6.916200000	C	-3.144301000	-3.276490000	-5.707550000
C	-1.070442000	-4.883256000	6.447870000	C	-4.297250000	-4.083355000	-5.084530000
C	-1.619798000	-3.899105000	5.400650000	C	-5.399498000	-3.117401000	-4.617900000
C	1.265373000	-4.361290000	5.707550000	C	-5.921408000	-2.313136000	-5.821150000
C	0.711835000	-3.382067000	4.658910000	C	-4.764245000	-1.514598000	-6.447870000
C	-0.685884000	-3.824711000	4.166740000	C	-3.666218000	-2.483567000	-6.916200000
C	-0.957469000	-6.284657000	5.821150000	C	-4.819443000	-2.152664000	-3.571840000
C	1.387664000	-5.763205000	5.084530000	C	-4.186623000	-0.546766000	-5.400650000
C	0.000000000	-6.234803000	4.617900000	C	-3.883092000	0.750812000	-2.697740000
C	-0.545460000	-5.250092000	3.571840000	C	-3.421421000	1.623457000	-1.699960000
C	-4.273983000	3.097428000	3.571840000	C	-4.211596000	2.887264000	-1.363560000
C	-2.969354000	2.506349000	4.166740000	C	-3.583020000	3.681807000	-0.199250000
C	-2.566825000	3.352339000	5.400650000	C	-4.388054000	4.955479000	0.101220000
C	-5.399498000	3.117401000	4.617900000	C	-4.398918000	5.853786000	-1.147320000
C	-3.284873000	1.074567000	4.658910000	C	-5.049002000	5.092738000	-2.316070000
C	-4.963938000	3.971521000	5.821150000	C	-6.491614000	4.707074000	-1.943770000
C	-3.693802000	3.368658000	6.447870000	C	-6.478757000	3.817220000	-0.688020000
C	-5.684914000	1.679850000	5.084530000	C	-5.832715000	4.584884000	0.476960000
C	-4.409675000	1.084800000	5.707550000	C	-4.243796000	3.816428000	-2.605860000
C	-3.983941000	1.933254000	6.916200000	C	-5.669825000	2.539522000	-0.969700000
C	2.573039000	2.307500000	4.658910000	C	-2.201645000	1.340477000	-1.078910000
C	3.655239000	1.318362000	4.166740000	H	-1.917608000	0.420615000	2.762320000
C	4.819443000	2.152664000	3.571840000	H	-1.590153000	4.667168000	3.183460000
C	3.144301000	3.276490000	5.707550000	H	0.843003000	2.592323000	0.335640000
C	4.186623000	0.546766000	5.400650000	H	0.877790000	4.577941000	-0.698410000
C	4.297250000	4.083355000	5.084530000	H	2.155808000	4.187033000	0.451330000
C	5.399498000	3.117401000	4.617900000	H	-1.375480000	6.311277000	1.775480000
C	3.666218000	2.483567000	6.916200000	H	-1.191649000	5.845266000	0.077910000

H	0.501739000	5.693992000	3.464940000	H	2.840634000	1.921118000	7.385100000
H	1.925113000	4.816870000	2.883130000	H	5.138716000	0.933659000	7.307090000
H	2.798577000	6.129223000	-0.939050000	H	6.722441000	1.626391000	5.497120000
H	1.553863000	8.302233000	-0.700110000	H	6.360809000	2.993895000	6.570190000
H	0.512016000	7.040231000	-1.386520000	H	2.666519000	0.566099000	-0.335640000
H	3.636586000	5.987646000	1.413160000	H	4.403508000	1.528782000	0.698410000
H	3.398401000	7.683664000	0.943610000	H	4.703981000	0.226532000	-0.451330000
H	-0.691637000	8.274675000	0.421300000	H	6.707351000	0.640973000	0.939050000
H	2.434655000	7.241819000	3.216760000	H	7.003747000	-0.155553000	-1.413160000
H	1.316529000	8.948408000	1.757250000	H	8.353449000	0.898731000	-0.943610000
H	0.128604000	8.118657000	2.783440000	H	7.488927000	1.512436000	-3.216760000
H	5.054272000	-5.729383000	3.216760000	H	8.407813000	3.334056000	-1.757250000
H	4.680273000	-3.281515000	3.464940000	H	7.095265000	3.947954000	-2.783440000
H	3.208975000	-4.075632000	2.883130000	H	6.820260000	4.736313000	-0.421300000
H	3.367160000	-6.143199000	1.413160000	H	7.966876000	2.805432000	0.700110000
H	4.955048000	-6.784934000	0.943610000	H	6.353027000	3.076696000	1.386520000
H	7.091284000	-5.614352000	1.757250000	H	5.182012000	2.412478000	-3.464940000
H	6.966661000	-4.170703000	2.783440000	H	5.134089000	0.741238000	-2.883130000
H	4.836963000	-0.956472000	3.183460000	H	4.777986000	4.346839000	-1.775480000
H	3.908775000	-5.488250000	-0.939050000	H	4.466324000	3.954632000	-0.077910000
H	3.525719000	-3.049159000	-0.698410000	H	3.246810000	3.710697000	-3.183460000
H	2.548173000	-3.960501000	0.451330000	H	1.724348000	2.891088000	-5.836990000
H	1.323068000	1.450390000	2.762320000	H	2.627260000	4.222415000	-5.096540000
H	1.823516000	-2.026224000	0.335640000	H	1.760786000	4.917088000	-7.307090000
H	7.511898000	-3.538362000	0.421300000	H	1.952725000	6.635000000	-5.497120000
H	6.153466000	-1.964438000	1.775480000	H	0.587615000	7.005570000	-6.570190000
H	5.657974000	-1.890635000	0.077910000	H	-0.079902000	7.236716000	-4.163640000
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H	-6.820260000	-4.736313000	0.421300000	H	-2.260588000	4.012323000	-6.029210000
H	-4.777986000	-4.346839000	1.775480000	H	-0.714310000	5.107385000	-7.680250000
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H	-8.407813000	-3.334056000	1.757250000	H	1.524769000	5.591758000	-3.199260000
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H	-7.966876000	-2.805432000	-0.700110000	H	-1.412848000	3.334485000	-3.812450000
H	-6.353027000	-3.076696000	-1.386520000	H	-0.653400000	2.364408000	-5.080550000
H	-3.246810000	-3.710697000	3.183460000	H	-0.594541000	1.871005000	-2.762320000
H	-7.488927000	-1.512436000	3.216760000	H	1.917608000	-0.420615000	-2.762320000
H	-5.182012000	-2.412478000	3.464940000	H	3.594172000	-0.443680000	-3.812450000
H	-5.134089000	-0.741238000	2.883130000	H	2.374338000	-0.616343000	-5.080550000
H	0.594541000	-1.871005000	2.762320000	H	4.605068000	-0.048435000	-6.029210000
H	-2.666519000	-0.566099000	0.335640000	H	6.505458000	-1.674220000	-5.822300000
H	-6.707351000	-0.640973000	-0.939050000	H	6.012507000	-1.063071000	-4.230000000
H	-4.403508000	-1.528782000	-0.698410000	H	6.307131000	-3.549160000	-4.163640000
H	-4.703981000	-0.226532000	0.451330000	H	4.769716000	-5.008609000	-5.497120000
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H	-8.353449000	-0.898731000	0.943610000	H	3.377930000	-3.983429000	-7.307090000
H	0.714310000	-5.107385000	7.680250000	H	4.780281000	-1.935082000	-7.680250000
H	0.243420000	-3.420621000	7.385100000	H	3.084054000	-1.499502000	-7.385100000
H	-1.760786000	-4.917088000	7.307090000	H	4.080220000	-4.116368000	-3.199260000
H	-1.724348000	-5.836990000	5.836990000	H	4.576138000	-2.492331000	-2.701150000
H	-2.627260000	-4.222415000	5.096540000	H	1.641582000	-2.938873000	-5.836990000
H	2.260588000	-4.012323000	6.029210000	H	2.343089000	-4.386481000	-5.096540000
H	1.412848000	-3.334485000	3.812450000	H	1.590153000	-4.667168000	-3.183460000
H	0.653400000	-2.364408000	5.080550000	H	1.375480000	-6.311277000	-1.775480000
H	-1.952725000	-6.635000000	5.497120000	H	1.191649000	-5.845266000	-0.077910000
H	-0.587615000	-7.005570000	6.570190000	H	0.691637000	-8.274675000	-0.421300000
H	1.802812000	-6.471002000	5.822300000	H	-1.553863000	-8.302233000	0.700110000
H	2.085607000	-5.738520000	4.230000000	H	-0.512016000	-7.040231000	1.386520000
H	0.079902000	-7.236716000	4.163640000	H	-2.798577000	-6.129223000	0.939050000
H	-1.524769000	-5.591758000	3.199260000	H	-3.636586000	-5.987646000	-1.413160000
H	0.129648000	-5.209218000	2.701150000	H	-3.398401000	-7.683664000	-0.943610000
H	-4.080220000	4.116368000	3.199260000	H	-2.434655000	-7.241819000	-3.216760000
H	-4.576138000	2.492331000	2.701150000	H	-1.316529000	-8.948408000	-1.757250000
H	-1.641582000	2.938873000	5.836990000	H	-0.128604000	-8.118657000	-2.783440000
H	-2.343089000	4.386481000	5.096540000	H	-0.877790000	-4.577941000	0.698410000
H	-6.307131000	3.549160000	4.163640000	H	-2.155808000	-4.187033000	-0.451330000
H	-3.594172000	0.443680000	3.812450000	H	-0.501739000	-5.693992000	-3.464940000
H	-2.374338000	0.616343000	5.080550000	H	-1.925113000	-4.816870000	-2.883130000
H	-4.769716000	5.008609000	5.497120000	H	-0.843003000	-2.592323000	-0.335640000
H	-5.773194000	4.011675000	6.570190000	H	-1.323068000	-1.450390000	-2.762320000
H	-3.377930000	3.983429000	7.307090000	H	-2.181324000	-2.890804000	-3.812450000
H	-6.505458000	1.674220000	5.822300000	H	-1.720938000	-1.748065000	-5.080550000
H	-6.012507000	1.063071000	4.230000000	H	-2.344480000	-3.963888000	-6.029210000
H	-4.605068000	0.048435000	6.029210000	H	-4.702646000	-4.796781000	-5.822300000
H	-4.780281000	1.935082000	7.680250000	H	-3.926900000	-4.675449000	-4.230000000
H	-3.084054000	1.499502000	7.385100000	H	-6.227228000	-3.687555000	-4.163640000
H	2.181324000	2.890804000	3.812450000	H	-6.722441000	-1.626391000	-5.497120000
H	1.720938000	1.748065000	5.080550000	H	-6.360809000	-2.993895000	-6.570190000
H	5.604989000	1.475390000	3.199260000	H	-5.138716000	-0.933659000	-7.307090000
H	4.446491000	2.716887000	2.701150000	H	-4.065970000	-3.172304000	-7.680250000
H	2.344480000	3.963888000	6.029210000	H	-2.840634000	-1.921118000	-7.385100000
H	3.365929000	-0.047785000	5.836990000	H	-5.604989000	-1.475390000	-3.199260000
H	4.970349000	-0.164066000	5.096540000	H	-4.446491000	-2.716887000	-2.701150000
H	4.702646000	4.796781000	5.822300000	H	-3.365929000	0.047785000	-5.836990000
H	3.926900000	4.675449000	4.230000000	H	-4.970349000	0.164066000	-5.096540000
H	6.227228000	3.687555000	4.163640000	H	-4.836963000	0.956472000	-3.183460000
H	4.065970000	3.172304000	7.680250000	H	-3.525719000	3.049159000	0.698410000

H	-2.548173000	3.960501000	-0.451330000	C	3.626987000	-1.563340000	4.101900000
H	-3.908775000	5.488250000	0.939050000	C	5.023802000	-1.736303000	3.464440000
H	-3.367160000	6.143199000	-1.413160000	C	4.626723000	0.191166000	5.636070000
H	-4.955048000	6.784934000	-0.943610000	C	3.522099000	-2.505312000	5.322510000
H	-5.054272000	5.729383000	-3.216760000	C	5.999778000	0.002453000	4.975480000
H	-7.091284000	5.614352000	-1.757250000	C	6.133123000	-1.444289000	4.482030000
H	-6.966661000	4.170703000	-2.783440000	C	4.500008000	-0.759509000	6.832330000
H	-7.511898000	3.538362000	-0.421300000	C	4.630560000	-2.206182000	6.341070000
H	-6.413013000	5.496801000	0.700110000	C	5.999448000	-2.402979000	5.673420000
H	-5.841011000	3.963535000	1.386520000	C	-0.888388000	1.144373000	-1.422840000
H	-4.680273000	3.281515000	-3.464940000	C	0.000000000	0.000000000	-0.831710000
H	-3.208975000	4.075632000	-2.883130000	C	1.435250000	0.197180000	-1.422840000
H	-6.153466000	1.964438000	-1.775480000	C	2.494978000	-0.665769000	-1.089940000
H	-5.657974000	1.890635000	-0.077910000	C	3.750544000	-0.570900000	-1.693750000
H	-1.823516000	2.026224000	-0.335640000	C	4.871012000	-1.562037000	-1.385720000

M06-2X

C	0.000000000	0.000000000	0.831710000	C	6.360961000	-3.341545000	-2.416060000
C	-0.145994000	2.019448000	2.429520000	C	7.605448000	-2.571778000	-1.953230000
C	0.358025000	3.170675000	3.052570000	C	7.286634000	-1.815774000	-0.656140000
C	0.546862000	1.341553000	1.422840000	C	6.868268000	-2.818805000	0.425660000
C	1.609682000	3.639780000	2.657890000	C	5.222076000	-2.347451000	-2.671730000
C	1.824062000	1.827830000	1.089940000	C	6.140750000	-0.824157000	-0.904480000
C	2.369686000	2.962616000	1.693750000	C	3.956983000	0.425865000	-2.657890000
C	4.473883000	2.582998000	0.304530000	C	2.924897000	1.275279000	-3.052570000
C	3.788270000	3.437402000	1.385720000	C	3.167386000	2.359393000	-4.101900000
C	3.784116000	4.905967000	0.904480000	C	3.930713000	1.797572000	-5.322510000
C	4.643990000	3.348725000	2.671730000	C	4.225889000	2.907092000	-6.341070000
C	5.902716000	3.075704000	0.038070000	C	5.080765000	3.994185000	-5.673420000
C	5.875291000	4.538692000	-0.425660000	C	4.317353000	4.589296000	-4.482030000
C	6.725011000	2.970859000	1.329310000	C	2.997765000	5.197187000	-4.975480000
C	5.215824000	5.402523000	0.656140000	C	2.147807000	4.102442000	-5.636070000
C	6.074344000	3.837981000	2.416060000	C	2.907759000	3.517367000	-6.832330000
C	6.029949000	5.300622000	1.953230000	C	4.015583000	3.482589000	-3.464440000
C	0.286617000	-7.179527000	2.416060000	C	1.859703000	2.995377000	-4.612850000
C	0.578086000	-5.696176000	2.671730000	C	1.675896000	1.136158000	-2.429520000
C	-0.789666000	-7.309460000	1.329310000	C	-0.546862000	-1.341553000	-1.422840000
C	1.575498000	-7.872400000	1.953230000	C	0.145994000	-2.019448000	-2.429520000
C	2.347301000	-3.213915000	2.657890000	C	-0.358025000	-3.170675000	-3.052570000
C	1.082742000	-4.999439000	1.385720000	C	0.459602000	-3.922733000	-4.101900000
C	2.566872000	-1.895396000	3.052570000	C	1.664221000	-3.108239000	-4.612850000
C	-0.287720000	-6.649754000	0.038070000	C	2.478916000	-3.911277000	-5.636070000
C	1.380858000	-3.533516000	1.693750000	C	3.002014000	-5.194734000	-4.975480000
C	0.000000000	-5.165995000	0.304530000	C	1.815771000	-6.033585000	-4.482030000
C	1.821890000	-0.883290000	2.429520000	C	0.918683000	-6.397164000	-5.673420000
C	0.670916000	-2.493599000	1.089940000	C	0.404671000	-5.113274000	-6.341070000
C	0.888388000	-1.144373000	1.422840000	C	1.592250000	-4.276876000	-6.832330000
C	2.070811000	-7.218298000	0.656140000	C	1.008219000	-5.218891000	-3.464440000
C	2.356634000	-5.730124000	0.904480000	C	-0.408614000	-4.302883000	-5.322510000
C	0.992977000	-7.357497000	-0.425660000	C	-1.609682000	-3.639780000	-2.657890000
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C	-7.605448000	2.571778000	1.953230000	C	-3.784116000	-4.905967000	-0.904480000
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C	-3.956983000	-0.425865000	2.657890000	C	-5.875291000	-4.538692000	0.425660000
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C	-2.924897000	-1.275279000	3.052570000	C	-6.725011000	-2.970859000	-1.329310000
C	-6.360961000	3.341545000	2.416060000	C	-6.074344000	-3.837981000	-2.416060000
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C	-5.222076000	2.347451000	2.671730000	C	-4.473883000	-2.582998000	-0.304530000
C	-1.675896000	-1.136158000	2.429520000	C	-4.643990000	-3.348725000	-2.671730000
C	-2.494978000	0.665769000	1.089940000	C	-1.824062000	-1.827830000	-1.089940000
C	-1.435250000	-0.197180000	1.422840000	C	-1.821890000	0.883290000	-2.429520000
C	-5.614996000	3.574050000	0.038070000	C	-2.566872000	1.895396000	-3.052570000
C	-4.473883000	2.582997000	0.304530000	C	-3.626987000	1.563340000	-4.101900000
C	-5.935345000	4.338601000	1.329310000	C	-3.523924000	0.112861000	-4.612850000
C	-2.907759000	-3.517367000	6.832330000	C	-4.626723000	-0.191166000	-5.636070000
C	-4.225889000	-2.907092000	6.341070000	C	-5.999778000	-0.002453000	-4.975480000
C	-3.930713000	-1.797572000	5.322510000	C	-6.133123000	1.444289000	-4.482030000
C	-2.147807000	-4.102442000	5.636070000	C	-5.999448000	2.402979000	-5.673420000
C	-1.859703000	-2.995377000	4.612850000	C	-4.630560000	2.206182000	-6.341070000
C	-3.167386000	-2.359393000	4.101900000	C	-4.500008000	0.759509000	-6.832330000
C	-5.080765000	-3.994185000	5.673420000	C	-5.023802000	1.736303000	-3.464440000
C	-2.997765000	-5.197187000	4.975480000	C	-3.522099000	2.505312000	-5.322510000
C	-4.317353000	-4.589296000	4.482030000	C	-2.347301000	3.213915000	-2.657890000
C	-4.015583000	-3.482589000	3.464440000	C	-1.380858000	3.533516000	-1.693750000
C	-1.008219000	5.218891000	3.464440000	C	-1.082742000	4.999439000	-1.385720000
C	-0.459602000	3.922733000	4.101900000	C	0.000000000	5.165995000	-0.304530000
C	0.408614000	4.302883000	5.322510000	C	0.287720000	6.649754000	-0.038070000
C	-1.815771000	6.033585000	4.482030000	C	0.789666000	7.309460000	-1.329310000
C	-1.664221000	3.108239000	4.612850000	C	-0.286617000	7.179527000	-2.416060000
C	-0.918683000	6.397164000	5.673420000	C	-1.575498000	7.872400000	-1.953230000
C	-0.404671000	5.113274000	6.341070000	C	-2.070811000	7.218298000	-0.656140000
C	-3.002014000	5.194734000	4.975480000	C	-0.992977000	7.357497000	0.425660000
C	-2.478916000	3.911277000	5.636070000	C	-0.578086000	5.696176000	-2.671730000
C	-1.592250000	4.276876000	6.832330000	C	-2.356634000	5.730124000	-0.904480000
C	3.523924000	-0.112861000	4.612850000	C	-0.670916000	2.493599000	-1.089940000

H	-1.101153000	1.637686000	2.765930000	H	4.520090000	1.233840000	5.974730000
H	2.021135000	4.537410000	3.123530000	H	2.528971000	-2.383224000	5.787200000
H	2.428279000	1.283200000	0.375270000	H	3.605057000	-3.555546000	5.002530000
H	3.882961000	2.608956000	-0.626980000	H	6.801070000	0.231493000	5.697550000
H	4.505103000	1.528448000	0.631890000	H	6.111466000	0.701715000	4.128860000
H	3.295740000	5.547188000	1.656620000	H	7.113609000	-1.584965000	3.999810000
H	3.188916000	4.981428000	-0.022760000	H	5.282224000	-0.539118000	7.577660000
H	4.180019000	3.947823000	3.472450000	H	3.524896000	-0.616410000	7.326660000
H	4.659184000	2.301722000	3.018270000	H	4.532897000	-2.897719000	7.192400000
H	6.355383000	2.445122000	-0.744580000	H	6.105048000	-3.446160000	5.331320000
H	6.902654000	4.891617000	-0.616450000	H	6.804985000	-2.213307000	6.401880000
H	5.315975000	4.629302000	-1.370110000	H	2.325423000	-1.461351000	-0.375270000
H	6.771269000	1.919720000	1.663330000	H	4.200903000	-2.058265000	0.626980000
H	7.760326000	3.304331000	1.148370000	H	3.576226000	-3.137310000	-0.631890000
H	5.180003000	6.451518000	0.322610000	H	5.295229000	-4.281363000	0.744580000
H	6.654475000	3.760302000	3.349360000	H	5.048161000	-4.904231000	-1.663330000
H	7.052772000	5.676094000	1.784930000	H	6.741797000	-5.068474000	-1.148370000
H	5.573789000	5.928355000	2.736800000	H	6.583754000	-3.882793000	-3.349360000
H	-0.070720000	-7.643095000	3.349360000	H	8.442028000	-3.269833000	-1.784930000
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H	-0.336242000	-5.185833000	3.018270000	H	8.177180000	-1.260255000	-0.322610000
H	-1.723108000	-6.823951000	1.663330000	H	7.687592000	-3.532065000	0.616450000
H	-1.018529000	-8.372805000	1.148370000	H	6.667080000	-2.289118000	1.370110000
H	1.389256000	-8.945927000	1.784930000	H	5.508925000	-1.646091000	-3.472450000
H	2.347211000	-7.791220000	2.736800000	H	4.322942000	-2.884111000	-3.018270000
H	2.918945000	-4.019059000	3.123530000	H	6.451876000	-0.080601000	-1.656620000
H	-1.060154000	-6.726484000	-0.744580000	H	5.908501000	-0.270969000	0.022760000
H	0.317942000	-4.667221000	-0.626980000	H	4.940080000	0.518351000	-3.123530000
H	-0.928877000	-4.665758000	0.631890000	H	3.328418000	0.998541000	-5.787200000
H	1.968855000	0.134783000	2.765930000	H	4.881722000	1.344298000	-5.002530000
H	-0.102856000	-2.744551000	0.375270000	H	4.775946000	2.476744000	-7.192400000
H	2.997177000	-7.711773000	0.322610000	H	6.036986000	3.564047000	-5.331320000
H	3.156136000	-5.627789000	1.656620000	H	5.319273000	4.786637000	-6.401880000
H	2.719585000	-5.252396000	-0.022760000	H	4.929425000	5.368083000	-3.999810000
H	0.784938000	-8.423683000	-0.616450000	H	3.200056000	6.005646000	-5.697550000
H	1.351105000	-6.918420000	-1.370110000	H	2.448030000	5.643542000	-4.128860000
H	-8.177180000	1.260255000	0.322610000	H	1.191509000	4.531433000	-5.974730000
H	-6.451876000	0.080601000	1.656620000	H	3.108002000	4.304981000	-7.577660000
H	-5.908501000	0.270969000	-0.022760000	H	2.296274000	2.744444000	-7.326660000
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H	-5.295229000	4.281363000	-0.744580000	H	3.663436000	-4.941828000	-4.128860000
H	-4.200903000	2.058265000	-0.626980000	H	2.184184000	-6.953049000	-3.999810000
H	-3.576226000	3.137310000	0.631890000	H	0.068062000	-7.010207000	-5.331320000
H	-5.048161000	4.904231000	1.663330000	H	1.485713000	-6.999944000	-6.401880000
H	-6.741797000	5.068474000	1.148370000	H	-0.243050000	-5.374463000	-7.192400000
H	-3.108002000	-4.304981000	7.577660000	H	2.174222000	-4.844099000	-7.577660000
H	-2.296274000	-2.744444000	7.326660000	H	1.228621000	-3.360854000	-7.326660000
H	-4.775946000	-2.476744000	7.192400000	H	0.169704000	-5.817723000	-3.067300000
H	-3.328418000	-0.998541000	5.787200000	H	1.646394000	-4.946173000	-2.604160000
H	-4.881722000	-1.344298000	5.002530000	H	-0.799447000	-3.381765000	-5.787200000
H	-1.191509000	-4.531433000	5.974730000	H	-1.276664000	-4.899844000	-5.002530000
H	-1.301271000	-3.428814000	3.767900000	H	-2.021135000	-4.537410000	-3.123530000
H	-1.216986000	-2.218182000	5.060810000	H	-3.295740000	-5.547188000	-1.656620000
H	-6.036986000	-3.564047000	5.331320000	H	-3.188916000	-4.981428000	0.022760000
H	-5.319273000	-4.786637000	6.401880000	H	-5.180003000	-6.451518000	-0.322610000
H	-3.200056000	-6.005646000	5.697550000	H	-6.902654000	-4.891617000	0.616450000
H	-2.448030000	-5.643542000	4.128860000	H	-5.315975000	-4.629302000	1.370110000
H	-4.929425000	-5.368083000	3.999810000	H	-6.355383000	-2.445122000	0.744580000
H	-4.953443000	-3.055830000	3.067300000	H	-6.771269000	-1.919720000	-1.663330000
H	-3.460314000	-3.898906000	2.604160000	H	-7.760326000	-3.304331000	-1.148370000
H	-0.169704000	5.817723000	3.067300000	H	-6.654475000	-3.760302000	-3.349360000
H	-1.646394000	4.946173000	2.604160000	H	-7.052772000	-5.676094000	-1.784930000
H	0.799447000	3.381765000	5.787200000	H	-5.573789000	-5.928355000	-2.736800000
H	1.276664000	4.899844000	5.002530000	H	-3.882961000	-2.608956000	0.626980000
H	-2.184184000	6.953049000	3.999810000	H	-4.505103000	-1.528448000	-0.631890000
H	-2.318805000	2.841341000	3.767900000	H	-4.180019000	-3.947823000	-3.472450000
H	-1.312509000	2.163032000	5.060810000	H	-4.659184000	-2.301722000	-3.018270000
H	-0.068062000	7.010207000	5.331320000	H	-2.428279000	-1.283200000	-0.375270000
H	-1.485713000	6.999944000	6.401880000	H	-1.968855000	-0.134783000	-2.765930000
H	0.243050000	5.374463000	7.192400000	H	-3.620076000	-0.587474000	-3.767900000
H	-3.601014000	5.774153000	5.697550000	H	-2.529495000	-0.055150000	-5.060810000
H	-3.663436000	4.941828000	4.128860000	H	-4.520090000	-1.233840000	-5.974730000
H	-3.328582000	3.297593000	5.974730000	H	-6.801070000	-0.231493000	-5.697550000
H	-2.174222000	4.844099000	7.577660000	H	-6.111466000	-0.701715000	-4.128860000
H	-1.228621000	3.360854000	7.326660000	H	-7.113609000	1.584965000	-3.999810000
H	3.620076000	0.587474000	3.767900000	H	-6.105048000	3.446160000	-5.331320000
H	2.529495000	0.055150000	5.060810000	H	-6.804985000	2.213307000	-6.401880000
H	5.123148000	-2.761893000	3.067300000	H	-4.532897000	2.897719000	-7.192400000
H	5.106709000	-1.047267000	2.604160000	H	-5.282224000	0.539118000	-7.577660000

H	-3.524896000	0.616410000	-7.326660000	H	-1.389256000	8.945927000	-1.784930000
H	-5.123148000	2.761893000	-3.067300000	H	-2.347211000	7.791220000	-2.736800000
H	-5.106709000	1.047267000	-2.604160000	H	-2.997177000	7.711773000	-0.322610000
H	-2.528971000	2.383224000	-5.787200000	H	-0.784938000	8.423683000	0.616450000
H	-3.605057000	3.555546000	-5.002530000	H	-1.351105000	6.918420000	1.370110000
H	-2.918945000	4.019059000	-3.123530000	H	-1.328906000	5.593914000	-3.472450000
H	-0.317942000	4.667221000	0.626980000	H	0.336242000	5.185833000	-3.018270000
H	0.928877000	4.665758000	-0.631890000	H	-3.156136000	5.627789000	-1.656620000
H	1.060154000	6.726484000	0.744580000	H	-2.719585000	5.252396000	0.022760000
H	1.723108000	6.823951000	-1.663330000	H	0.102856000	2.744551000	-0.375270000
H	1.018529000	8.372805000	-1.148370000				
H	0.070720000	7.643095000	-3.349360000				

NMR computations

Symmetry for ^tBu-1₂ was restricted to S₆, for tetramethylsilane to T_d. Throughout cc-pVDZ was used as basis set.

Table S18. Tetramethylsilane NMR shifts computed with GIAO:B3LYP-D3(BJ)/6-31G(d,p) and C-PCM:cyclohexane.

Atom (Count)	δ [ppm]
H(12)	31.5159
C(4)	190.4201
Si(1)	411.4509

Table S19. ^tBu-1₂ NMR shifts computed with GIAO:B3LYP-D3(BJ)/6-31G(d,p) and C-PCM:cyclohexane in S₆ symmetry.

Atom (Count)	δ [ppm]	δ(rel. to TMS) [ppm]	H(1)	30.5336	0.9868
H(1)	30.9663	0.5541	H(1)	30.5336	0.9868
H(1)	30.9663	0.5541	H(1)	30.5327	0.9877
H(1)	30.9659	0.5545	H(1)	30.5327	0.9877
H(1)	30.9659	0.5545	H(1)	30.5319	0.9885
H(1)	30.9656	0.5548	H(1)	30.5319	0.9885
H(1)	30.9656	0.5548	H(1)	30.5271	0.9933
H(1)	30.9170	0.6034	H(1)	30.5271	0.9933
H(1)	30.9170	0.6034	H(1)	30.5265	0.9939
H(1)	30.9165	0.6039	H(1)	30.5265	0.9939
H(1)	30.9165	0.6039	H(1)	30.5265	0.9939
H(1)	30.9160	0.6044	H(1)	30.5265	0.9939
H(1)	30.9160	0.6044	H(1)	30.4849	1.0355
H(1)	30.8679	0.6525	H(1)	30.4849	1.0355
H(1)	30.8679	0.6525	H(1)	30.4847	1.0357
H(1)	30.8678	0.6526	H(1)	30.4847	1.0357
H(1)	30.8678	0.6526	H(1)	30.4838	1.0366
H(1)	30.8671	0.6533	H(1)	30.4838	1.0366
H(1)	30.8671	0.6533	H(1)	30.4392	1.0812
H(1)	30.8216	0.6988	H(1)	30.4392	1.0812
H(1)	30.8216	0.6988	H(1)	30.4374	1.0830
H(1)	30.8206	0.6998	H(1)	30.4374	1.0830
H(1)	30.8206	0.6998	H(1)	30.4369	1.0835
H(1)	30.8204	0.7000	H(1)	30.4369	1.0835
H(1)	30.8204	0.7000	H(1)	30.4200	1.1004
H(1)	30.6704	0.8500	H(1)	30.4200	1.1004
H(1)	30.6704	0.8500	H(1)	30.4191	1.1013
H(1)	30.6700	0.8504	H(1)	30.4191	1.1013
H(1)	30.6700	0.8504	H(1)	30.4185	1.1019
H(1)	30.6695	0.8509	H(1)	30.4185	1.1019
H(1)	30.6695	0.8509	H(1)	30.1966	1.3238
H(1)	30.5653	0.9551	H(1)	30.1966	1.3238
H(1)	30.5653	0.9551	H(1)	30.1951	1.3253
H(1)	30.5649	0.9555	H(1)	30.1951	1.3253
H(1)	30.5649	0.9555	H(1)	30.1944	1.3260
H(1)	30.5628	0.9576	H(1)	30.1944	1.3260
H(1)	30.5628	0.9576	H(1)	30.1400	1.3804
H(1)	30.5531	0.9673	H(1)	30.1400	1.3804
H(1)	30.5531	0.9673	H(1)	30.1330	1.3874
H(1)	30.5529	0.9675	H(1)	30.1330	1.3874
H(1)	30.5529	0.9675	H(1)	30.1240	1.3964
H(1)	30.5528	0.9676	H(1)	30.1240	1.3964
H(1)	30.5528	0.9676	H(1)	30.1109	1.4095
H(1)	30.5365	0.9839	H(1)	30.1109	1.4095
H(1)	30.5365	0.9839	H(1)	30.1105	1.4099
H(1)	30.5361	0.9843	H(1)	30.1105	1.4099
H(1)	30.5361	0.9843	H(1)	30.1100	1.4104
H(1)	30.5351	0.9853	H(1)	30.1100	1.4104
H(1)	30.5351	0.9853	H(1)	29.9754	1.5450

H(1)	29.9754	1.5450	C(1)	155.4680	34.9089
H(1)	29.9737	1.5467	C(1)	155.4680	34.9089
H(1)	29.9737	1.5467	C(1)	155.4555	34.9214
H(1)	29.9735	1.5469	C(1)	155.4555	34.9214
H(1)	29.9735	1.5469	C(1)	155.4487	34.9282
H(1)	29.9567	1.5637	C(1)	155.4487	34.9282
H(1)	29.9567	1.5637	C(1)	153.8288	36.5481
H(1)	29.9561	1.5643	C(1)	153.8288	36.5481
H(1)	29.9561	1.5643	C(1)	153.8134	36.5635
H(1)	29.9557	1.5647	C(1)	153.8134	36.5635
H(1)	29.9557	1.5647	C(1)	153.8109	36.5660
H(1)	25.2600	6.2604	C(1)	153.8109	36.5660
H(1)	25.2600	6.2604	C(1)	153.5193	36.8576
H(1)	25.2599	6.2605	C(1)	153.5193	36.8576
H(1)	25.2599	6.2605	C(1)	153.5190	36.8579
H(1)	25.2582	6.2622	C(1)	153.5190	36.8579
H(1)	25.2582	6.2622	C(1)	153.5189	36.8580
H(1)	23.9909	7.5295	C(1)	153.5189	36.8580
H(1)	23.9909	7.5295	C(1)	117.9551	72.4218
H(1)	23.9889	7.5315	C(1)	117.9551	72.4218
H(1)	23.9889	7.5315	C(1)	73.8151	116.5618
H(1)	23.9887	7.5317	C(1)	73.8151	116.5618
H(1)	23.9887	7.5317	C(1)	73.8040	116.5729
H(1)	23.3480	8.1724	C(1)	73.8040	116.5729
H(1)	23.3480	8.1724	C(1)	73.7991	116.5778
H(1)	23.3473	8.1731	C(1)	73.7991	116.5778
H(1)	23.3473	8.1731	C(1)	67.8038	122.5731
H(1)	23.3467	8.1737	C(1)	67.8038	122.5731
H(1)	23.3467	8.1737	C(1)	67.8001	122.5768
C(1)	161.7969	28.5800	C(1)	67.8001	122.5768
C(1)	161.7969	28.5800	C(1)	67.7977	122.5792
C(1)	161.7899	28.5870	C(1)	67.7977	122.5792
C(1)	161.7899	28.5870	C(1)	65.6515	124.7254
C(1)	161.7888	28.5881	C(1)	65.6515	124.7254
C(1)	161.7888	28.5881	C(1)	65.6460	124.7309
C(1)	161.4918	28.8851	C(1)	65.6460	124.7309
C(1)	161.4918	28.8851	C(1)	65.6456	124.7313
C(1)	161.4914	28.8855	C(1)	65.6456	124.7313
C(1)	161.4914	28.8855	C(1)	47.8934	142.4835
C(1)	161.4894	28.8875	C(1)	47.8934	142.4835
C(1)	161.4894	28.8875	C(1)	47.8902	142.4867
C(1)	158.8161	31.5608	C(1)	47.8902	142.4867
C(1)	158.8161	31.5608	C(1)	47.8836	142.4933
C(1)	158.8080	31.5689	C(1)	47.8836	142.4933
C(1)	158.8080	31.5689	C(1)	47.4038	142.9731
C(1)	158.8077	31.5692	C(1)	47.4038	142.9731
C(1)	158.8077	31.5692	C(1)	47.4007	142.9762
C(1)	157.1310	33.2459	C(1)	47.4007	142.9762
C(1)	157.1310	33.2459	C(1)	47.3977	142.9792
C(1)	157.1247	33.2522	C(1)	47.3977	142.9792
C(1)	157.1247	33.2522	C(1)	44.1428	146.2341
C(1)	157.1228	33.2541	C(1)	44.1428	146.2341
C(1)	157.1228	33.2541	C(1)	44.1387	146.2382
C(1)	156.8415	33.5354	C(1)	44.1387	146.2382
C(1)	156.8415	33.5354	C(1)	44.1367	146.2402
C(1)	156.8353	33.5416	C(1)	44.1367	146.2402
C(1)	156.8353	33.5416			
C(1)	156.8321	33.5448			
C(1)	156.8321	33.5448			

Table S20. Comparison of experimental and computed relative, per group averaged (GIAO:B3LYP-D3(BJ)/6-31G(d,p) and C-PCM:cyclohexane) chemical shifts of ¹Bu-1₂.

Group	δ (Comp.) [ppm]	δ (Found) [ppm]	Position ^{a)}
C(CH ₃) ₃	1.01	0.95	outside
C(CH ₃) ₃	1.07	0.98	inside
<i>o</i> -Ph CH	6.26	6.03	outside
<i>p</i> -Ph CH	7.53	7.20	
<i>o</i> -Ph CH	8.17	7.76	inside
C(CH ₃) ₃	31.2	31.8	outside
C(CH ₃) ₃	32.4	32.1	inside
C(CH ₃) ₃	36.6	35.2	inside
C(CH ₃) ₃	36.9	35.3	outside
R ₃ CCR ₃	72.4	71.5	
<i>p</i> -Ph C _q	116.6	120.3	
<i>o</i> -Ph CH	122.6	128.1	outside
<i>o</i> -Ph CH	124.7	128.6	inside
<i>m</i> -Ph C _q	142.5	149.5	inside
<i>m</i> -Ph C _q	143.0	149.9	outside
<i>ipso</i> -Ph C _q	146.2	151.1	

^{a)} outside groups point towards a phenyl moiety within the same trityl group, inside groups point towards an opposite phenyl moiety of the other trityl group.

Table S21. Coordinates of optimized structures (in Å) of the NMR computation (GIAO:B3LYP-D3(BJ)/6-31G(d,p) with C-PCM:cyclohexane).

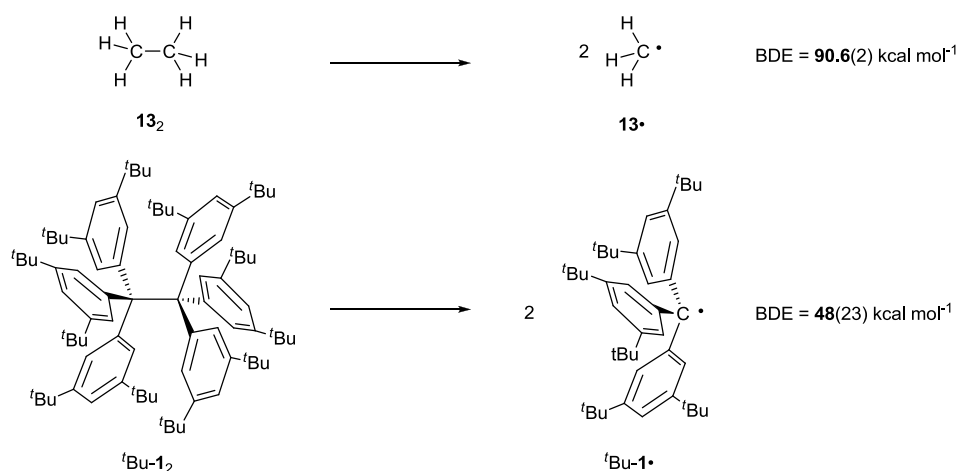
Tetramethylsilane			
Si	0.00000000	0.00000000	0.00000000
C	1.09425000	-1.09425000	-1.09425000
C	-1.09425000	1.09425000	-1.09425000
C	1.09425000	1.09425000	1.09425000
C	-1.09425000	-1.09425000	1.09425000
H	1.74191000	-0.47996000	-1.74191000
H	0.47996000	-1.74191000	-1.74191000
H	1.74191000	-1.74191000	-0.47996000
H	-0.47996000	1.74191000	-1.74191000
H	-1.74191000	1.74191000	-0.47996000
H	-1.74191000	0.47996000	-1.74191000
H	1.74191000	1.74191000	0.47996000
H	1.74191000	0.47996000	1.74191000
H	0.47996000	1.74191000	1.74191000
H	-1.74191000	-1.74191000	0.47996000
H	-1.74191000	-0.47996000	1.74191000
H	-0.47996000	-1.74191000	1.74191000
¹ Bu-1 ₂			
C	1.91149900	-3.47201500	2.69854000
C	0.98695700	-3.67667600	1.66986000
C	0.40274400	-2.55405000	1.06344000
C	0.73996700	-1.24394700	1.42711000
C	1.66003000	-1.08927800	2.47718000
C	2.24215900	-2.17935800	3.13165000
C	-1.44727300	-0.01885700	1.42711000
C	-2.41324400	0.92823900	1.06344000
C	-3.67757300	0.98360800	1.66986000
C	-3.96260300	0.08060000	2.69854000
C	-3.00845900	-0.85208800	3.13165000
C	-1.77335800	-0.89298900	2.47718000
C	0.76630000	3.03144600	3.13165000
C	0.11332800	1.98226700	2.47718000
C	0.70730600	1.26280300	1.42711000
C	2.01050100	1.62581200	1.06344000
C	2.69061600	2.69306800	1.66986000
C	2.05110300	3.39141500	2.69854000
C	0.00000000	0.00000000	0.83107000
C	-1.91149900	3.47201500	-2.69854000
C	-2.24215900	2.17935800	-3.13165000
C	-1.66003000	1.08927800	-2.47718000
C	-0.73996700	1.24394700	-1.42711000
C	-0.40274400	2.55405000	-1.06344000
C	-0.98695700	3.67667600	-1.66986000
C	-0.70730600	-1.26280300	-1.42711000
C	-2.01050100	-1.62581200	-1.06344000
C	-2.69061600	-2.69306800	-1.66986000
C	-2.05110300	-3.39141500	-2.69854000
C	-0.76630000	-3.03144600	-3.13165000
C	-0.11332800	-1.98226700	-2.47718000
C	3.00845900	0.85208800	-3.13165000
C	1.77335800	0.89298900	-2.47718000
C	1.44727300	0.01885700	-1.42711000
C	2.41324400	-0.92823900	-1.06344000
C	3.67757300	-0.98360800	-1.66986000
C	3.96260300	-0.08060000	-2.69854000
C	0.00000000	0.00000000	-0.83107000
C	0.53608900	-5.07926800	1.22952000
C	3.19121200	-1.98918900	4.32561000
C	-4.66681900	2.07536700	1.22952000
C	-3.31829500	-1.76907600	4.32561000
C	0.12708200	3.75826600	4.32561000
C	4.13073000	3.00390100	1.22952000
C	-3.19121200	1.98918900	-4.32561000
C	-0.53608900	5.07926800	-1.22952000
C	-4.13073000	-3.00390100	-1.22952000
C	-0.12708200	-3.75826600	-4.32561000
C	3.31829500	1.76907600	-4.32561000
C	4.66681900	-2.07536700	-1.22952000
C	1.36034000	-6.19324500	1.89193000
C	0.66887800	-5.22113000	-0.29934000
C	-0.94423000	-5.26091600	1.62536000
C	3.41972800	-0.50575700	4.65676000
C	4.55875200	-2.63199000	4.01588000
C	2.57073000	-2.67092000	5.56420000
C	-6.04367800	1.91853400	1.89193000
C	-4.85607000	2.03129900	-0.29934000
C	-4.08397200	3.44818500	1.62536000
C	-2.14786200	-2.70869300	4.65676000
C	-4.55874600	-2.63200000	4.01588000

C	-3.598449000	-0.890858000	5.564200000	H	5.038782000	1.676722000	2.718390000
C	-1.271866000	3.214450000	4.656760000	H	6.065255000	1.980004000	1.290290000
C	-0.000006000	5.263990000	4.015880000	H	4.670064000	0.877488000	1.171750000
C	1.027719000	3.561777000	5.564200000	H	-2.437096000	3.752362000	-5.409400000
C	4.683338000	4.274712000	1.891930000	H	-3.219500000	2.533117000	-6.444930000
C	4.187192000	3.189831000	-0.299340000	H	-1.583405000	2.237874000	-5.792320000
C	5.028202000	1.812731000	1.625360000	H	-4.461671000	3.701215000	-3.773710000
C	-2.570730000	2.670920000	-5.564200000	H	-5.039292000	2.133758000	-3.160380000
C	-4.558752000	2.631990000	-4.015880000	H	-5.229127000	2.542830000	-4.886470000
C	-3.419728000	0.505757000	-4.656760000	H	-3.859202000	-0.038064000	-3.807760000
C	-0.668878000	5.221130000	0.299340000	H	-2.483104000	-0.002076000	-4.934840000
C	-1.360340000	6.193245000	-1.891930000	H	-4.113164000	0.419537000	-5.507700000
C	0.944230000	5.260916000	-1.625360000	H	-0.294738000	6.205387000	0.624830000
C	-4.187192000	-3.189831000	0.299340000	H	-0.098757000	4.452471000	0.838000000
C	-4.683338000	-4.274712000	-1.891930000	H	-1.721935000	5.139586000	0.610170000
C	-5.028202000	-1.812731000	-1.625360000	H	-1.022202000	7.173643000	-1.521880000
C	-1.027719000	-3.561777000	-5.564200000	H	-2.432434000	6.096712000	-1.658870000
C	0.000006000	-5.263990000	-4.015880000	H	-1.244975000	6.195168000	-2.986770000
C	1.271866000	-3.214450000	-4.656760000	H	1.317893000	6.242667000	-1.290290000
C	3.598449000	0.890858000	-5.564200000	H	1.067307000	5.202074000	-2.718390000
C	4.558752000	2.632000000	-4.015880000	H	1.575105000	4.483138000	-1.171750000
C	2.147862000	2.708693000	-4.656760000	H	-5.226654000	-3.357944000	0.624830000
C	4.856070000	-2.031299000	0.299340000	H	-3.806575000	-2.311762000	0.838000000
C	6.043678000	-1.918534000	-1.891930000	H	-3.590044000	-4.061033000	0.610170000
C	4.083972000	-3.448185000	-1.625360000	H	-5.701456000	-4.472075000	-1.521880000
H	1.244975000	-6.195168000	2.986770000	H	-4.063691000	-5.154905000	-1.658870000
H	2.432434000	-6.096712000	1.658870000	H	-4.742685000	-4.175764000	-2.986770000
H	1.022202000	-7.173643000	1.521880000	H	-6.065255000	-1.980004000	-1.290290000
H	0.098757000	-4.452471000	-0.838000000	H	-5.038782000	-1.676722000	-2.718390000
H	0.294738000	-6.205387000	-0.624830000	H	-4.670064000	-0.877488000	-1.171750000
H	1.721935000	-5.139586000	-0.610170000	H	-2.031093000	-3.986768000	-5.409400000
H	-1.067307000	-5.202074000	2.718390000	H	-0.583994000	-4.054727000	-6.444930000
H	-1.317893000	-6.242667000	1.290290000	H	-1.146353000	-2.490206000	-5.792320000
H	-1.575105000	-4.483138000	1.171750000	H	-0.974511000	-5.714528000	-3.773710000
H	4.113164000	-0.419537000	5.507700000	H	0.671757000	-5.431034000	-3.160380000
H	2.483104000	0.002076000	4.934840000	H	0.412408000	-5.799972000	-4.886470000
H	3.859202000	0.038064000	3.807760000	H	1.962565000	-3.323135000	-3.807760000
H	5.229127000	-2.542830000	4.886470000	H	1.243349000	-2.149393000	-4.934840000
H	5.039292000	-2.133758000	3.160380000	H	1.693253000	-3.771873000	-5.507700000
H	4.461671000	-3.701215000	3.773710000	H	4.468189000	0.234406000	-5.409400000
H	3.219500000	-2.533117000	6.444930000	H	3.803494000	1.521610000	-6.444930000
H	2.437096000	-3.752362000	5.409400000	H	2.729758000	0.252332000	-5.792320000
H	1.583405000	-2.237874000	5.792320000	H	5.436182000	2.013313000	-3.773710000
H	-5.987661000	2.019404000	2.986770000	H	4.367535000	3.297276000	-3.160380000
H	-6.496124000	0.941807000	1.658870000	H	4.816719000	3.257142000	-4.886470000
H	-6.723658000	2.701569000	1.521880000	H	1.896636000	3.361199000	-3.807760000
H	-3.905332000	2.140709000	-0.838000000	H	1.239754000	2.151469000	-4.934840000
H	-5.521392000	2.847443000	-0.624830000	H	2.419911000	3.352336000	-5.507700000
H	-5.311980000	1.078553000	-0.610170000	H	5.521392000	-2.847443000	0.624830000
H	-3.971475000	3.525352000	2.718390000	H	3.905332000	-2.140709000	0.838000000
H	-4.747361000	4.262663000	1.290290000	H	5.311980000	-1.078553000	0.610170000
H	-3.094959000	3.605650000	1.171750000	H	6.723658000	-2.701569000	-1.521880000
H	-2.419911000	-3.352336000	5.507700000	H	6.496124000	-0.941807000	-1.658870000
H	-1.239754000	-2.151469000	4.934840000	H	5.987661000	-2.019404000	-2.986770000
H	-1.896636000	-3.361199000	3.807760000	H	4.747361000	-4.262663000	-1.290290000
H	-4.816719000	-3.257142000	4.886470000	H	3.971475000	-3.525352000	-2.718390000
H	-4.367535000	-3.297276000	3.160380000	H	3.094959000	-3.605650000	-1.171750000
H	-5.436182000	-2.013313000	3.773710000	H	2.365756000	-4.328560000	3.192610000
H	-3.803494000	-1.521610000	6.444930000	H	-0.351453000	-2.715799000	0.304750000
H	-4.468189000	-0.234406000	5.409400000	H	1.913196000	-0.092396000	2.810390000
H	-2.729758000	-0.252332000	5.792320000	H	-2.176224000	1.662267000	0.304750000
H	-1.693253000	3.771873000	5.507700000	H	-4.931521000	0.115476000	3.192610000
H	-1.243349000	2.149393000	4.934840000	H	-1.036615000	-1.610678000	2.810390000
H	-1.962565000	3.323135000	3.807760000	H	-0.876581000	1.703074000	2.810390000
H	-0.412408000	5.799972000	4.886470000	H	2.527677000	1.053532000	0.304750000
H	-0.671757000	5.431034000	3.160380000	H	2.565766000	4.213085000	3.192610000
H	0.974511000	5.714528000	3.773710000	H	-2.365756000	4.328560000	-3.192610000
H	0.583994000	4.054727000	6.444930000	H	-1.913196000	0.092396000	-2.810390000
H	2.031093000	3.986768000	5.409400000	H	0.351453000	2.715799000	-0.304750000
H	1.146353000	2.490206000	5.792320000	H	-2.527677000	-1.053532000	-0.304750000
H	4.742685000	4.175764000	2.986770000	H	-2.565766000	-4.213085000	-3.192610000
H	4.063691000	5.154905000	1.658870000	H	0.876581000	-1.703074000	-2.810390000
H	5.701456000	4.472075000	1.521880000	H	1.036615000	1.610678000	-2.810390000
H	3.806575000	2.311762000	-0.838000000	H	2.176224000	-1.662267000	-0.304750000
H	5.226654000	3.357944000	-0.624830000	H	4.931521000	-0.115476000	-3.192610000
H	3.590044000	4.061033000	-0.610170000				

Estimation of the covalent contribution of the overall dissociation energy

Estimation from heat of formation

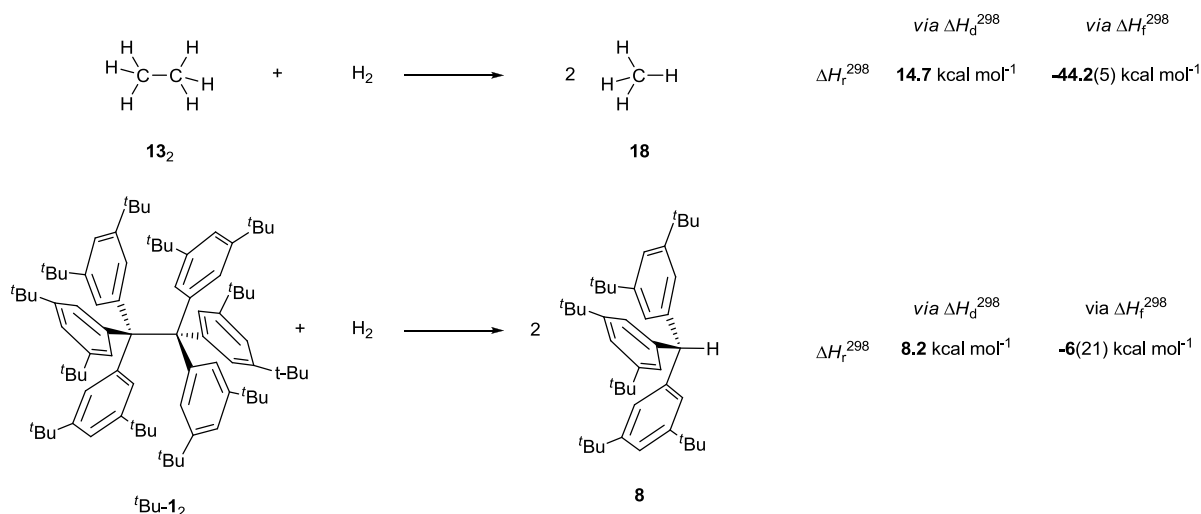
To estimate the covalent contribution (BDE) of the dissociation energy of HPE into two TPM radicals from heats of formation (ΔH_f^0) a reference molecule needed to be chosen. The common example for exclusively covalent element–element bonds are the simple stable representative molecules which bare this bond type. In case of a carbon–carbon single bond this is ethane **13₂**. The BDEs were derived for the carbon–carbon dissociations of **13₂** and ^tBu-**1₂** (Scheme S2). The unknown ΔH_f^0 of ^tBu-**1₂** and ^tBu-**1•** were calculated from isodesmic reactions (Scheme S4). Reaction enthalpies were derived from optimized structures with B3YLP-D3(BJ)/cc-pVDZ computations. Heats of formation of ethane **13₂**, methyl radical **13•**, methane **14**, triphenylmethane **15**, 2,2,3,3-tetramethylbutane **16** and *tert*-butyl radical **17** are listed in Table S24. Here 53% of covalent bonding are left in ^tBu-**1₂** regarding **13₂**.



Scheme S2. The strength of the central bond estimated for **13₂** and ^tBu-**1₂**.

Estimation from enthalpy of hydrogenation

Likewise the determination of aromatization energy *via* the enthalpy of hydrogenation, can the theoretical hydrogenation of a carbon–carbon single bonds be utilized to estimate the covalent bond strength upon stretching the bond relative to ethane. Bond dissociation energies ΔH_d^{298} were derived from optimized structures with B3YLP-D3(BJ)/cc-pVDZ computations (Table S25 and Table S26). Regarding the hydrogenation of ^tBu-**1₂** *via* ΔH_d^{298} remain 56%, *via* ΔH_f^{298} remain 14% of covalent bonding strength (Scheme S3).



Scheme S3. Hydrogenation of ethanes derivatives leads to methanes.

Estimation from bond vibration

Regarding Hooke's law depend the frequency of a harmonic oscillator on the reduced mass μ and the stiffness K_H . This stiffness correlates direct with bond strength and can therefore serve as a gauge for the covalent contribution relative to ethane. Due to the symmetric weight distribution is the reduced mass deduced from the half molecular weight. The specific symmetric bond stretching frequency $\nu_s(\text{C}-\text{C})$ was obtained from B3YLP-D3(BJ)/cc-pVDZ frequency computations (${}^t\text{Bu}-1_2$:Table S12 and Table S16 / 13_2 :Table S25 and Table S26). Regarding 13_2 were 46% bond strength in ${}^t\text{Bu}-1_2$ preserved.

Table S22. Specifications of the harmonic oscillators 12_2 and ${}^t\text{Bu}-1_2$.

Compound	Half mass (u)	μ (g)	$\tilde{\nu}$ (cm^{-1})	ν (GHz)	K_H (nN m)
13_2	15.02	$0.13 \cdot 10^{-22}$	1013	304.7	45.4
${}^t\text{Bu}-1_2$	579.49	$4.81 \cdot 10^{-22}$	111	33.3	21.0

Estimation via ISAPT computations

The intramolecular SAPT method allowed Sherrill *et al.* to compute the non-covalent contributions within ${}^t\text{Bu}-1_2$.⁹ The total non-covalent energy was determined to be repulsive by $E^{\text{non-cov. tot}} = -44.97 \text{ kcal mol}^{-1}$. Herein the overall dissociation enthalpy $\Delta H_d^{298} = 7.94(3) \text{ kcal mol}^{-1}$ was determined. A ruff estimation of the covalent contribution is obtained by subtracting all non-covalent contributions from the overall enthalpy. This give $52.91 \text{ kcal mol}^{-1}$; 59% of the BDE for ethane.

Conclusions

On one hand are these estimations no quantitative calculation of the true covalent contribution but rather a qualitative analysis of how much covalent bonding should be expected. The error bars for the heat of formations are quite large and further are attractive interactions lost during the reaction. As these attractions are only within ${}^t\text{Bu}-1_2$ and on side of the starting materials is the determined bond strength likely too strong. This loss of interactions accounts also for the enthalpy of hydrogenation. The bond strength from hydrogenation *via* ΔH_d^{298} should appear overestimated, too. The bond strength from hydrogenation *via* ΔH_f^{298} bares for ${}^t\text{Bu}-1_2$ an uncertainty of $\pm 21 \text{ kcal mol}^{-1}$, more than three times larger than the value. The estimation from bond vibrations depends on an isolated pure $\nu_s(\text{C}-\text{C})$. This indeed is obtained for ethane. In case of ${}^t\text{Bu}-1_2$ instead little mixing with wagging, rocking and deformation vibrations cannot be avoided. In the estimation from the ISAPT computation are energies mixed with enthalpies. In general appear energies to a little stronger relative to the enthalpies. Hence are these derived bond strength likely to be overestimated.

On the other hand, if the heat of hydrogenation *via* ΔH_f^{298} is because of the prohibitive uncertainty omitted match the here estimated covalent bond strengths roughly and are placed between 46% and 59% regarding ethane as reference system. This gives an averaged BDE of $48(+5/-7) \text{ kcal mol}^{-1}$ which should be taken as an upper limit. The 0.13 Å elongation of the central bond in ${}^t\text{Bu}-1_2$ at least halve its strength, it still appears to be essential to the overall stability of ${}^t\text{Bu}-1_2$ against dissociation.

Computational details for estimations of covalent C–C bond contribution

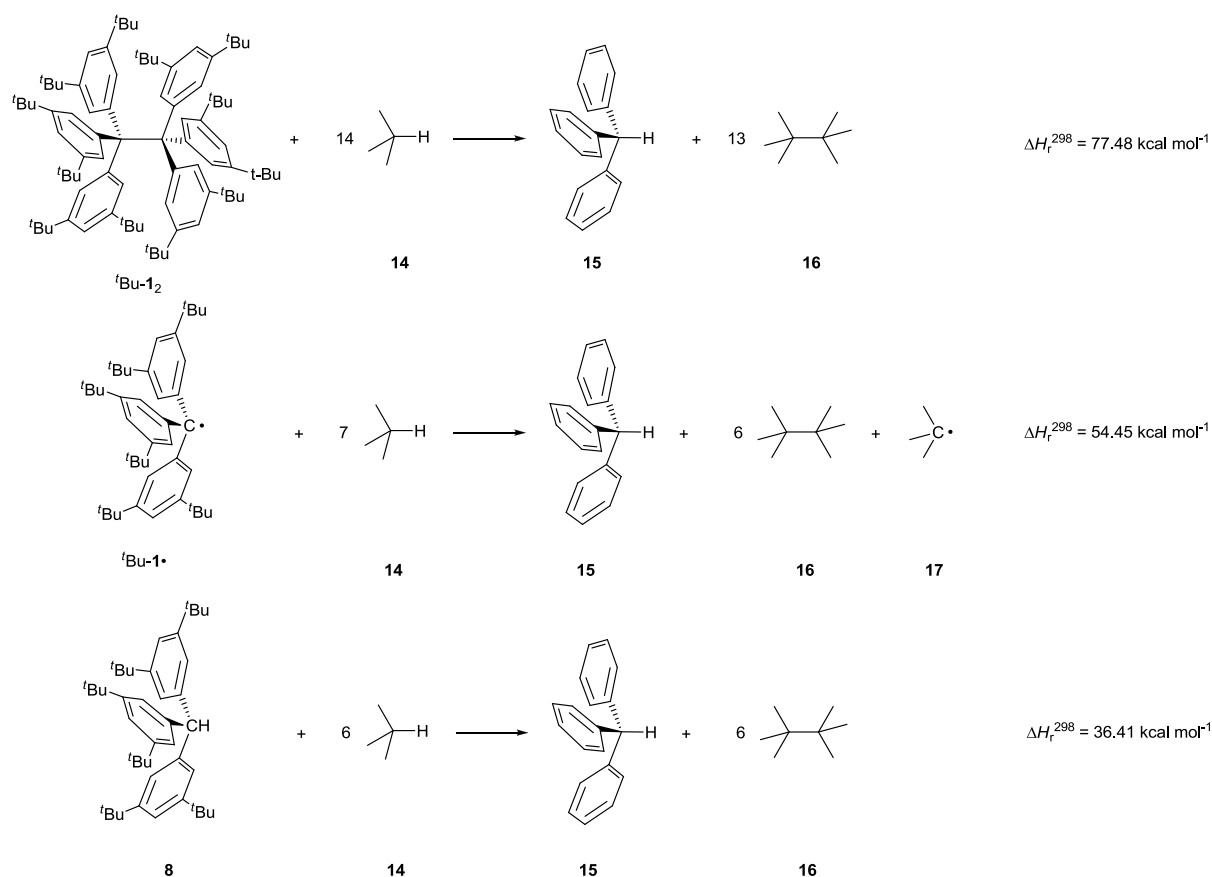
Dissociation energies, heats of formation and isodesmic reactions

Table S23. Computed dissociation enthalpies with B3YLP-D3(BJ)/cc-pVDZ.

Compound	Concerned Bond	ΔH_d^{298} (kcal mol ⁻¹)
H ₂	H–H	99.14
13 ₂	H ₃ C–CH ₃	89.17
18	H ₃ C–H	101.54
^t Bu- 1 ₂	Ar ₃ C–CAr ₃	37.96
8	Ar ₃ C–H	72.64

Table S24. Calculated and literature known heats of formation.

Compound	ΔH_f^{298} (kcal mol ⁻¹)	Reference
^t Bu- 1 ₂	–198(11)	
^t Bu- 1 •	–75(6)	
8	–102(5)	
13 ₂	–20.04(7)	10
13 •	35.3(5)	11
14	–32.1(2)	10
15	66(2)	12
16	–54.0(3)	13
17	12.3(4)	14



Scheme S4. The isodesmic reactions balance the occurrence of bonding situations in starting materials and products to minimize errors.

Energies

Energies of the optimized structures are given in hartree. Throughout cc-pVDZ was used as basis set. Energies and Cartesian coordinates of ^tBu-1₂ and ^tBu-1• are listed in section “computations”.

Table S25. Computed energies from B3YLP-D3(BJ)/cc-pVDZ.

Compound	EE	ZPVE	H^{298}
H•	-0.501258	0	-0.501258
H ₂	-1.173745	0.009933	-1.160508
8	-1677.480586	0.958430	-1676.474814
13•	-39.840451	0.029368	-39.807036
13₂	-79.834689	0.074095	-79.756170
14	-158.474946	0.130565	-158.337727
15	-315.747236	0.242372	-315.493939
16	-733.785857	0.290371	-733.479513
17	-157.814456	0.115387	-157.691690
18	-40.518262	0.044344	-40.470101

H	-1.537818000	-0.887860000	-1.090228000
H	-2.136484000	-0.200817000	0.432669000
H	-1.242155000	-1.749841000	0.432669000

15

C	0.121253000	4.170479000	-0.422976000
C	-0.654890000	3.264296000	-1.148034000
C	-0.717122000	1.921104000	-0.762902000
C	0.000000000	1.464615000	0.349596000
C	0.776113000	2.383390000	1.071583000
C	0.837602000	3.724436000	0.692471000
C	-1.268394000	-0.732308000	0.349596000
C	-2.452133000	-0.519561000	1.071583000
C	-3.644257000	-1.136833000	0.692471000
C	-3.672368000	-1.980231000	-0.422976000
C	-2.499518000	-2.199300000	-1.148034000
C	-1.305164000	-1.581598000	-0.762902000
C	3.154409000	-1.064997000	-1.148034000
C	2.022286000	-0.339506000	-0.762902000
C	1.268394000	-0.732308000	0.349596000

C	1.676020000	-1.863828000	1.071583000
C	2.806655000	-2.587602000	0.692471000
C	3.551114000	-2.190248000	-0.422976000
C	0.000000000	0.000000000	0.777683000
H	0.165516000	5.219977000	-0.721527000
H	-1.221518000	3.602682000	-2.018442000
H	-1.333752000	1.221895000	-1.329264000
H	1.344417000	2.036814000	1.938630000
H	1.444680000	4.425144000	1.270043000
H	-2.436141000	0.145892000	1.938630000
H	-4.554627000	-0.961443000	1.270043000
H	-4.603391000	-2.466647000	-0.721527000
H	-2.509255000	-2.859207000	-2.018442000
H	-0.391316000	-1.766011000	-1.329264000
H	3.730773000	-0.743475000	-2.018442000
H	1.725068000	0.544116000	-1.329264000
H	1.091724000	-2.182706000	1.938630000
H	3.109948000	-3.463701000	1.270043000
H	4.437875000	-2.753330000	-0.721527000
H	0.000000000	0.000000000	1.880300000

Appendix

Thermodynamic data of C–C bond dissociations equilibria

An enthalpy–entropy compensation is found for dissociation of C–C single bonds in solution with low ΔH_d^{298} (below 15 kcal mol⁻¹) in an ensemble of 36 hydrocarbons (Table S27 and Figure S4). Here the ΔH_d^{298} ranges from 6.2 kcal mol⁻¹ to 67.4 kcal mol⁻¹. The term $T\Delta S_d^{298}$ at 298 K instead varies around $\emptyset(T\Delta S_d^{298}) = 6(3)$ kcal mol⁻¹. In this ensemble occurs the compensation phenomenon only in systems with a very low carbon–carbon bond dissociation energy.

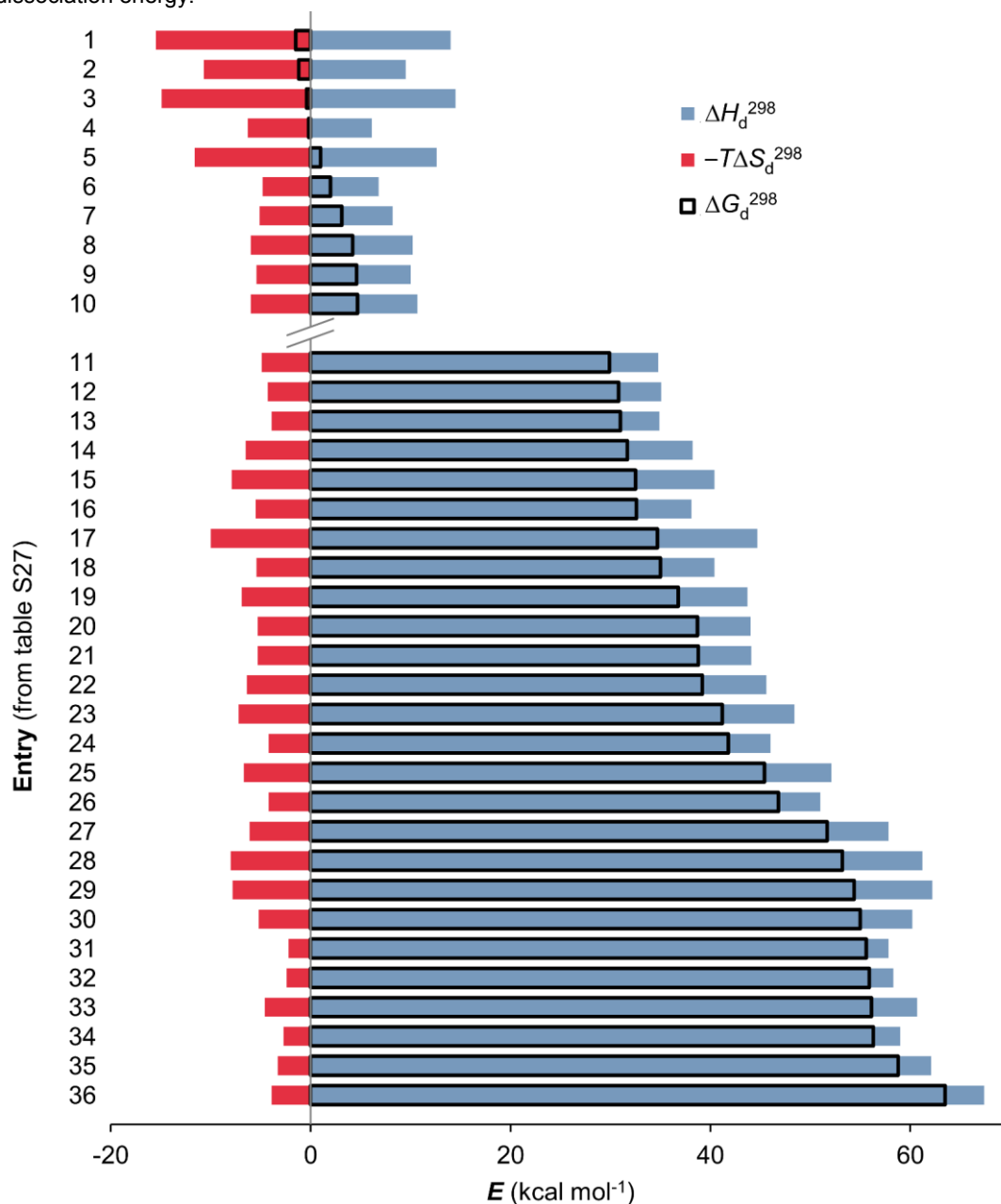


Figure S4. Thermodynamic data from table S27 reveal an enthalpy–entropy compensation for low ΔH_d^{298} . With rising ΔH_d^{298} becomes the term $T\Delta S_d^{298}$ more negligible.

Table S27. A list of homolytic C–C bond dissociations in solution.

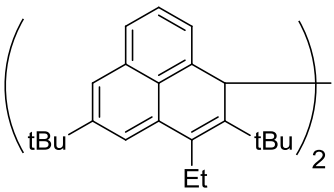
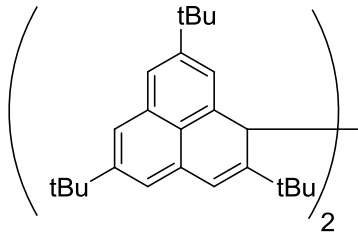
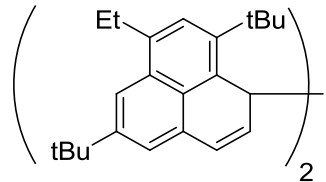
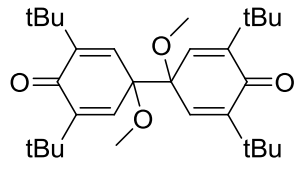
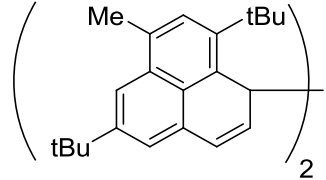
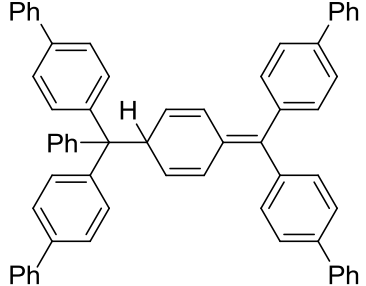
Entry	Compound	R_{CC} [Å]	ΔH [Kcal mol ⁻¹]	$298K \cdot \Delta S$ [Kcal mol ⁻¹]	ΔG [Kcal mol ⁻¹]	Reference
1			14	15.5	-1.5	15
2			9.5	10.7	-1.2	15
3			14.5	14.9	-0.4	16
4		1.606	6.1	6.3	-0.2	17
5			12.6	11.6	1.0	16
6			6.8	4.8	2	18

Table S27 Continued...

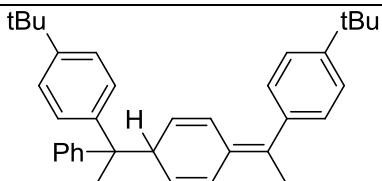
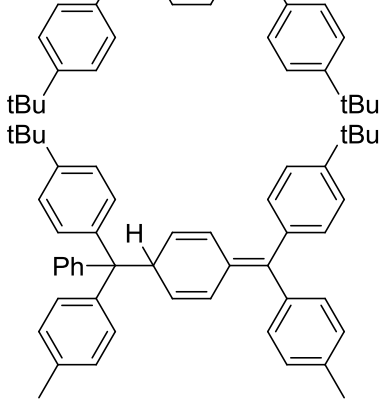
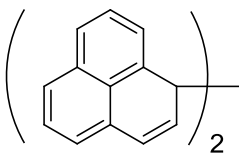
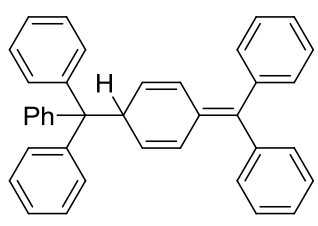
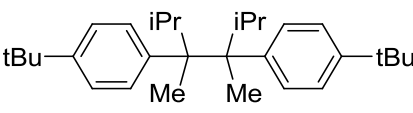
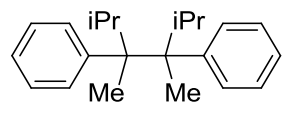
Entry	Compound	R_{CC} [Å]	ΔH [Kcal mol ⁻¹]	$298K \cdot \Delta S$ [Kcal mol ⁻¹]	ΔG [Kcal mol ⁻¹]	Reference
7			8.2	5.1	3.1	18
8			10.2	6.0	4.2	18
9			10	5.4	4.6	15
10		1.60	10.7	6.0	4.7	18
11			34.8	4.9	29.9	19
12			35.1	4.3	30.8	19

Table S27 Continued...

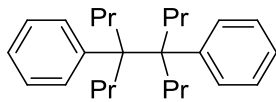
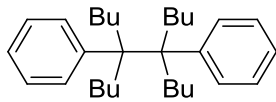
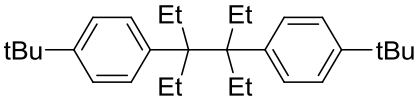
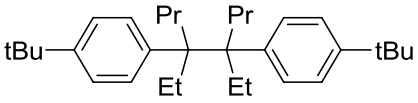
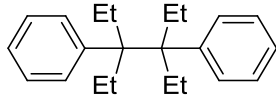
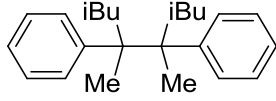
Entry	Compound	R_{CC} [Å]	ΔH [Kcal mol ⁻¹]	$298K \cdot \Delta S$ [Kcal mol ⁻¹]	ΔG [Kcal mol ⁻¹]	Reference
13			34.9	3.9	31	19
14		1.638	38.2	6.5	31.7	19
15			40.4	7.9	32.5	19
16			38.1	5.5	32.6	19
17		1.622	44.7	10.0	34.7	19
18			40.4	5.4	35	19

Table S27 Continued...

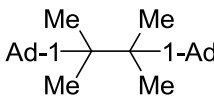
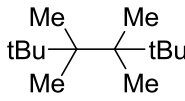
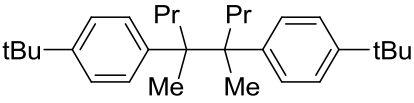
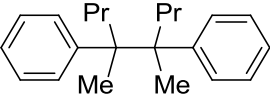
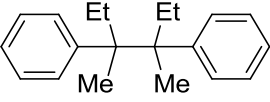
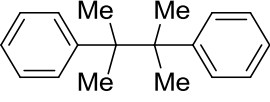
Entry	Compound	R_{CC} [Å]	ΔH [Kcal mol ⁻¹]	$298K \cdot \Delta S$ [Kcal mol ⁻¹]	ΔG [Kcal mol ⁻¹]	Reference
19		1.639	43.7	6.9	36.8	20
20			44.0	5.3	38.7	21
21			44.1	5.3	38.8	19
22			45.6	6.4	39.2	19
23			48.4	7.2	41.2	19
24		1.585	46.0	4.2	41.8	19

Table S27 Continued...

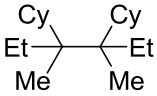
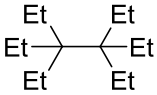
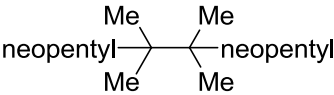
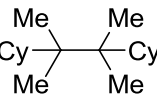
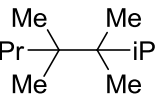
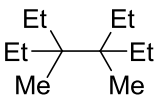
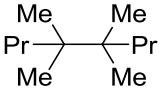
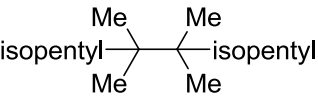
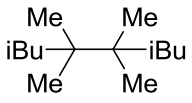
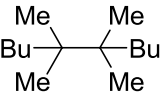
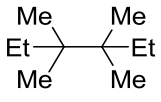
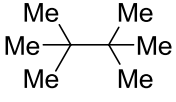
Entry	Compound	R_{CC} [Å]	ΔH [Kcal mol ⁻¹]	$298K \cdot \Delta S$ [Kcal mol ⁻¹]	ΔG [Kcal mol ⁻¹]	Reference
25			52.1	6.7	45.4	21
26			51.0	4.2	46.8	21
27			57.8	6.1	51.7	21
28			61.2	8.0	53.2	21
29			62.2	7.8	54.4	21
30		1.626	60.2	5.2	55	21

Table S27 Continued...

Entry	Compound	R_{CC} [Å]	ΔH [Kcal mol ⁻¹]	$298K \cdot \Delta S$ [Kcal mol ⁻¹]	ΔG [Kcal mol ⁻¹]	Reference
31			57.8	2.2	55.6	21
32			58.3	2.4	55.9	21
33			60.7	4.6	56.1	21
34			59.0	2.7	56.3	21
35			62.1	3.3	58.8	21
36		1.582	67.4	3.9	63.5	21

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