Supporting Information

Probing Substituent Effects in Aryl-Aryl Interactions Using Stereoselective Diels-Alder Cycloadditions

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Materials: Silica gel (40 μm) was purchased from SiliCycle. Commercial grade anthracene (97%, Lancaster) was purified by recrystallization in hexanes (2x) followed by vacuum sublimation. All other reagent grade materials were purchased from Aldrich, Lancaster, Alfa Aesar, or Acros and used without further purification unless otherwise noted.

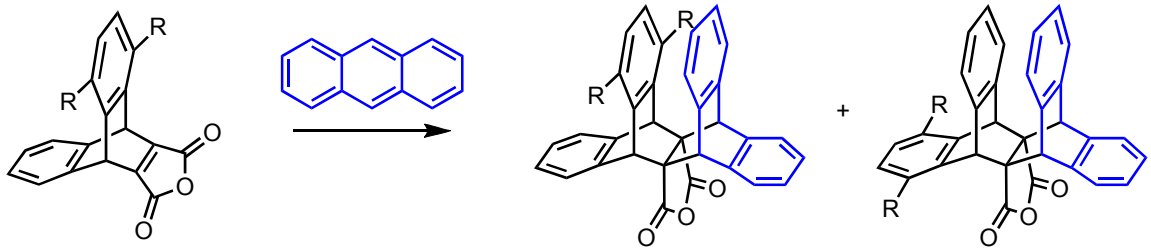
Experimental:

NMR Spectroscopy: ^{1}H and ^{13}C NMR spectra for all compounds were acquired in $CDCl_3$ or d_6-DMSO on a Bruker Avance Spectrometer operating at 400 and 100 MHz, respectively. The chemical shift data are reported in units of δ (ppm) relative to tetramethylsilane (TMS) and referenced with residual $CHCl_3$ or DMSO.

X-ray Crystallography: Low temperature (100 K) diffraction data were collected on a Siemens Platform three-circle diffractometer coupled to a Bruker-AXS Smart Apex CCD detector with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å), performing φ- and ω-scans. All structures were solved by direct methods using SHELXS[1] and refined against F^2 on all data by full-matrix least squares with SHELXL-97[2] using established refinement strategies.[3] All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups).

The crystal on which the structure for **2c** is based on was non-merohedrally twinned. Two independent orientation matrices for the unit cell were found using the program CELL_NOW,[4] and data reduction taking into account the twinning was performed with SAINT.[5] The program TWINABS[6] was used to perform absorption correction and to set up the HKLF5 format file for structure refinement. The twin ratio was refined freely and converged at a value of 0.463(2).

General Procedure for Diels–Alder Reaction



1a: R = H
1b: R = Me
1c: R = OMe
1d: R = Br

2a: R = H
2b: R = Me
2c: R = OMe
2d: R = Br

3b: R = Me
3c: R = OMe
3d: R = Br

In a 20 mL RBF was placed **1** (50 mg), anthracene (10 equiv), and decane (4 mL). The flask was equipped with a stir bar and an N_2 inlet. The heterogeneous mixture was heated to 140-150 ^{o}C for 12-15 h. (The reaction becomes homogeneous with heating.) After cooling to room temperature, a sample was taken for ^{1}H NMR spectroscopic analysis to determine the product ratio (**2**:**3**, see **Figure S1**). Subsequent purification via column chromatography using 50/50 CH_2Cl_2/hexanes → neat CH_2Cl_2 as the eluent provided the product. See **Table 1** for product ratios and isolated yields.

Table 1. Product Ratios and Isolated Yields

Substrate	2:3[a]	Average 2:3	Total Isolated Yield	Average Yield
1a (run 1)	--	--	45 mg (56%)	64%
1a (run 2)	--		58 mg (71%)	
1a (run 3)	--		53 mg (65%)	
1b (run 1)	1:2	1:3	52 mg (66%)	62%
1b (run 2)	1:4		53 mg (67%)	
1b (run 3)	1:2		43 mg (54%)	
1c (run 1)	4:1	5:1	44 mg (58%)	62%
1c (run 2)	4:1		46 mg (61%)	
1c (run 3)	5:1		56 mg (74%)	
1c (run 4)	6:1		42 mg (54%)	
1d (run 1)	12:1	17:1	49 mg (67%)	77%
1d (run 2)	20:1		62 mg (85%)	
1d (run 3)	20:1		57 mg (78%)	

[a]Ratio is based on ^{1}H NMR spectral integration of the crude reaction mixture (see **Figure S1**).

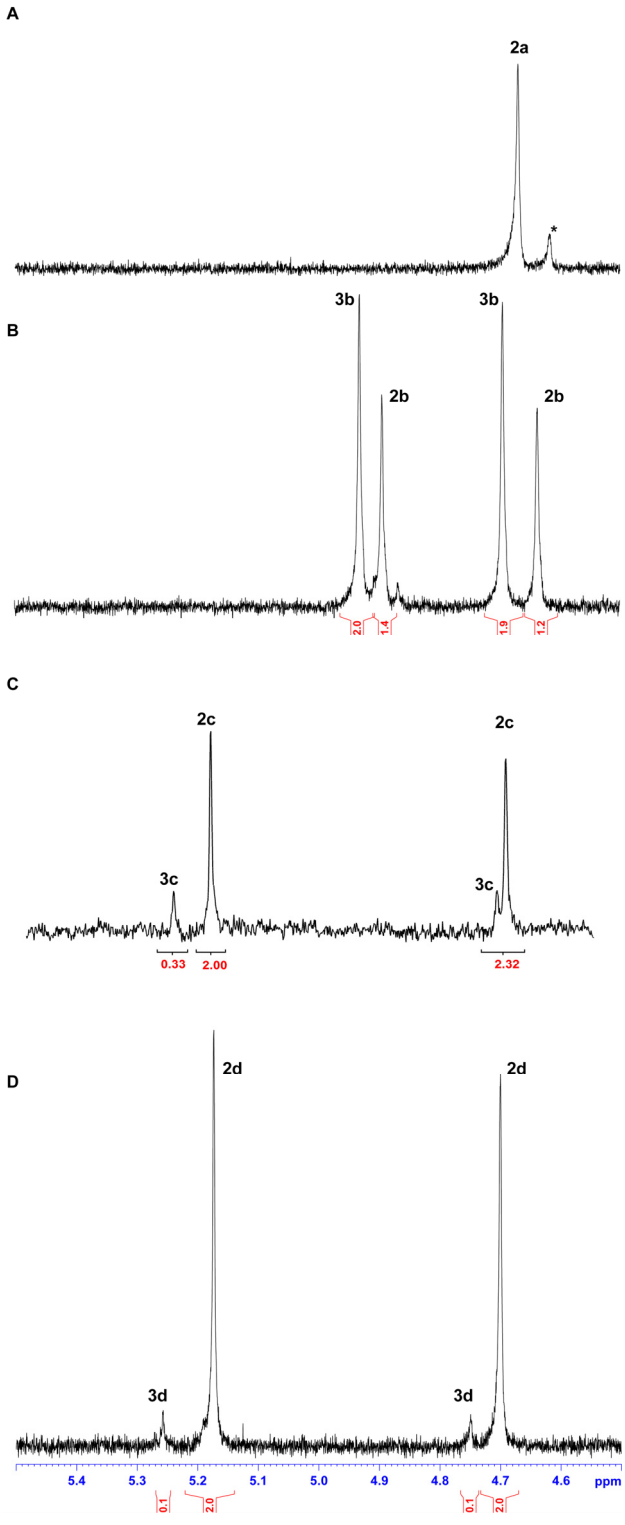
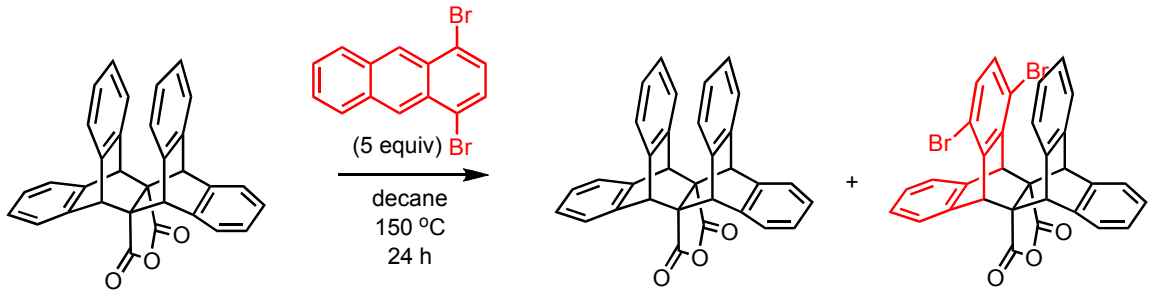


Figure S1. ^{1}H NMR Spectra of the crude reaction mixture from the general procedure. The resonances correspond to the bridgehead protons for products **2** and **3**. (A) R = H; (B) R = Me; (C) R = OMe; (D) R = Br. * denotes an unidentified impurity.

Control Experiment #1



2a **2a** **2d**

In a 20 mL RBF was placed **2a** (12 mg), 1,4-dibromoanthracene (5 equiv), and decane (2 mL). The flask was equipped with a stir bar and an N_2 inlet. The heterogeneous mixture was heated to 150 °C for 24 h. (The reaction becomes homogeneous with heating.) After cooling to room temperature, a sample was taken for ^{1}H NMR spectroscopic analysis to determine the product ratio (**2a**:**2d**). As shown in **Figure S2**, **2d** was not observed, indicating the retro-Diels-Alder reaction is not occurring under the reaction conditions.

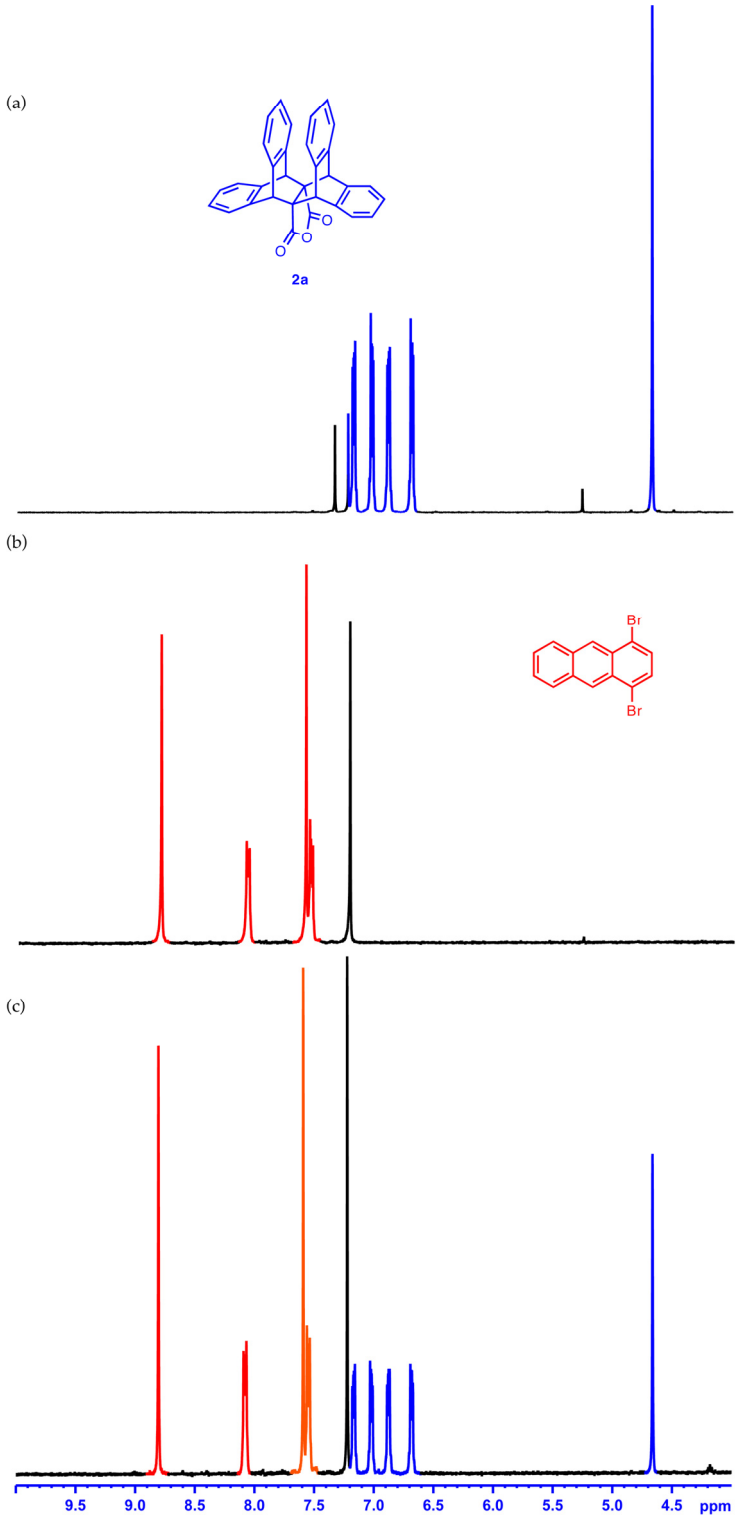
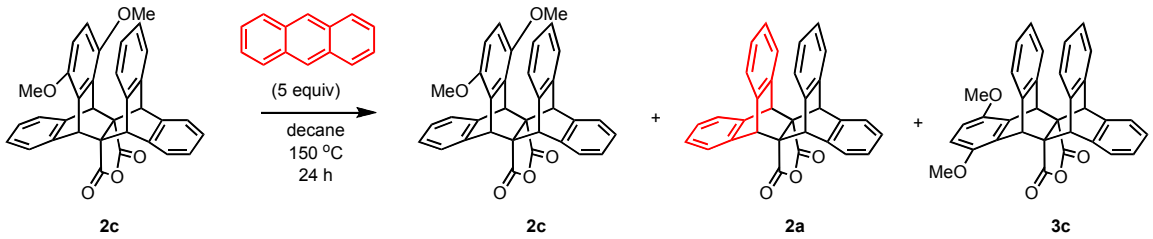


Figure S2. ^{1}H NMR Spectra of (a) **2a**, (b) 1,4-dibromoanthracene, and (c) the crude reaction mixture of **2a** with excess 1,4-dibromoanthracene.

Control Experiment #2



2c **2c** **2a** **3c**

In a 10 mL vial was placed **2c** (15 mg), anthracene (5 equiv), and decane (2 mL). The vial was equipped with a stir bar and sealed. The heterogeneous mixture was heated to 150 °C for 24 h. (The reaction becomes homogeneous with heating.) After cooling to room temperature, a sample was taken for ^{1}H NMR spectroscopic analysis to determine the product ratio (**2c**:**2a**:**3c**). As shown in **Figure S3**, neither **2a** nor **3c** was observed, indicating that a retro-Diels-Alder reaction is not occurring under the reaction conditions.

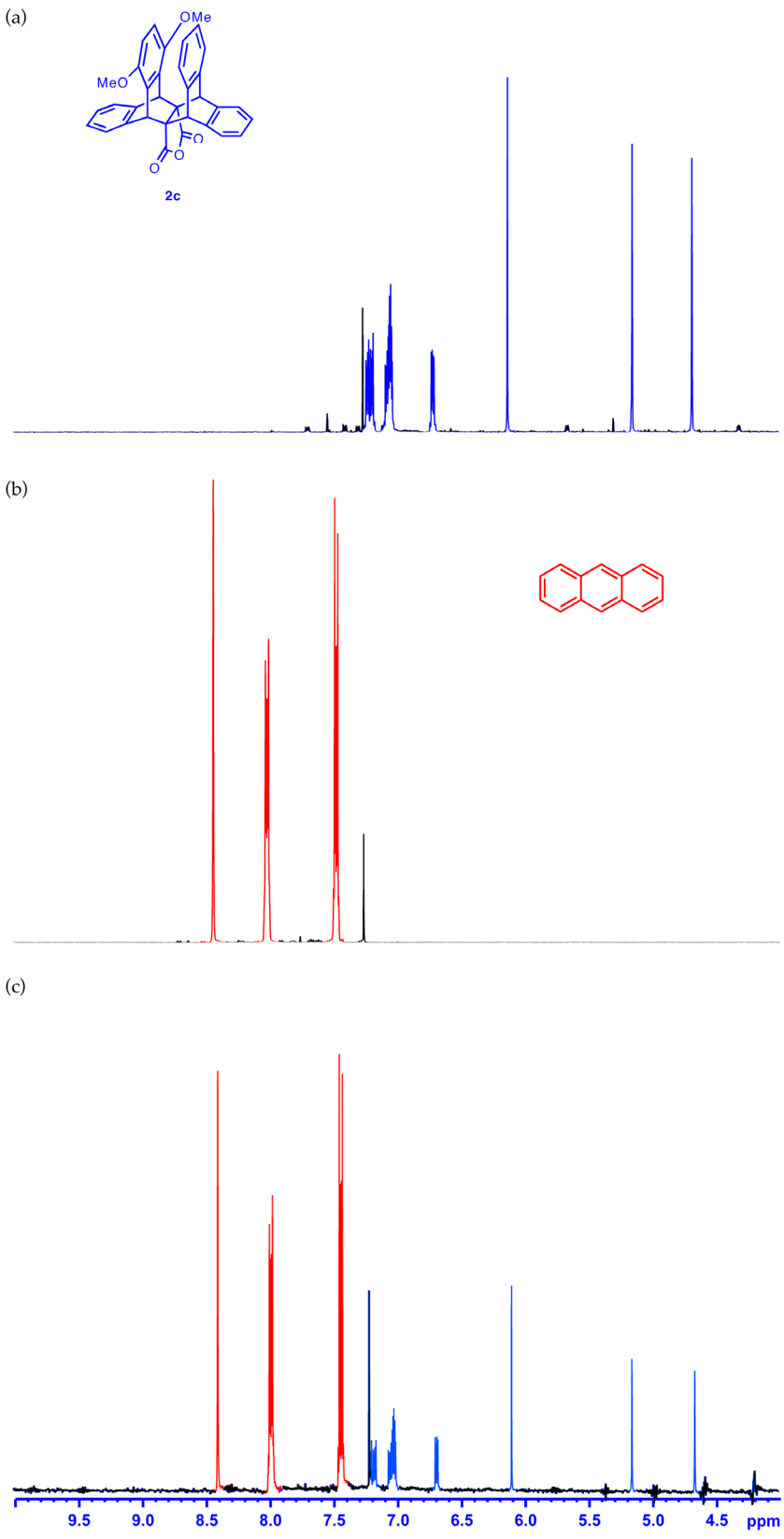
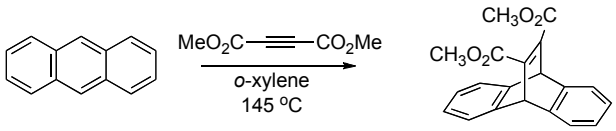


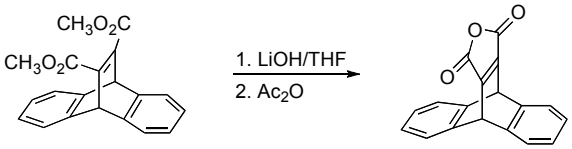
Figure S3. ^{1}H NMR Spectra of (a) **2c**, (b) anthracene, and (c) the crude reaction mixture of **2c** with excess anthracene.

Synthesis of 1a



S1

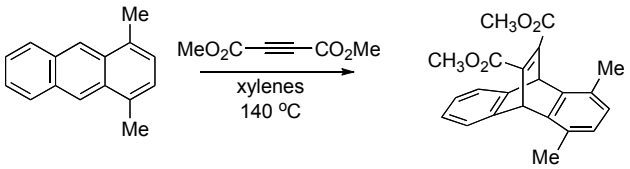
S1: A 100 mL round-bottom flask was equipped with a stir bar, reflux condenser, and an argon inlet. Sequentially, anthracene (1.0 g, 5.6 mmol), dimethylacetylene dicarboxylate (6.9 mL, 56 mmol) and *o*-xylene (15 mL) were added to the flask. The reaction mixture was heated to 145 ^{o}C overnight. After cooling to room temperature, the reaction mixture was concentrated in vacuo and then purified by column chromatography using 50/50 hexanes/CH_2Cl_2 as the eluent to give a sticky off-white solid. MeOH was added to dissolve the excess acetylene and the mixture was filtered to give 1.13 g of pure **S1** as a white, crystalline solid (63% yield). HRMS (ESI): Calcd. for $C_{20}H_{16}O_4$, 343.0941 $[M+Na]^+$; found, 343.0931.



S1 **1a**

1a: A 50 mL round-bottom flask was equipped with a stir bar. Sequentially, lithium hydroxide (0.75 g, 30 mmol), **S1** (1.0 g, 3.0 mmol), THF (15 mL) and water (5 mL) were added to the flask. The heterogeneous mixture was loosely capped and heated to 40 ^{o}C overnight. After cooling to room temperature, EtOAc was added and an aq. HCl solution (10%) until the pH strip indicated the aqueous layer was acidic. The aqueous layer was extracted with EtOAc (3 x 50 mL) and dried over Na_2SO_4. The solution was concentrated in vacuo to produce a sticky solid. Acetic anhydride (~50 mL) was added and the flask was capped and stirred at 60 ^{o}C overnight. After cooling to room temperature, toluene (50 mL) was added and the solution was concentrated in vacuo to yield an off-white solid. Hexanes were added and the mixture was filtered to give a white precipitate (0.55 g, 66% yield). HRMS (ESI): Calcd. for $C_{18}H_{10}O_3$, 275.0703 $[M+H]^+$; found, 275.0699.

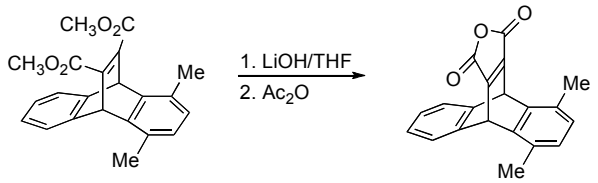
Synthesis of 1b



S2

1,4-dimethylanthracene was prepared according to a literature procedure.[7]

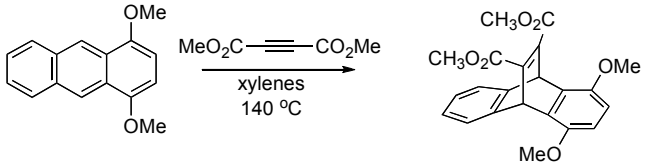
S2: A 75 mL bomb flask was equipped with a stir bar. Sequentially, 1,4-dimethylanthracene (0.75 g, 3.6 mmol), dimethylacetylene dicarboxylate (4.5 mL, 36 mmol) and *o*-xylene (6 mL) were added to the flask. The reaction mixture was heated to 140 °C overnight. After cooling to room temperature, the reaction mixture was concentrated in vacuo and then purified by column chromatography using 50/50 hexanes/CH_2Cl_2 → neat CH_2Cl_2 as the eluent to give a sticky off-white solid. MeOH was added to dissolve the excess acetylene and the mixture was filtered to give 0.67 g of pure **S2** as an off-white, crystalline solid (54% yield). HRMS (ESI): Calcd. for $C_{22}H_{20}O_4$, 371.1254 $[M+Na]^+$; found, 371.1256.



S2 **1b**

1b: A 50 mL round-bottom flask was equipped with a stir bar. Sequentially, lithium hydroxide (0.46 g, 19 mmol), **S2** (0.67 g, 1.9 mmol), THF (10 mL) and water (5 mL) were added to the flask. The heterogeneous mixture was loosely capped and heated to 40 °C overnight. After cooling to room temperature, EtOAc was added and an aq. HCl solution (10%) until the pH strip indicated the aqueous layer was acidic. The aqueous layer was extracted with EtOAc (3 x 50 mL) and dried over Na_2SO_4. The solution was concentrated in vacuo to produce an oil. Acetic anhydride (~50 mL) was added and the flask was capped and stirred at 60 °C overnight. After cooling to room temperature, toluene (50 mL) was added and the solution was concentrated in vacuo to yield an light yellow solid. Hexanes were added and the mixture was filtered to give a light yellow precipitate (0.44 g, 67% yield). HRMS (ESI): Calcd. for $C_{20}H_{14}O_3$, 303.1016 $[M+H]^+$; found, 303.1012.

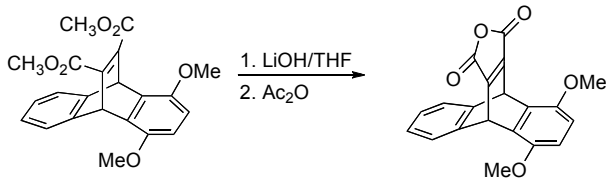
Synthesis of 1c



S3

1,4-dimethoxyanthracene was synthesized according to literature protocol.[8]

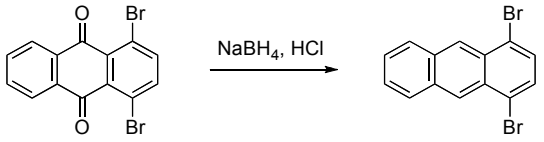
S3: A 50 mL round-bottom flask was equipped with a stir bar and reflux condensor. Sequentially, 1,4-dimethoxyanthracene (0.69 g, 2.9 mmol), dimethylacetylene dicarboxylate (3.5 mL, 29 mmol) and *o*-xylene (10 mL) were added to the flask. The reaction mixture was heated to 140 °C overnight. After cooling to room temperature, the reaction mixture was concentrated in vacuo and then purified by column chromatography using 50/50 hexanes/CH_2Cl_2 → neat CH_2Cl_2 as the eluent to give a yellow solid. MeOH was added to dissolve the excess acetylene and the mixture was filtered to give 307 mg of pure **S3** as a yellow crystalline solid (28% yield). HRMS (ESI): Calcd. for $C_{22}H_{20}O_6$, 381.1333 $[M+H]^+$; found, 381.1344.



S3 **1c**

1c: A 50 mL round-bottom flask was equipped with a stir bar. Sequentially, lithium hydroxide (0.19 g, 8.1 mmol), **S3** (0.31 g, 0.81 mmol), THF (10 mL) and water (5 mL) were added to the flask. The heterogeneous mixture was loosely capped and heated to 40 °C overnight. After cooling to room temperature, EtOAc was added and an aq. HCl solution (10%) until the pH strip indicated the aqueous layer was acidic. The aqueous layer was extracted with EtOAc (3 x 50 mL) and dried over Na_2SO_4. The solution was concentrated in vacuo to produce a yellow solid. Acetic anhydride (~40 mL) was added and the flask was capped and stirred at 60 °C overnight. After cooling to room temperature, toluene (50 mL) was added and the solution was concentrated in vacuo to yield a bright yellow solid (0.27 g, 99% yield). HRMS (ESI): Calcd. for $C_{20}H_{14}O_5$, 335.0914 $[M+H]^+$; found, 335.0923.

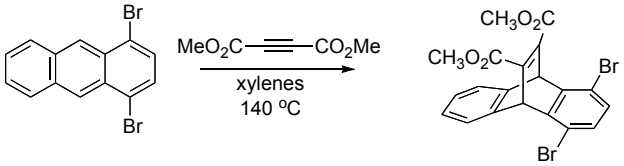
Synthesis of 1d



S4

1,4-dibromoanthraquinone was synthesized via literature procedure.[9]

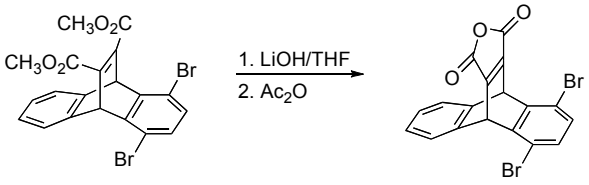
S4: A 25 mL round-bottom flask was equipped with a stir bar. Sequentially, 1,4-dibromoanthraquinone (0.50 g, 1.4 mmol), $NaBH_4$ (0.212 g, 5.6 mmol), and *i*-PrOH (5 mL) were added to the flask. The heterogeneous mixture was capped and stirred at rt overnight. The mixture was poured into ice-water and filtered. The solid was placed in a 100 mL round-bottom flask and 3M HCl (20 mL) was added and the mixture was heated at 75 ^{o}C overnight. The solid was collected via filtration and placed in a 25 mL round-bottom flask. $NaBH_4$ (0.33 g, 8.6 mmol) and *i*-PrOH (10 mL) were added and the mixture was heated to reflux overnight. 3 M HCl was then added until bubbling ceased and the solid was collected via filtration. The product was purified by column chromatography using 80/20 hexanes/CH_2Cl_2 as the eluent to give a yellow, fluffy solid (0.21 g, 42% yield).



S4 **S5**

S5: A 75 mL bomb flask was equipped with a stir bar. Sequentially, **S4** (236 mg, 0.78 mmol), dimethylacetylene dicarboxylate (0.96 mL, 7.8 mmol) and *o*-xylene (10 mL) were added to the flask. The reaction mixture was heated to 145 ^{o}C overnight. After cooling to room temperature, the reaction mixture was concentrated in vacuo and then purified by column chromatography using 50/50 hexanes/CH_2Cl_2

neat CH_2Cl_2 as the eluent to give an oil. MeOH/CH_2Cl_2 (50 mL) was added and subsequent concentration led to a sticky solid. MeOH was added to dissolve the excess acetylene and the mixture was filtered to give 225 mg of pure **S5** as an off-white solid (61% yield). HRMS (ESI): Calcd. for $C_{20}H_{14}Br_2O_4$, 498.9151 $[M+Na]^+$; found, 498.9167.



S5 **1d**

1d: A 50 mL round-bottom flask was equipped with a stir bar. Sequentially, lithium hydroxide (100 mg, 4.2 mmol), **S5** (200 mg, 0.42 mmol), THF (5 mL) and water (5 mL) were added to the flask. The heterogeneous mixture was loosely capped and heated to 40 ^{o}C overnight. After cooling to room temperature, EtOAc was added and an aq. HCl solution (10%) until the pH strip indicated the aqueous layer was acidic. The aqueous layer was extracted with EtOAc (3 x 50 mL) and dried over Na_2SO_4. The solution was concentrated in vacuo to produce a sticky solid. Acetic anhydride (~15 mL) was added and the flask was capped and stirred at 60 ^{o}C overnight. After cooling to room temperature, toluene (50 mL) was added and the solution was concentrated in vacuo to yield an off-white solid. Hexanes were added and the mixture was filtered to give a white precipitate (114 mg, 63% yield). HRMS (ESI): Calcd. for $C_{18}H_8Br_2O_3$, 430.8913 $[M+H]^+$; found, 430.8907.

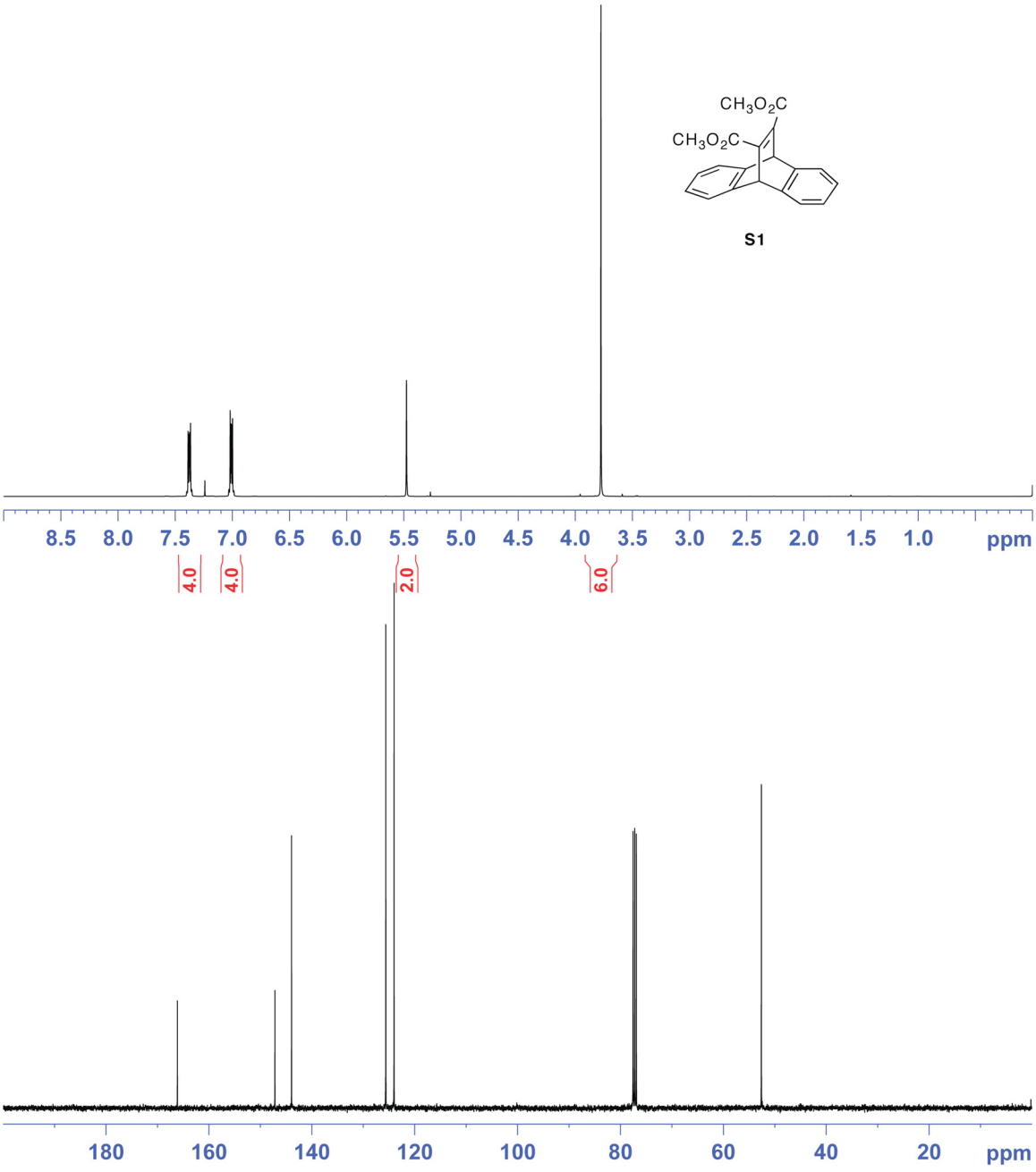


Figure S4. ^{1}H and ^{13}C NMR spectra of **S1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (m, 4H), 7.01 (m, 4H), 5.48 (s, 2H), 3.77 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.12, 147.17, 143.93, 125.61, 124.01, 52.61, 52.60.

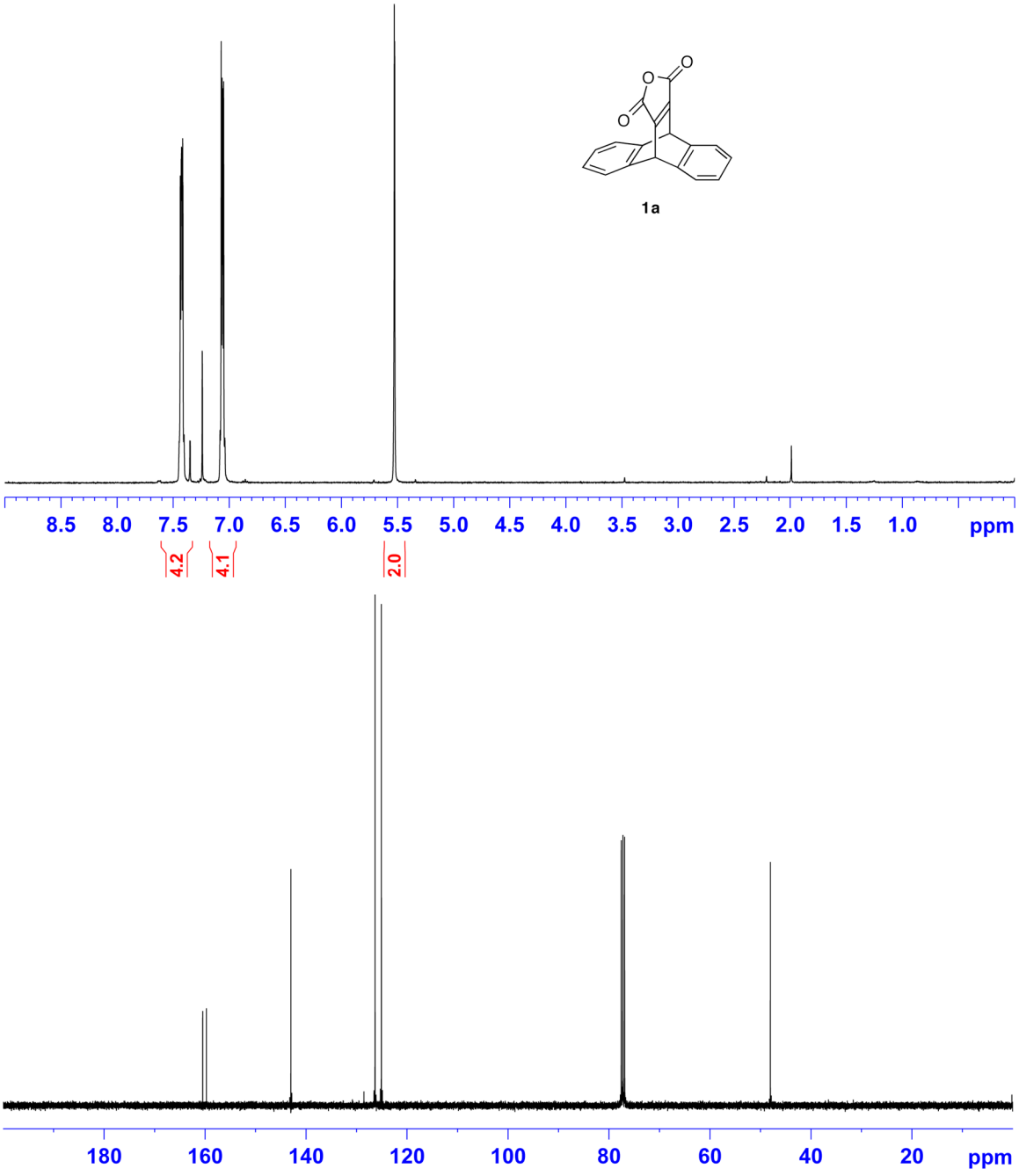


Figure S5. ^{1}H and ^{13}C NMR spectra of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (m, 4H), 7.06 (m, 4H), 5.53 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.45, 159.71, 143.01, 126.33, 125.08, 48.03.

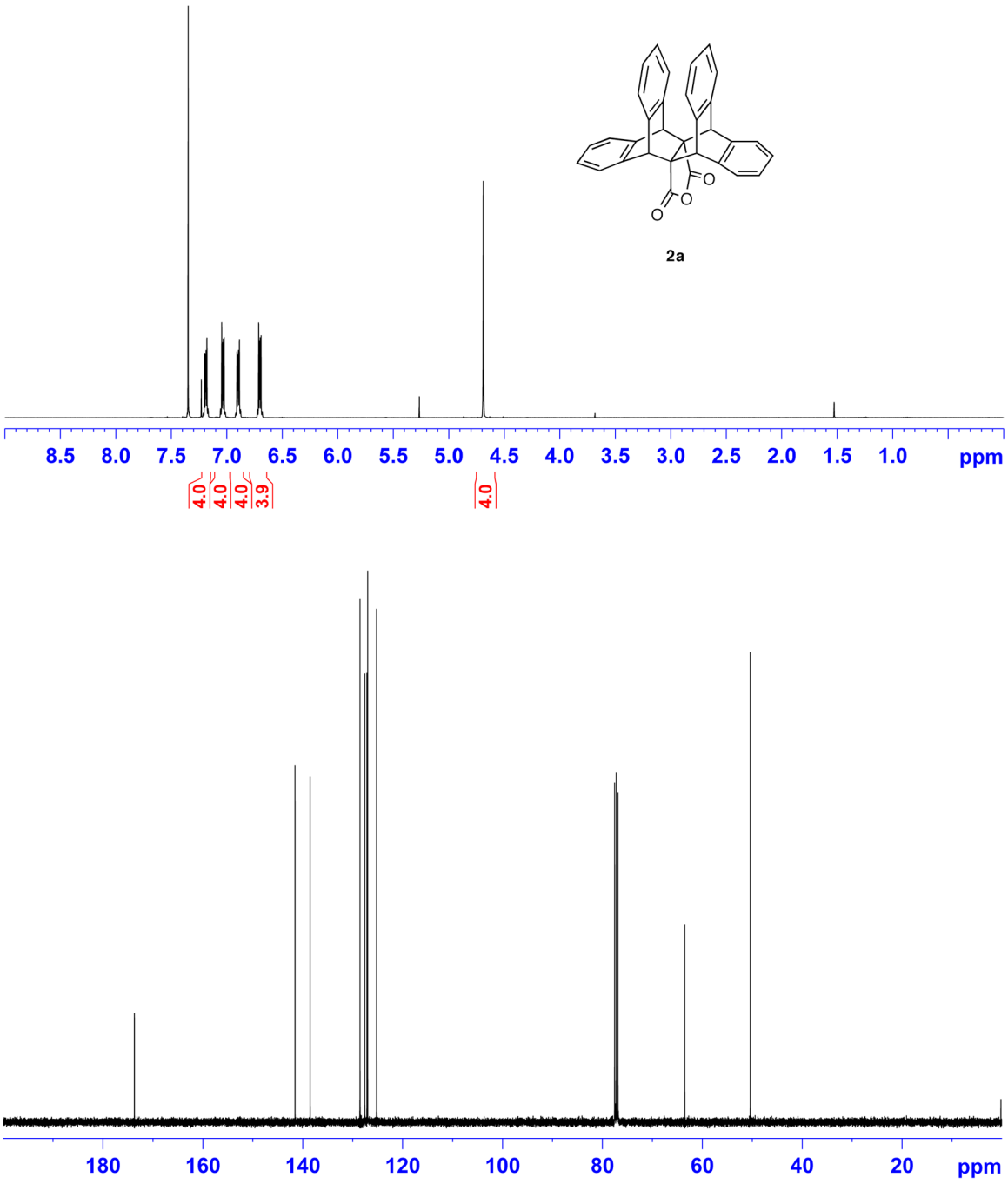


Figure S6. ^{1}H and ^{13}C NMR spectra of **2a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (m, 4H), 7.04 (m, 4H), 6.89 (m, 4H), 6.70 (m, 4H), 4.69 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.68, 141.54, 138.51, 128.53, 127.59, 127.14, 126.98, 125.20, 63.51, 50.38.

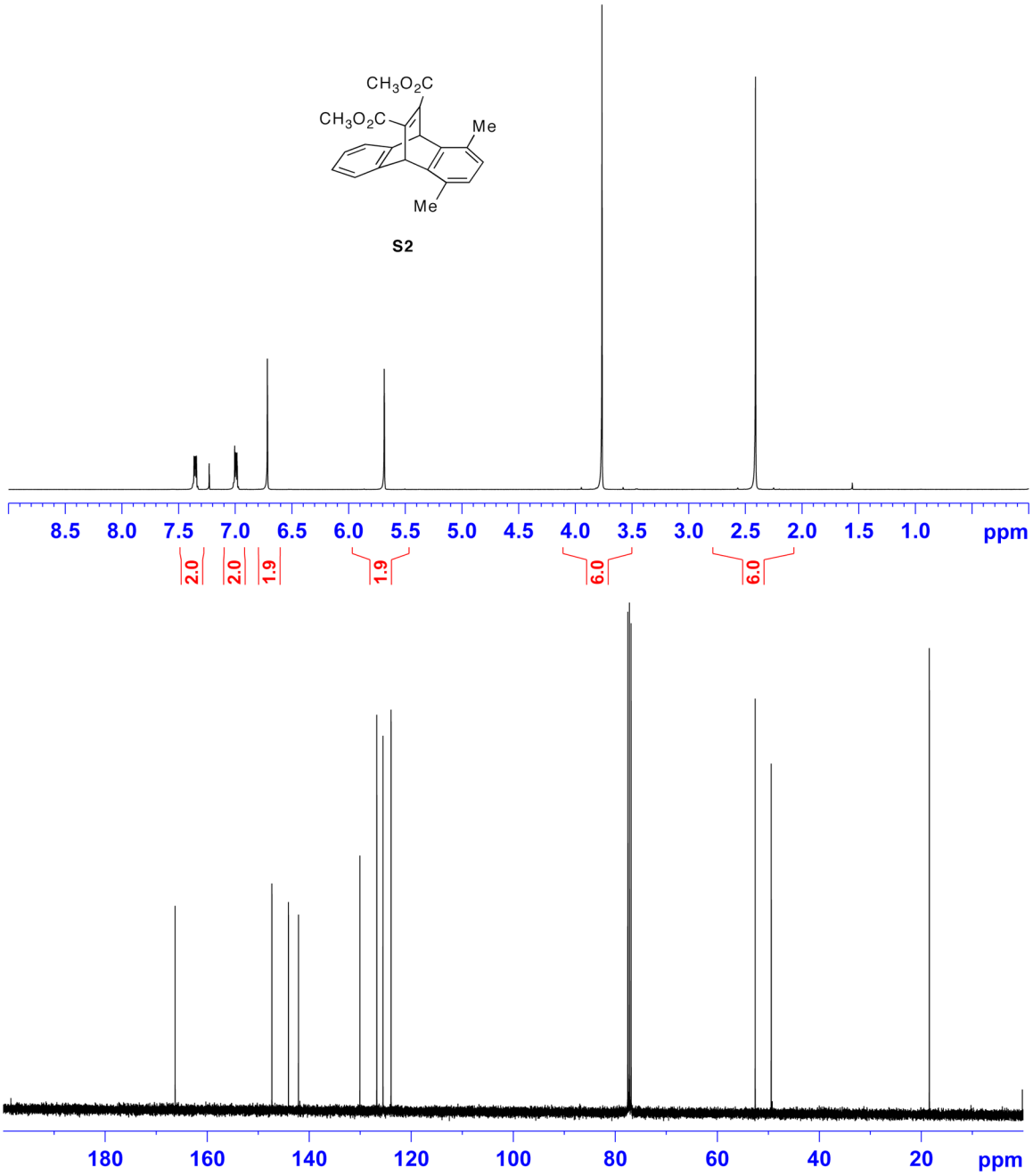


Figure S7. ^{1}H and ^{13}C NMR spectra of **S2**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (m, 2H), 6.99 (m, 2H), 6.71 (s, 2H), 5.68 (s, 2H), 3.77 (s, 6H), 2.41 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.27, 147.30, 144.06, 142.09, 130.06, 126.75, 125.53, 123.95, 52.56, 49.43, 18.41.

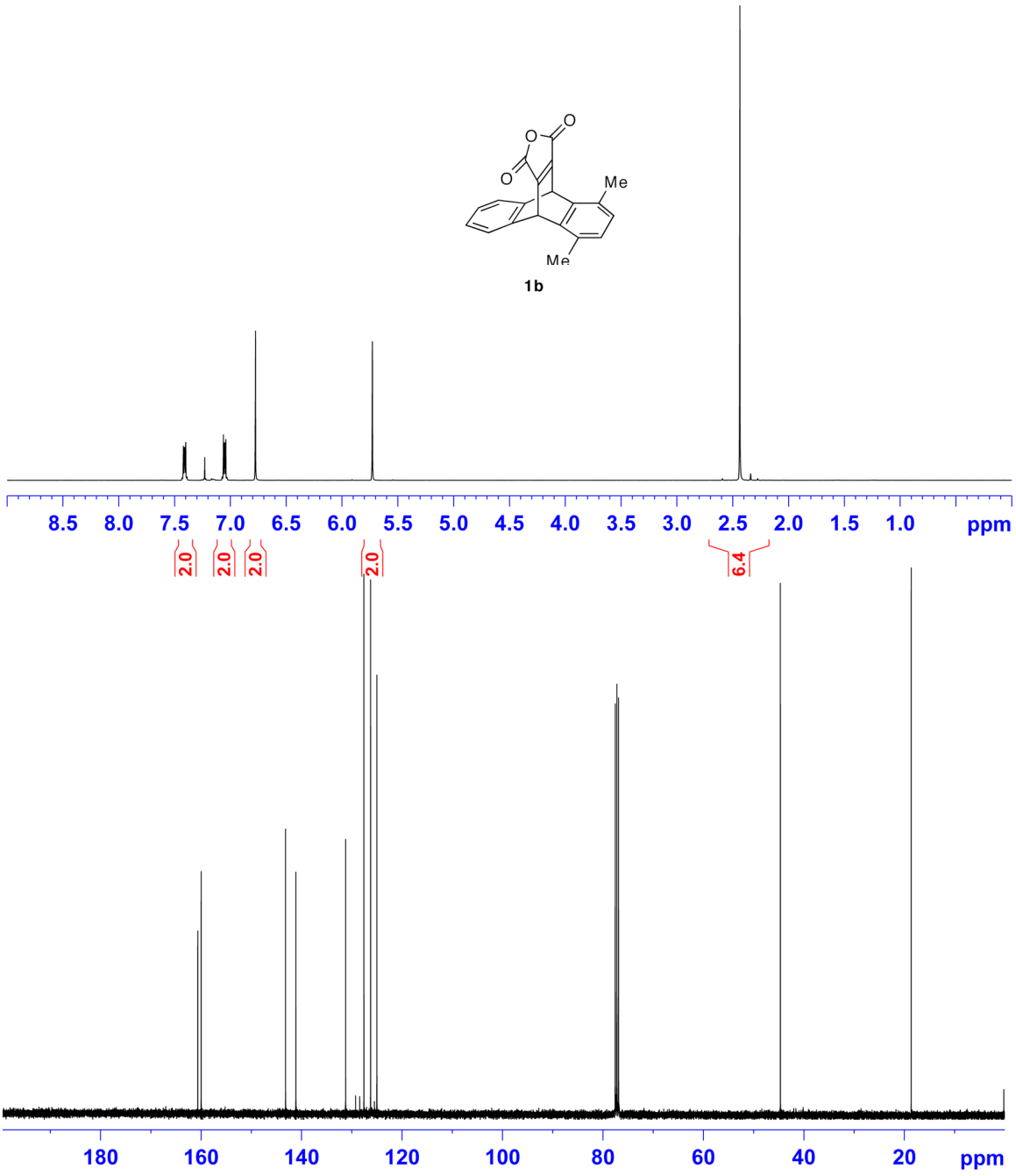


Figure S8. ^{1}H and ^{13}C NMR spectra of **1b**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (m, 2H), 7.05 (m, 2H), 6.77 (S, 2H), 5.73 (s, 2H), 2.44 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.65, 159.97, 143.41, 141.13, 131.22, 127.58, 126.24, 124.99, 44.68, 18.63.

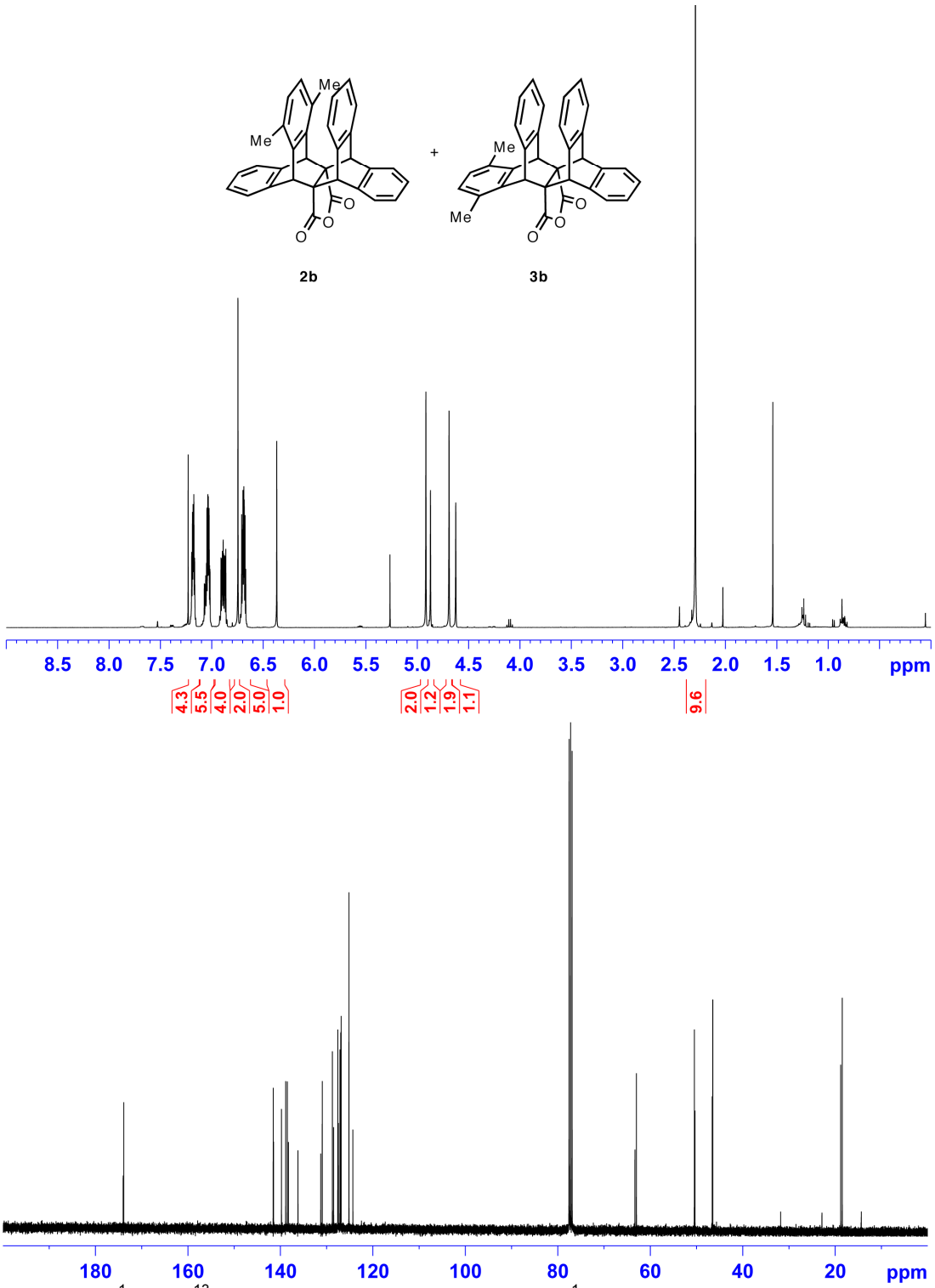


Figure S9. ^{1}H and ^{13}C NMR spectra of **2b/3b** (1/2 ratio). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (m, 2H, 2H), 7.04 (m, 4H, 1H), 6.89 (m 2H, 2H), 6.70 (s, 2H), 6.69 (m, 4H, 1H), 6.37 (s, 1H), 4.91 (s, 2H), 4.87 (s, 1H), 4.69 (s, 2H), 4.62 (s, 1H), 2.29 (s, 6H, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.99, 173.88, 141.56, 141.54, 141.53, 141.48, 139.76, 138.85, 138.49, 138.25, 136.19, 131.27, 130.93, 128.74, 128.49, 127.58, 127.53, 127.45, 127.11, 126.98, 126.95, 126.85, 125.17, 124.31, 63.31, 62.98, 50.45, 50.32, 46.58, 46.48, 18.81, 18.47.

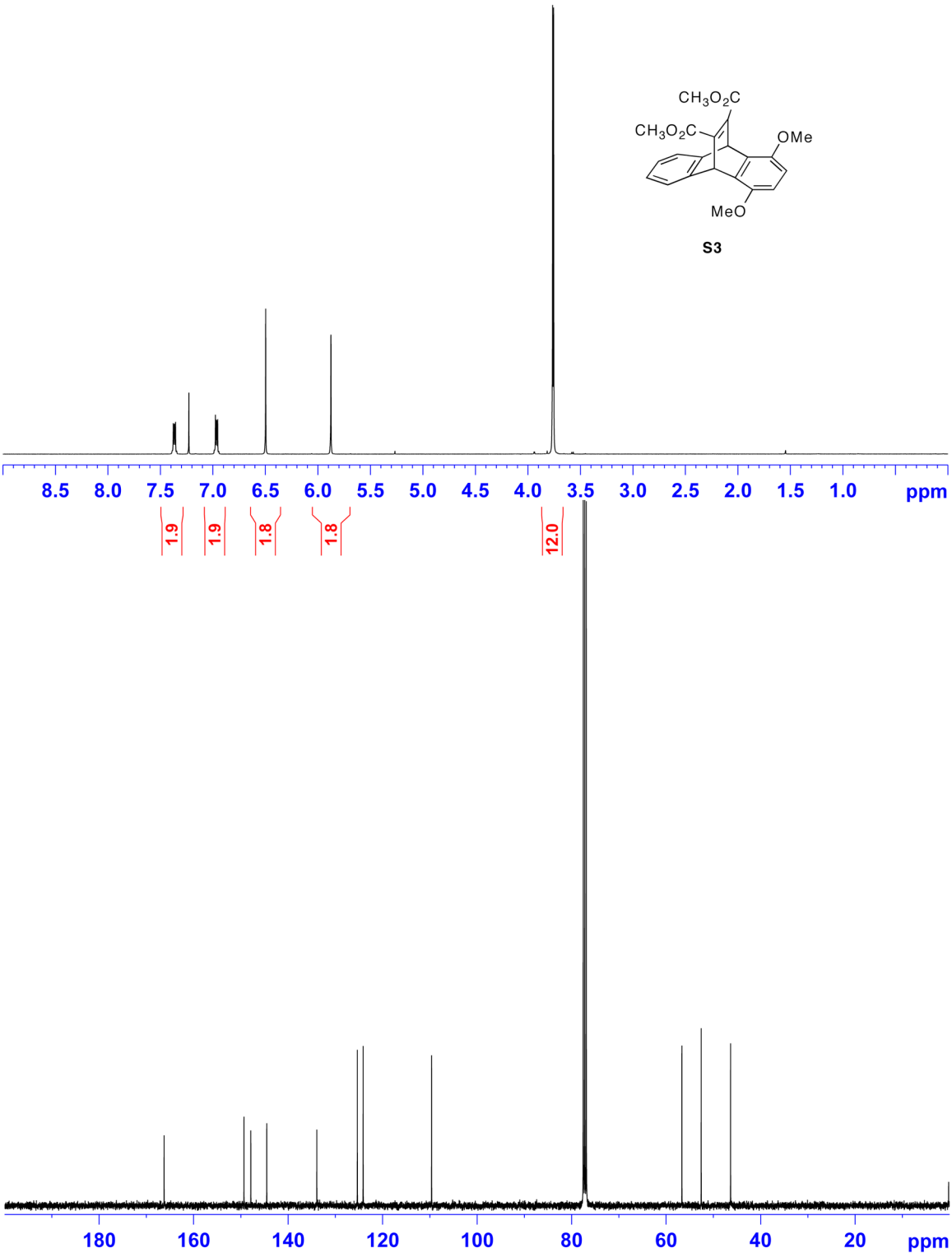


Figure S10. ^{1}H and ^{13}C NMR spectra of **S3**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (m, 2H), 6.96 (m, 2H), 6.50 (s, 2H), 5.88 (s, 2H), 3.76 (s, 6H), 3.75 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.23, 149.34, 147.88, 144.50, 133.91, 125.33, 124.11, 109.63, 56.65, 52.56, 46.34.

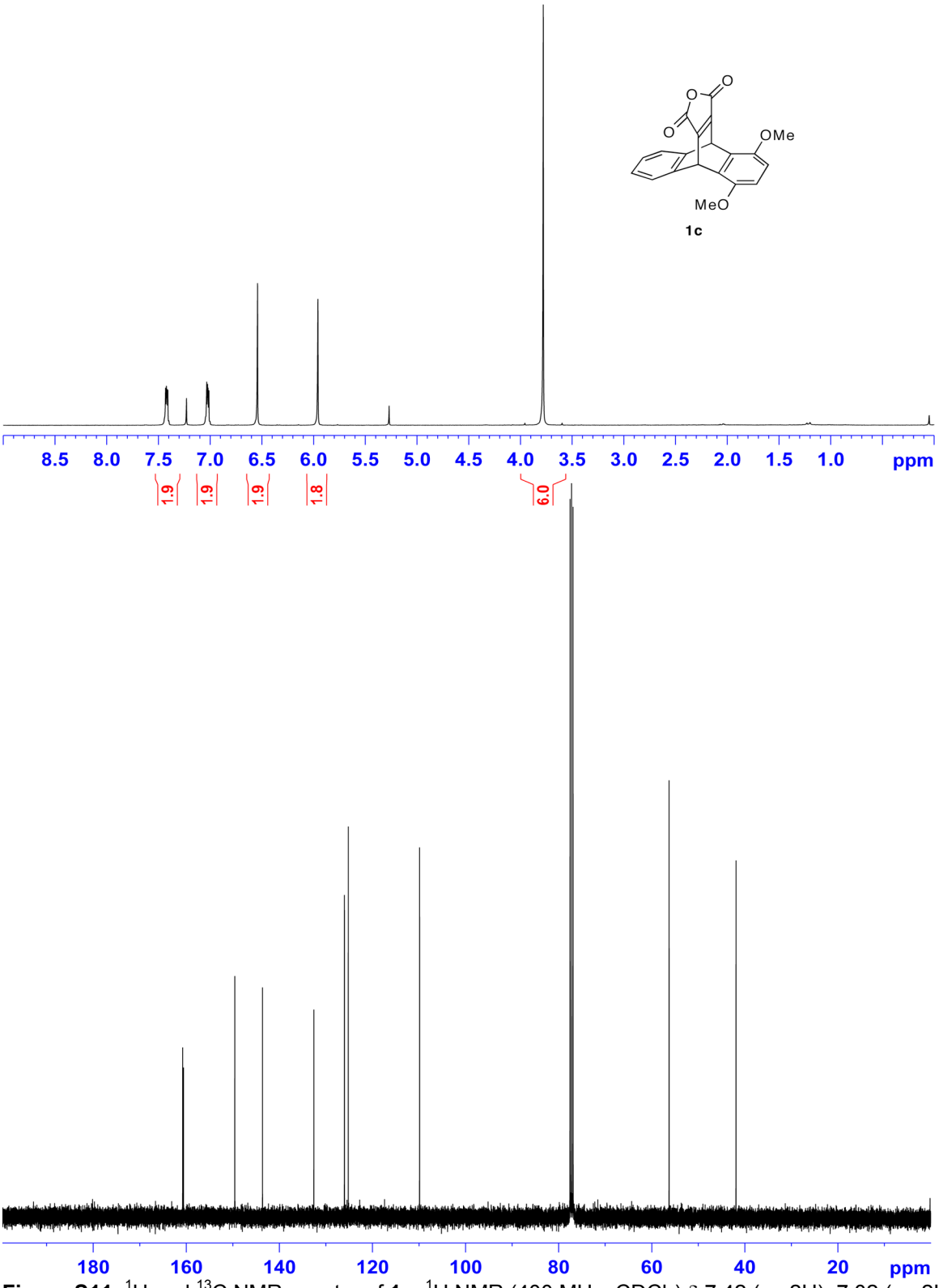


Figure S11. ^{1}H and ^{13}C NMR spectra of **1c**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (m, 2H), 7.02 (m, 2H), 6.54 (s, 2H), 5.96 (s, 2H), 3.78 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.77, 160.57, 149.57, 143.61, 132.59, 126.01, 125.19, 109.87, 56.27, 41.88.

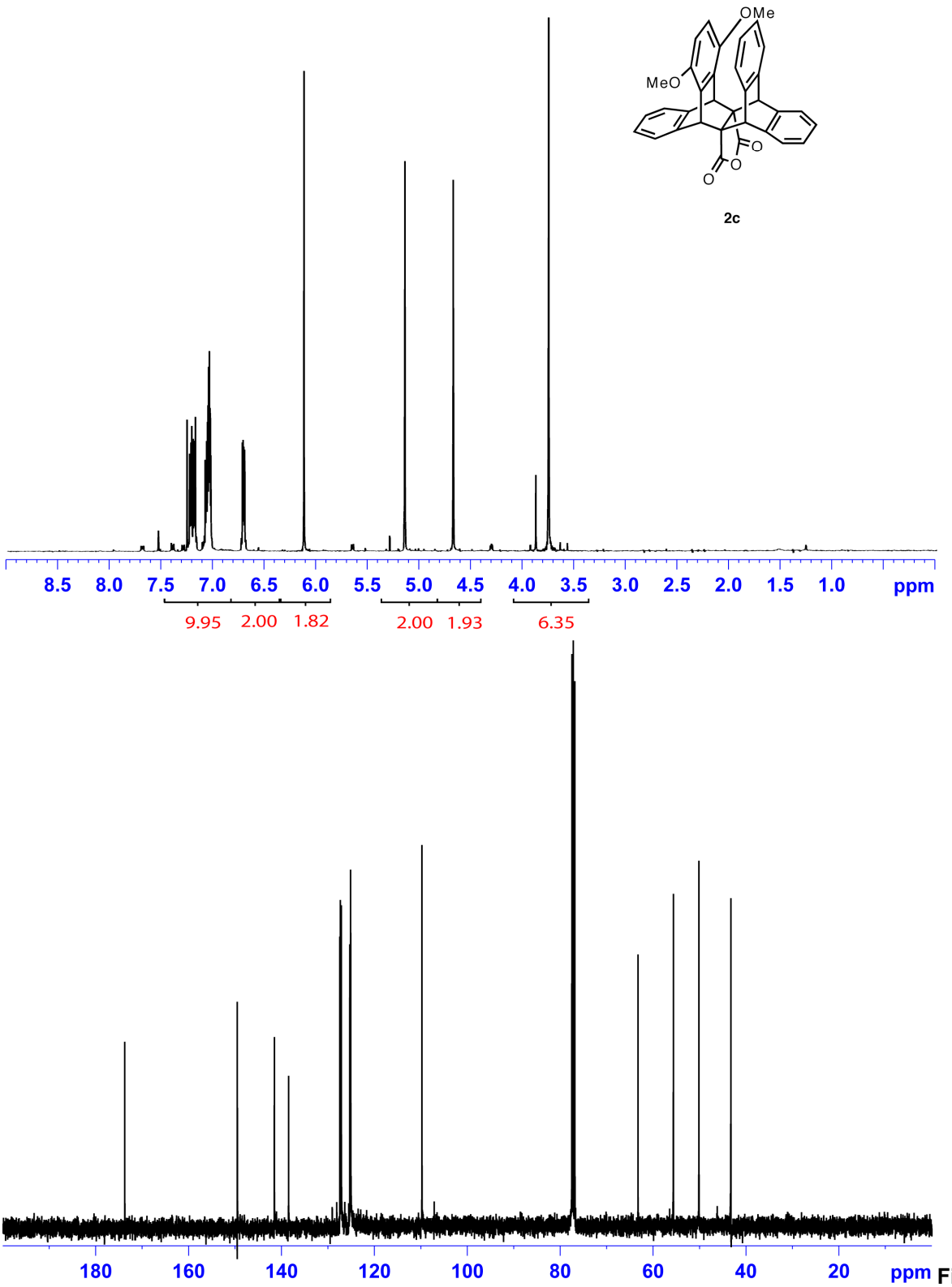


Figure S12. ^{1}H and ^{13}C NMR spectra of **2c**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (m, 4H), 7.06 (m, 6H), 6.72 (m, 2H), 6.13 (s, 2H), 5.15 (s, 2H), 4.68 (s, 2H), 3.76 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.80, 149.57, 141.62, 141.59, 138.55, 127.51, 127.47, 127.40, 127.18, 125.37, 125.20, 125.14, 109.83, 63.30, 55.69, 50.19, 43.31.

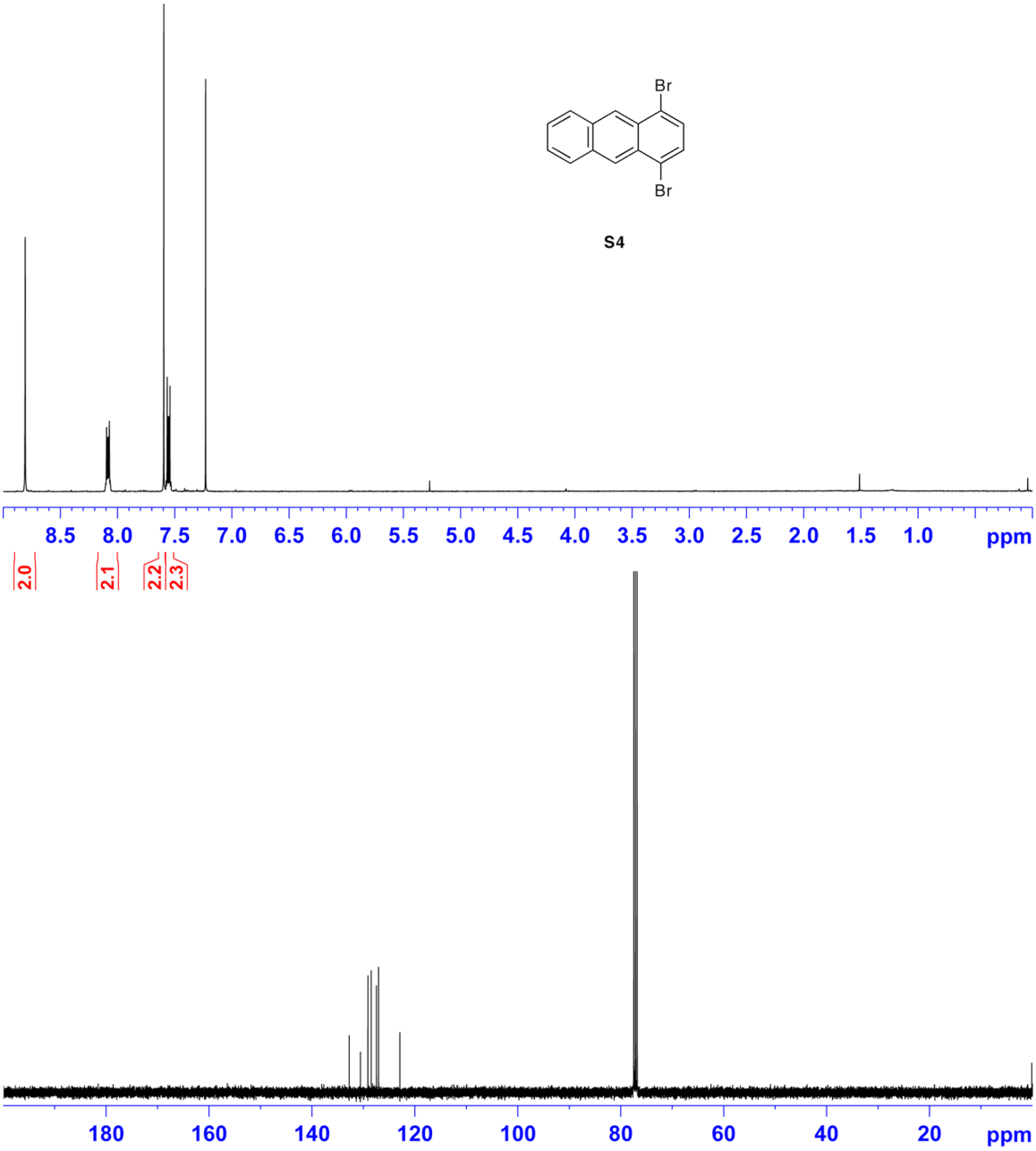


Figure S13. ^{1}H and ^{13}C NMR spectra of **S4**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (s, 2H), 8.08 (m, 2H), 7.59 (s, 2H), 7.55 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.80, 130.62, 129.16, 128.53, 127.50, 127.10, 122.94.

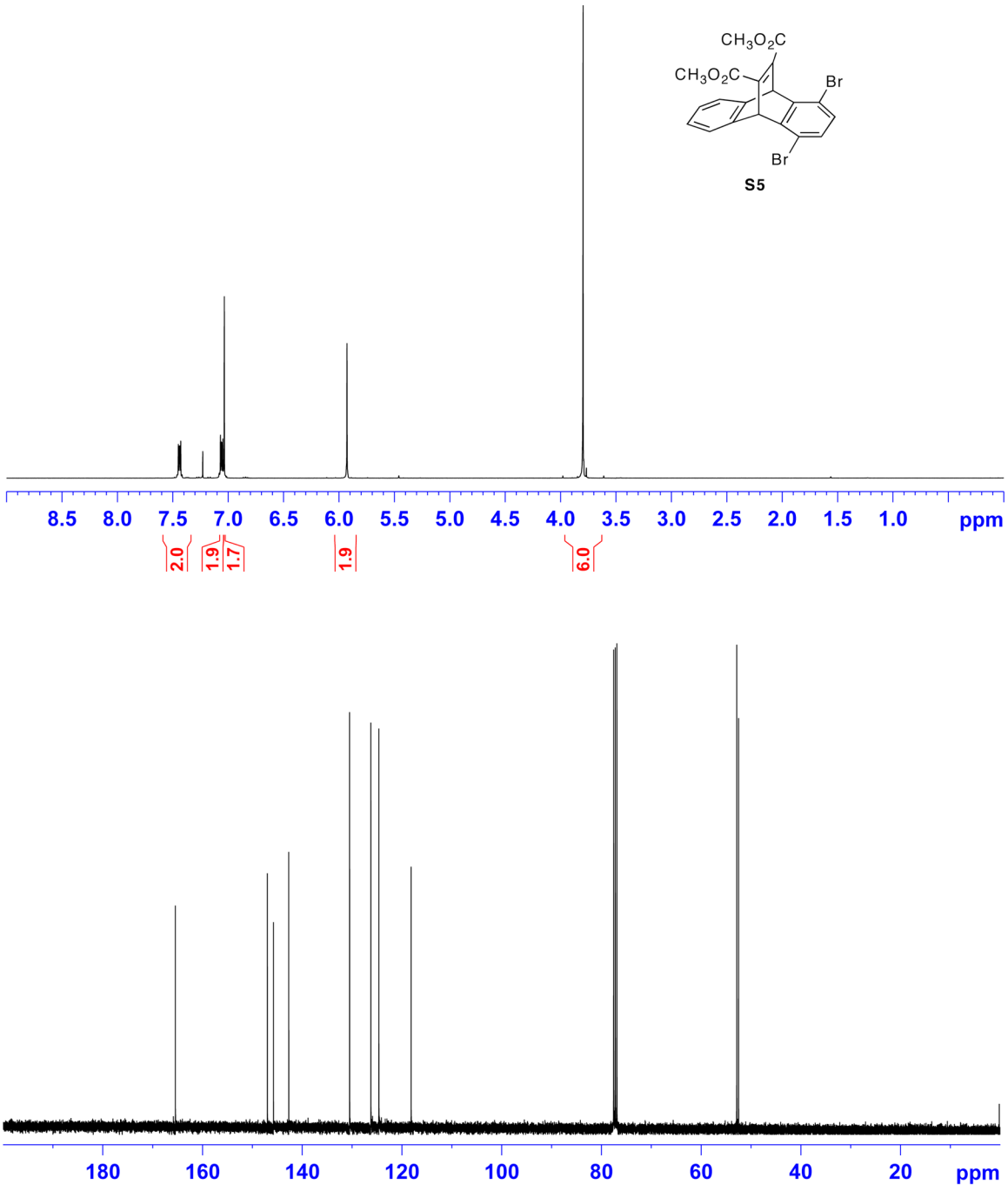


Figure S14. ^{1}H and ^{13}C NMR spectra of **S5**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (m, 2H), 7.06 (m, 2H), 7.03 (s, 2H), 5.93 (s, 2H), 3.80 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.43, 146.99, 145.77, 142.70, 130.49, 126.23, 124.63, 118.15, 52.84, 52.49.

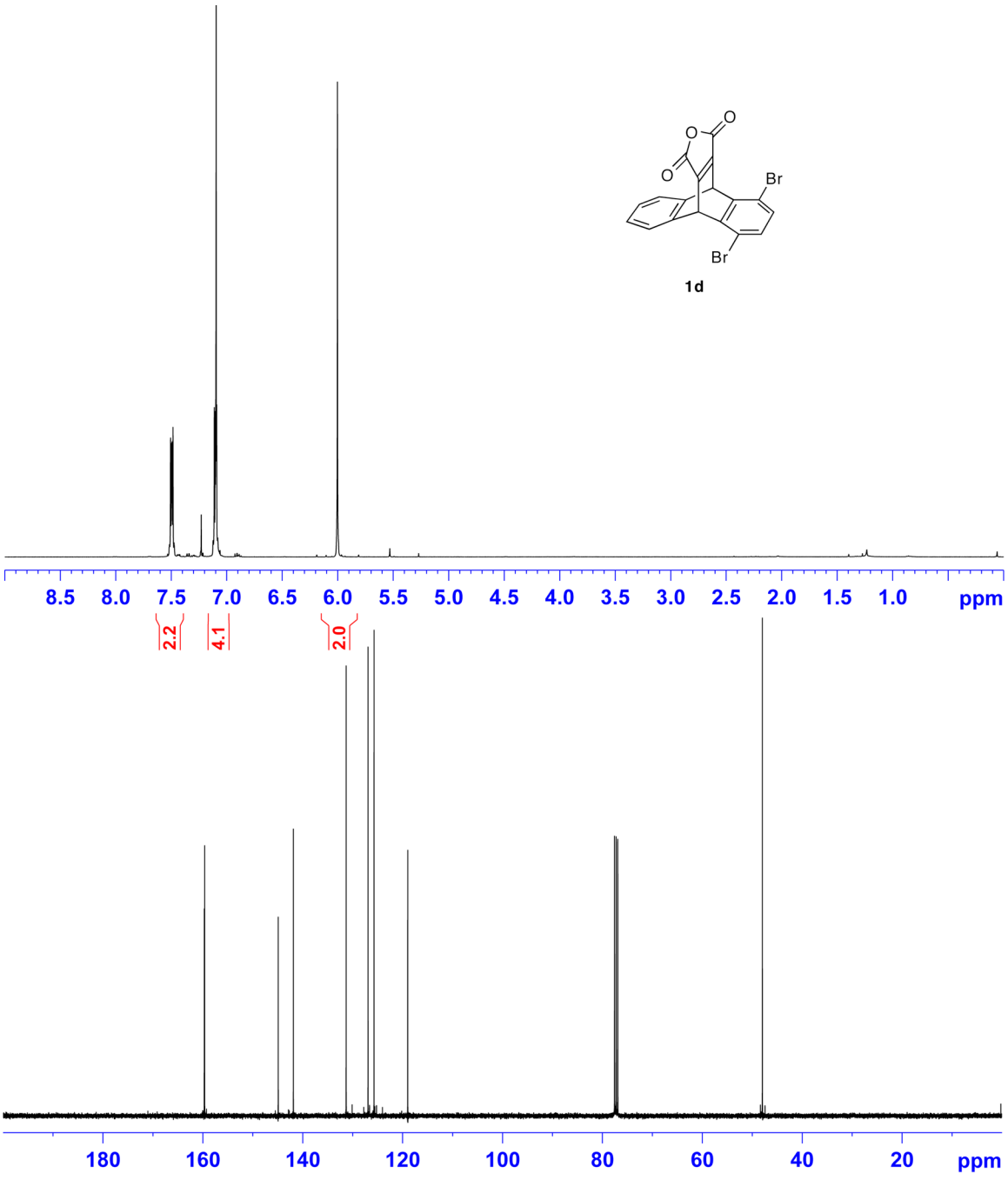


Figure S15. ^{1}H and ^{13}C NMR spectra of **1d**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (m, 2H), 7.10 (m, 2H), 7.09 (s, 2H), 6.00 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.71, 159.63, 144.90, 141.88, 131.31, 126.92, 125.72, 118.97, 47.97.

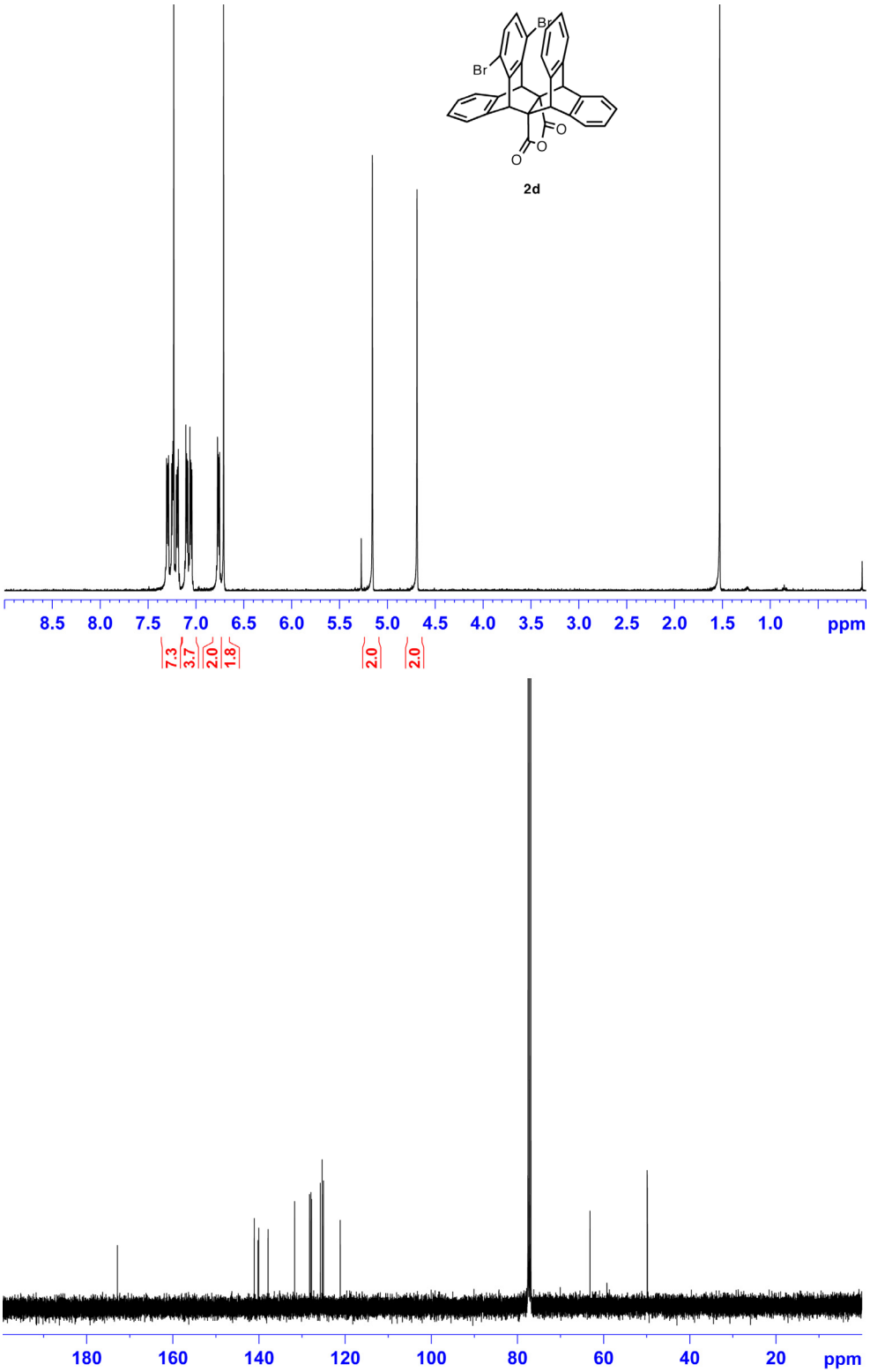


Figure S16. ^{1}H and ^{13}C NMR spectra of **2d**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.19 (m, 6H), 7.09-7.05 (m, 4H), 6.76 (m, 2H), 6.71 (s, 2H), 5.16 (s, 2H), 4.69 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.86, 141.08, 140.22, 140.06, 137.88, 131.73, 128.25, 127.93, 127.81, 125.74, 125.31, 125.02, 121.14, 63.14, 49.89, 49.83.

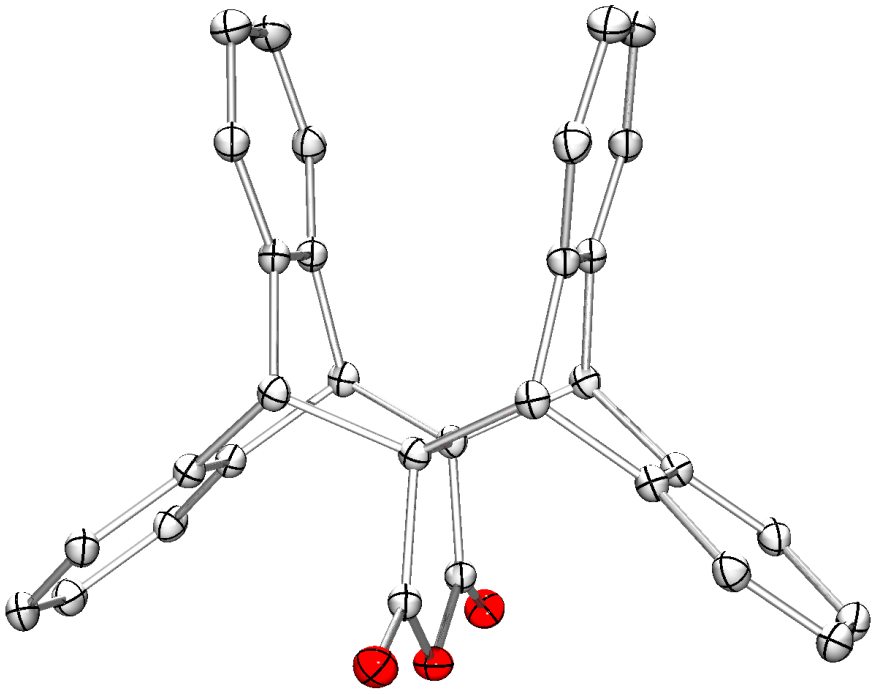


Figure S17. Crystal Structure of **2a**.

Table S2. Summary of Bond Distances and Angles for **2a**.

centroid distance	3.51 Å
angle between the planes of rings	22.20 ± 0.05
shortest C-C arene-arene distance	3.048 Å
middle C-C arene-arene distance	3.514 Å
longest C-C arene-arene distance	3.972 Å

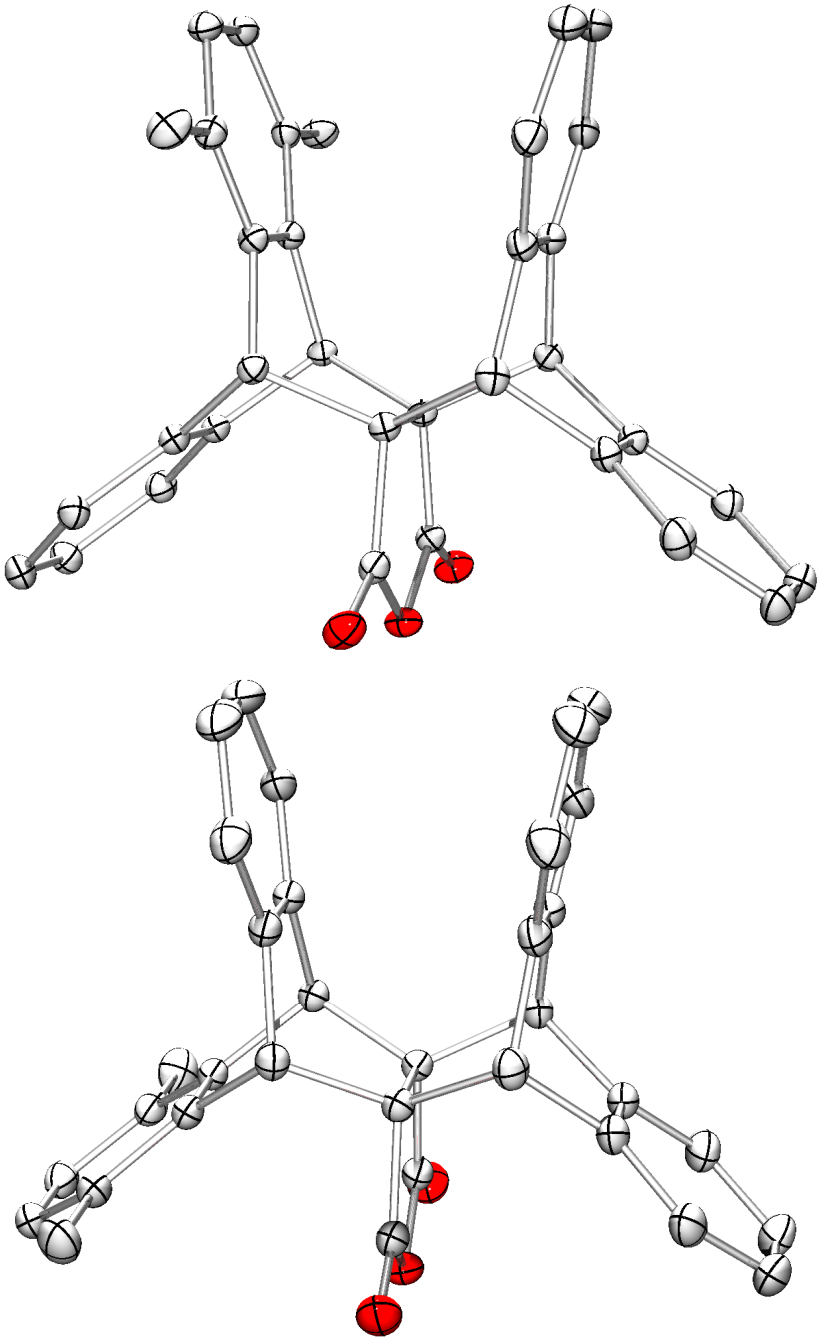


Figure S18. Crystal Structures of **2b** (top) and **3b** (bottom).

Table S3. Summary of Bond Distances and Angles for **2b and 3b**.

	2b	**3b**
centroid distance	3.54 Å	3.48 Å
angle between the planes of rings	24.97 ± 0.06	21.40 ± 0.05
shortest C-C arene-arene distance	3.036 Å	3.027 Å
middle C-C arene-arene distance	3.538 Å	3.452 Å
longest C-C arene-arene distance	4.074 Å	3.913 Å

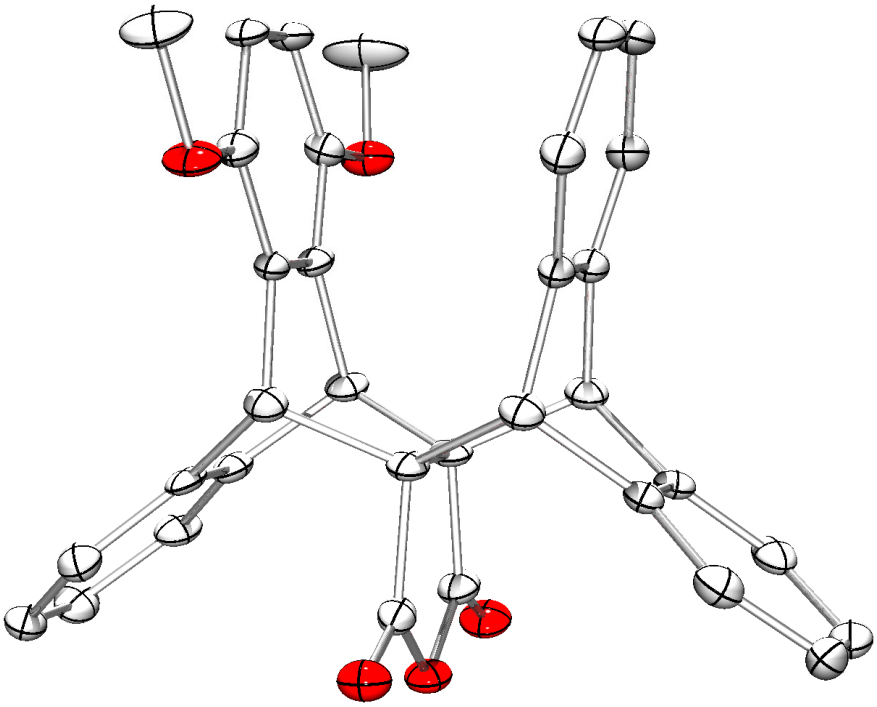


Figure S19. Crystal Structure of **2c**.

Table S4. Summary of Bond Distances and Angles for **2c**.

centroid distance	3.38 Å
angle between the planes of rings	17.26 ± 0.08
shortest C-C arene-arene distance	3.023 Å
middle C-C arene-arene distance	3.380 Å
longest C-C arene-arene distance	3.739 Å

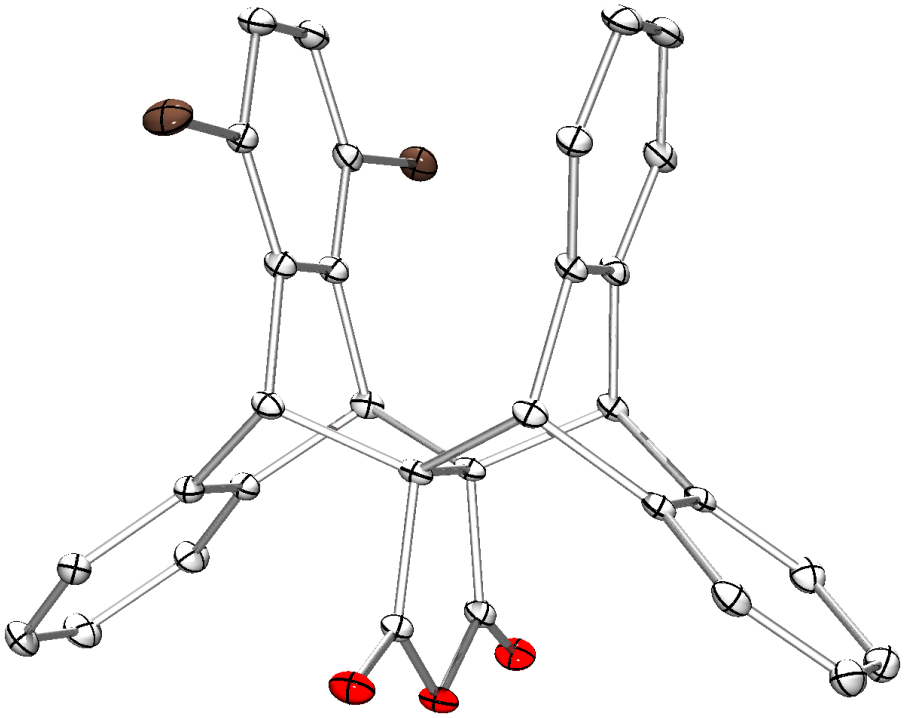


Figure S20. Crystal Structure of **2d**.

Table S5. Summary of Bond Distances and Angles for **2d**.

centroid distance	3.41 Å
angle between the planes of rings	18.52 ± 0.08
shortest C-C arene-arene distance	3.022 Å
middle C-C arene-arene distance	3.411 Å
longest C-C arene-arene distance	3.802 Å

Computational Results

Complete citations for Refs. 44 and 48.

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Table S6. DFT and CBS-QB3 computed free energy barriers ($\Delta G^{\ddagger}$, 298 K, kcal mol^{-1}) and free energy of reaction (ΔG) for the 1,4-cycloaddition of benzene and maleic anhydride.[a]

	M05-2X	M06-2X	B3LYP	CBS-QB3
$\Delta G^{\ddagger}$	35.5	37.5	49.4	34.8
ΔG	11.0	12.4	29.8	11.6

[a] The 6-31+G(d) basis set was used with M05-2X, M06-2X, and B3LYP. M05-2X harmonic vibrational frequencies were used to compute free energy corrections to the M06-2X electronic energies.

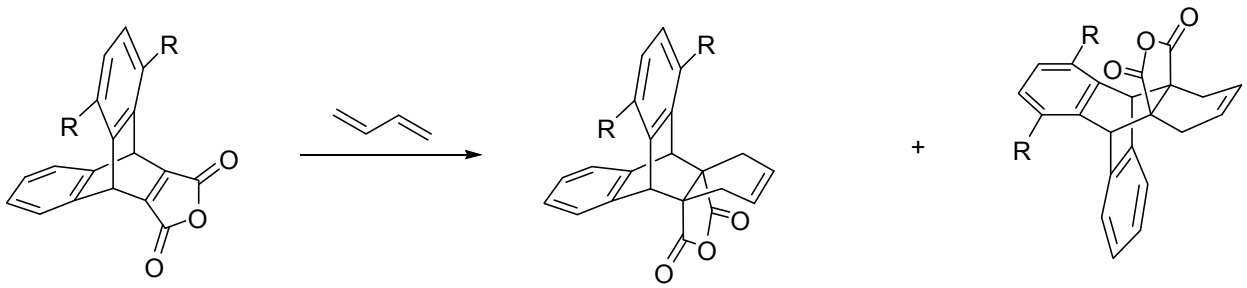
Table S7. Gas-phase energy barriers [$\Delta E^{\ddagger}$] and free energy barriers [$\Delta G^{\ddagger}$, 423K)]. All energies given in kcal mol^{-1}.

Product		M05-2X		M06-2X		B3LYP	
		$\Delta E^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta G^{\ddagger}$
H	**2a**	12.8	32.8	12.1	32.1	35.1	54.2
Me	**2b**	11.9	32.9	10.9	31.9	35.4	56.3
Me	**3b**	11.9	33.0	11.2	32.3	34.7	55.0
OMe	**2c**	10.9	29.4	10.0	28.5	34.3	55.0
OMe	**3c**	13.4	34.0	12.7	33.3	35.7	55.5
Br	**2d**	8.6	29.4	8.1	28.9	32.8	53.1
Br	**3d**	12.1	32.6	12.0	32.5	34.9	54.6
Cl	**2e**	8.7	29.8	7.8	28.9	32.6	52.9
Cl	**3e**	12.0	33.0	11.3	32.3	34.8	54.9
F	**2f**	9.7	29.4	9.2	28.8	32.4	52.5
F	**3f**	12.3	33.2	11.8	32.6	34.6	54.3

Table S8. Inter-ring distances (Å) between interacting rings in TS2, TS3, and the corresponding disubstituted gas-phase dimer, evaluated at the M05-2X/6-31+G(d) or M05-2X/AVDZ′ level of theory.

Substrate		TS2			TS3		
		short	long	gas phase	short	long	gas phase
Me	**1b**	3.23	3.49	3.90	3.26	3.54	4.05
OMe	**1c**	3.23	3.42	3.85	3.24	3.53	4.05
Br	**1d**	3.24	3.45	3.65	3.26	3.52	4.05
Cl	**1e**	3.23	3.43	3.80	3.25	3.51	4.05
F	**1f**	3.23	3.44	3.85	3.24	3.53	4.05

Scheme S1. Reactions of 1,3-butadiene + Substrates 1a – 1f.



1a: R = H
1b: R = Me
1c: R = OMe
1d: R = Br
1e: R = CN

4a: R = H
4b: R = Me
4c: R = OMe
4d: R = Br
4e: R = CN

5b: R = Me
5c: R = OMe
5d: R = Br
5e: R = CN

Table S9. M05-2X/6-31+G(d) predicted energy barriers ($\Delta E^{\ddagger}$, kcal mol^{-1}) and relative energy barriers [$\Delta\Delta E_{sub}$ = $\Delta E^{\ddagger}$(TS5) - $\Delta E^{\ddagger}$(TS4)] for the addition of butadiene to substrates **1a**-**1e**.

Product		$\Delta E^{\ddagger}$	$\Delta\Delta E_{sub}$
H	**4a**	5.6	
Me	**4b**	5.2	
Me	**5b**	5.3	0.1
OMe	**4c**	5.0	
OMe	**5c**	6.0	1.0
Br	**4d**	5.6	
Br	**5d**	6.5	0.9
Cl	**4e**	4.6	
Cl	**5e**	5.4	0.8
F	**4f**	5.1	
F	**5f**	5.4	0.3

Table S10. M05-2X and M06-2X energies (in hartree) for substituted benzene dimers.

	M05-2X/6-31+G(d)		**M06-2X/6-31+G(d)**	
	Dimer	**Monomer**	**Dimer**	**Monomer**
H	-464.449702	-232.224432	-464.290572	-232.144460
Me	-503.760953	-271.535226	-503.588178	-271.441474
OH	-539.664749	-307.438898	-539.488518	-307.341650
OMe	-578.961134	-346.735326	-578.772553	-346.625497
Cl	-924.027009	-691.800414	-923.862522	-691.714788
F	-563.686969	-331.460889	-563.504871	-331.357742
CN	-556.692380	-324.465127	-556.510747	-324.362366
	M05-2X/AVDZ′		**M06-2X/ AVDZ′**	
H	-464.489655	-232.244271	-464.338359	-232.167882
Br	-3037.983350	-2805.736364	-3037.924961	-2805.752725

Table S11. B3LYP energies in hartree.

Substrate		**Reactant**	**TS2**	**TS3**	**Product2**	**Product3**
H	**1a**	-917.639447	-1457.132287		-1457.201169	
Me	**1b**	-996.274522	-1535.766868	-1535.767934	-1535.835592	-1535.837017
OMe	**1c**	-1146.689844	-1686.183982	-1686.181704	-1686.253017	-1686.251026
Br	**1d**	-6064.799655	-6604.318468	-6604.315094	-6604.376849	-6604.372598
Cl	**1e**	-1836.826150	-2376.322966	-2376.319424	-2376.391917	-2376.387760
F	**1f**	-1116.118104	-1655.615224	-1655.611712	-1655.683822	-1655.680400
Anthracene		-539.548722				

Table S12. B3LYP enthalpies (0 K) in hartree.

Substrate		**Reactant**	**TS2**	**TS3**	**Product2**	**Product3**
H	**1a**	-917.407648	-1456.705894		-1456.770427	
Me	**1b**	-995.987356	-1535.284737	-1535.285918	-1535.349440	-1535.350675
OMe	**1c**	-1146.392754	-1685.692093	-1685.690099	-1685.756905	-1685.755091
Br	**1d**	-6064.588891	-6603.913754	-6603.910438	-6603.967968	-6603.963890
Cl	**1e**	-1836.613614	-2375.915694	-2375.912218	-2375.980118	-2375.976210
F	**1f**	-1115.902733	-1655.205080	-1655.201723	-1655.269320	-1655.265977
Anthracene		-539.354531				

Table S13. B3LYP enthalpies (423 K) in hartree.

Substrate		Reactant	TS2	TS3	Product2	Product3
H	**1a**	-917.377771	-1456.65514		-1456.72069	
Me	**1b**	-995.951249	-1535.22798	-1535.22909	-1535.29354	-1535.29485
OMe	**1c**	-1146.35332	-1685.6319	-1685.62978	-1685.69763	-1685.69522
Br	**1d**	-6064.55418	-6603.858122	-6603.85477	-6603.912597	-6603.908517
Cl	**1e**	-1836.57962	-2375.86082	-2375.85736	-2375.92631	-2375.92237
F	**1f**	-1115.86983	-1655.15133	-1655.14794	-1655.21657	-1655.21324
Anthracene		-539.33376				

Table S14. B3LYP free energies (423 K) in hartree.

Substrate		Reactant	TS2	TS3	Product2	Product3
H	**1a**	-917.474319	-1456.7961		-1456.85737	
Me	**1b**	-996.062709	-1535.38106	-1535.38316	-1535.44366	-1535.44462
OMe	**1c**	-1146.47315	-1685.79367	-1685.79285	-1685.8563	-1685.85551
Br	**1d**	-6064.66681	-6604.013075	-6604.01072	-6604.066212	-6604.062366
Cl	**1e**	-1836.68838	-2376.01223	-2376.00905	-2376.07375	-2376.07002
F	**1f**	-1115.97474	-1655.29916	-1655.29626	-1655.36048	-1655.35715
Anthracene		-539.40813				

Table S15. B3LYP/6-31+G(d) CPCM-corrected free energies (423 K) in hartree.

Substrate		Reactant	TS2	TS3
H	**1a**	-917.480918	-1456.799078	
Me	**1b**	-996.067282	-1535.382254	-1535.383366
OMe	**1c**	-1146.478963	-1685.793214	-1685.793454
Br	**1d**	-6064.670770	-6604.010630	-6604.010953
Cl	**1e**	-1836.692402	-2376.009944	-2376.008555
F	**1f**	-1115.980176	-1655.298648	-1655.297496
Anthracene		-539.411413		

Table S16. M05-2X energies in hartree.

Substrate		Reactant	TS2	TS3	Product2	Product3
H	**1a**	-917.562544	-1457.033268		-1457.120125	
Me	**1b**	-996.184754	-1535.656946	-1535.656881	-1535.743591	-1535.744488
OMe	**1c**	-1146.582639	-1686.056403	-1686.052330	-1686.143500	-1686.140165
Br	**1d**	-6064.622264	-6604.141453	-6604.135857	-6604.211376	-6604.205340
Cl	**1e**	-1836.710422	-2376.187642	-2376.182365	-2376.274469	-2376.268689
F	**1f**	-1116.029411	-1655.504971	-1655.500827	-1655.591757	-1655.587292
Anthracene		-539.491078				

Table S17. M05-2X enthalpies (0 K) in hartree.

Substrate		Reactant	TS2	TS3	Product2	Product3
H	**1a**	-917.325908	-1456.598484		-1456.680678	
Me	**1b**	-995.891773	-1535.165721	-1535.165546	-1535.247683	-1535.248520
OMe	**1c**	-1146.279073	-1685.554565	-1685.550584	-1685.637253	-1685.634084
Br	**1d**	-6064.406925	-6603.728569	-6603.723152	-6603.796840	-6603.790961
Cl	**1e**	-1836.493260	-2375.772046	-2375.766919	-2375.854224	-2375.848696
F	**1f**	-1115.809260	-1655.086401	-1655.082406	-1655.168785	-1655.164379
Anthracene		-539.296887				

Table S18. M05-2X enthalpies (298 K) in hartree.

Substrate		Reactant	TS2	TS3	Product2	Product3
H	**1a**	-917.296509	-1456.548631		-1456.631832	
Me	**1b**	-995.856343	-1535.109904	-1535.109748	-1535.192896	-1535.19376
OMe	**1c**	-1146.240344	-1685.495426	-1685.491377	-1685.579048	-1685.575756
Br	**1d**	-6064.372773	-6603.673891	-6603.668430	-6603.742589	-6603.736703
Cl	**1e**	-1836.459812	-2375.718196	-2375.713035	-2375.801358	-2375.795769
F	**1f**	-1115.776901	-1655.033625	-1655.029621	-1655.116903	-1655.112537
Anthracene						

Table S19. M05-2X free energies (423 K) in hartree.

Substrate		Reactant	TS2	TS3	Product2	Product3
H	**1a**	-917.392346	-1456.687348		-1456.766339	
Me	**1b**	-995.96623	-1535.261168	-1535.26098	-1535.340857	-1535.341614
OMe	**1c**	-1146.358794	-1685.65931	-1685.65194	-1685.736241	-1685.733901
Br	**1d**	-6064.484379	-6603.827137	-6603.822079	-6603.892224	-6603.886352
Cl	**1e**	-1836.567612	-2375.867491	-2375.862412	-2375.947409	-2375.942347
F	**1f**	-1115.880872	-1655.181402	-1655.175246	-1655.259968	-1655.255415
Anthracene		-539.34734				

Table S20. M05-2X CPCM-corrected free energies (423 K) in hartree.

Substrate		Reactant	TS2	TS3
H	**1a**	-917.399281	-1456.691647	
Me	**1b**	-995.970561	-1535.265114	-1535.265080
OMe	**1c**	-1146.365212	-1685.659197	-1685.656271
Br	**1d**	-6064.503950	-6603.854269	-6603.852193
Cl	**1e**	-1836.587960	-2375.895782	-2375.892203
F	**1f**	-1115.887624	-1655.184212	-1655.179530
Anthracene		-539.353055		

Table S21. M06-2X energies in hartree.

Substrate		Reactant	TS2	TS3
H	**1a**	-917.278460	-1456.567454	
Me	**1b**	-995.873226	-1535.164067	-1535.163585
OMe	**1c**	-1146.238832	-1685.531134	-1685.526778
Br	**1d**	-6064.549319	-6603.898355	-6603.892206
Cl	**1e**	-1836.415459	-2375.711263	-2375.705671
F	**1f**	-1115.699277	-1654.992907	-1654.988783
Anthracene		-539.308234		

Table S22. M05-2X energies (in hartree) for the "truncated" stacked structures depicted in Fig. 3. "TS2" corresponds to the stacked geometry present in TS2, *etc*.

Substrate		TS2	Benzene1	Benzene2	TS3	Benzene1	Benzene2
Me	**1b**	-543.066051	-310.845535	-232.222450	-464.443944	-232.224249	-232.222337
OMe	**1c**	-693.464749	-461.243278	-232.222296	-464.443640	-232.224215	-232.222343
Br	**1d**	-5611.470898	-5379.226205	-232.242182	-464.484110	-232.244026	-232.242160
Cl	**1e**	-1383.598080	-1151.374525	-232.222390	-464.443658	-232.224207	-232.222305
F	**1f**	-662.916561	-430.694688	-232.222300	-464.443626	-232.224213	-232.222368

Table S23. M05-2X energies (in hartree) for the "truncated" structures depicted in Fig. 4.

Substrate		TS2	TS3
Me	**1b**	-996.058268	-996.058237
OMe	**1c**	-996.060570	-996.037701
Br	**1d**	-996.167805	-996.166452
Cl	**1e**	-996.058602	-996.057471
F	**1f**	-996.059135	-996.057634

Optimized Geometries

B3LYP optimized Cartesian Coordinates

Maleic Anhydride + Benzene

12
Benzene B3LYP/6-31+G(d) Optimized Geometry

C	0.0000000	1.3985480	0.0000000
C	1.2111780	0.6992740	0.0000000
C	1.2111780	-0.6992740	0.0000000
C	0.0000000	-1.3985480	0.0000000
C	-1.2111780	-0.6992740	0.0000000
C	-1.2111780	0.6992740	0.0000000
H	0.0000000	2.4858300	0.0000000
H	2.1527920	1.2429150	0.0000000
H	2.1527920	-1.2429150	0.0000000
H	0.0000000	-2.4858300	0.0000000
H	-2.1527920	-1.2429150	0.0000000
H	-2.1527920	1.2429150	0.0000000

9
maleic anhydride B3LYP/6-31+G(d) Optimized Geometry

C	0.0000000	0.6686910	-1.2588150
C	0.0000000	-0.6686910	-1.2588150
C	0.0000000	1.1319620	0.1581990
H	0.0000000	1.3620940	-2.0903670
H	0.0000000	-1.3620940	-2.0903670
O	0.0000000	0.0000000	0.9723990
O	0.0000000	2.2462550	0.6005590
C	0.0000000	-1.1319620	0.1581990
O	0.0000000	-2.2462550	0.6005590

21
cycloadduct B3LYP/6-31+G(d) Optimized Geometry

C	-0.5961580	2.3774650	0.6688290
H	-1.0470330	3.1462010	-1.2895340
H	-1.0470330	3.1462010	1.2895340
C	-0.5961580	2.3774650	-0.6688290
C	1.4555890	0.9878580	0.6690400
H	2.3347740	0.8407420	1.2889350
C	0.0745590	1.1570210	1.2884080
H	2.3347740	0.8407420	-1.2889350
C	-0.7854810	-0.0670660	-0.7685760
C	-0.7854810	-0.0670660	0.7685760
C	1.4555890	0.9878580	-0.6690400
C	0.0745590	1.1570210	-1.2884080
C	-0.1865420	-1.4115140	-1.1490740
H	0.0903710	1.1722960	-2.3791630
H	0.0903710	1.1722960	2.3791630
H	-1.7894660	-0.0065500	1.1993680
C	-0.1865420	-1.4115140	1.1490740
H	-1.7894660	-0.0065500	-1.1993680
O	0.0187350	-1.8603290	-2.2418940
O	0.1224180	-2.1331610	0.0000000
O	0.0187350	-1.8603290	2.2418940

21
transition state B3LYP/6-31+G(d) Optimized Geometry

C	-0.5820540	2.3802490	0.6797410
H	-1.2290620	3.0261290	-1.2668690
H	-1.2290620	3.0261290	1.2668690
C	-0.5820540	2.3802490	-0.6797410
C	1.4437710	0.9785600	0.6803540
H	2.2712260	0.5882240	1.2652310
C	0.2044280	1.3495950	1.3287770
H	2.2712260	0.5882240	-1.2652310
C	-0.9814330	-0.2394070	-0.7134060
C	-0.9814330	-0.2394070	0.7134060
C	1.4437710	0.9785600	-0.6803540
C	0.2044280	1.3495950	-1.3287770
C	-0.2017330	-1.4322270	-1.1399300
H	0.1586200	1.2748110	-2.4124940
H	0.1586200	1.2748110	2.4124940
H	-1.8424730	0.0270670	1.3136670
C	-0.2017330	-1.4322270	1.1399300
H	-1.8424730	0.0270670	-1.3136670
O	-0.0043460	-1.8775480	-2.2391910
O	0.3446450	-2.0291160	0.0000000
O	-0.0043460	-1.8775480	2.2391910

Reactions in Scheme 1: Anthracene + Substrates 1a-1e

24
Anthracene B3LYP/6-31+G(d) Optimized Geometry

C	0.0000000	2.4822450	1.4084520
C	0.0000000	2.4822450	-1.4084520
C	0.0000000	-2.4822450	-1.4084520
C	0.0000000	-2.4822450	1.4084520
C	0.0000000	0.0000000	-1.4046120
C	0.0000000	0.0000000	1.4046120
C	0.0000000	3.6654190	0.7139420
C	0.0000000	3.6654190	-0.7139420
C	0.0000000	-3.6654190	-0.7139420
C	0.0000000	-3.6654190	0.7139420
C	0.0000000	-1.2252350	-0.7230720
C	0.0000000	-1.2252350	0.7230720
C	0.0000000	1.2252350	-0.7230720
C	0.0000000	1.2252350	0.7230720
H	0.0000000	4.6122370	1.2480210
H	0.0000000	4.6122370	-1.2480210
H	0.0000000	-4.6122370	-1.2480210
H	0.0000000	-4.6122370	1.2480210
H	0.0000000	2.4802410	2.4964450
H	0.0000000	2.4802410	-2.4964450
H	0.0000000	-2.4802410	-2.4964450
H	0.0000000	-2.4802410	2.4964450
H	0.0000000	0.0000000	-2.4934550
H	0.0000000	0.0000000	2.4934550

55
2a B3LYP/6-31+G(d) Optimized Geometry

C	3.8025730	-2.1092980	0.6983270
C	3.8025730	-2.1092980	-0.6983270
C	-2.2431690	-4.3828110	-0.6983800
C	-2.2431690	-4.3828110	0.6983800
C	2.6255030	-1.8266930	-1.4043330
C	2.6255030	-1.8266930	1.4043330
C	-1.5139080	-3.4176150	-1.4066110
C	-1.5139080	-3.4176150	1.4066110
C	-0.7808480	-2.4658290	-0.7038550
C	-0.7808480	-2.4658290	0.7038550
C	1.4567720	-1.5478250	-0.7027840
C	1.4567720	-1.5478250	0.7027840
H	4.7170100	-2.3338890	1.2413400
H	4.7170100	-2.3338890	-1.2413400
H	-2.8153870	-5.1305580	-1.2411340
H	-2.8153870	-5.1305580	1.2411340
H	2.6234840	-1.8363170	-2.4923680
H	2.6234840	-1.8363170	2.4923680
H	-1.5255010	-3.4082410	-2.4939620
H	-1.5255010	-3.4082410	2.4939620
C	0.0745300	-1.3490980	-1.3020840
C	0.0745300	-1.3490980	1.3020840
C	-0.5583720	0.0000080	-0.7778890
C	-0.5583720	0.0000080	0.7778890
C	-2.0441920	0.0000330	-1.1445710
C	-2.0441920	0.0000330	1.1445710
O	-2.8281210	0.0000210	0.0000000
O	-2.5351550	-0.0000290	-2.2394540
O	-2.5351550	-0.0000290	2.2394540
H	0.0753690	-1.3667840	-2.3954240
H	0.0753690	-1.3667840	2.3954240
C	3.8026150	2.1092110	0.6983280
C	3.8026150	2.1092110	-0.6983280
C	1.4567940	1.5478160	-0.7027830
C	1.4567940	1.5478160	0.7027830
C	2.6255370	1.8266440	-1.4043320
C	2.6255370	1.8266440	1.4043320
C	0.0745510	1.3491250	-1.3020850
C	0.0745510	1.3491250	1.3020850
C	-0.7808120	2.4658590	-0.7038550
C	-0.7808120	2.4658590	0.7038550
C	-2.2431140	4.3828570	-0.6983810
C	-2.2431140	4.3828570	0.6983810
C	-1.5138640	3.4176530	-1.4066100
C	-1.5138640	3.4176530	1.4066100
H	4.7170600	2.3337740	1.2413390
H	4.7170600	2.3337740	-1.2413390
H	2.6235150	1.8362650	-2.4923680
H	2.6235150	1.8362650	2.4923680
H	0.0753850	1.3667980	-2.3954240
H	0.0753850	1.3667980	2.3954240
H	-2.8153240	5.1306100	-1.2411340
H	-2.8153240	5.1306100	1.2411340
H	-1.5254570	3.4082770	2.4939620
H	-1.5254570	3.4082770	-2.4939620

31
1a B3LYP/6-31+G(d) Optimized Geometry

C	-3.2846480	0.6975370	-2.0897840

C	-3.2846480	-0.6975370	-2.0897840
C	3.2846480	-0.6975370	-2.0897840
C	3.2846480	0.6975370	-2.0897840
C	-2.2465210	-1.4073090	-1.4648170
C	-2.2465210	1.4073090	-1.4648170
C	2.2465210	-1.4073090	-1.4648170
C	2.2465210	1.4073090	-1.4648170
C	1.2212770	-0.7036480	-0.8448350
C	1.2212770	0.7036480	-0.8448350
C	-1.2212770	-0.7036480	-0.8448350
C	-1.2212770	0.7036480	-0.8448350
H	-4.0925200	1.2408910	-2.5726350
H	-4.0925200	-1.2408910	-2.5726350
H	4.0925200	-1.2408910	-2.5726350
H	4.0925200	1.2408910	-2.5726350
H	-2.2473570	-2.4948920	-1.4644400
H	-2.2473570	2.4948920	-1.4644400
H	2.2473570	-2.4948920	-1.4644400
H	2.2473570	2.4948920	-1.4644400
C	0.0000000	-1.3149510	-0.1304590
C	0.0000000	1.3149510	-0.1304590
C	0.0000000	-0.6704970	1.2354890
C	0.0000000	0.6704970	1.2354890
C	0.0000000	-1.1446270	2.6358810
C	0.0000000	1.1446270	2.6358810
O	0.0000000	0.0000000	3.4488840
O	0.0000000	-2.2544450	3.0930450
O	0.0000000	2.2544450	3.0930450
H	0.0000000	-2.4059460	-0.1179790
H	0.0000000	2.4059460	-0.1179790

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TS2a B3LYP/6-31+G(d) Optimized Geometry

C	2.9631720	-3.1723480	0.6982240
C	2.9631720	-3.1723480	-0.6982240
C	-3.3649150	-3.7346070	-0.6972400
C	-3.3649150	-3.7346070	0.6972400
C	1.9326110	-2.5373760	-1.4038160
C	1.9326110	-2.5373760	1.4038160
C	-2.4208650	-2.9737940	-1.4074950
C	-2.4208650	-2.9737940	1.4074950
C	-1.4871280	-2.2233760	-0.7048770
C	-1.4871280	-2.2233760	0.7048770
C	0.9063990	-1.9103350	-0.7035380
C	0.9063990	-1.9103350	0.7035380
H	3.7600950	-3.6735360	1.2417830
H	3.7600950	-3.6735360	-1.2417830
H	-4.1024830	-4.3193320	-1.2407100
H	-4.1024830	-4.3193320	1.2407100
H	1.9239540	-2.5517140	-2.4917590
H	1.9239540	-2.5517140	2.4917590
H	-2.4265350	-2.9673690	-2.4950050
H	-2.4265350	-2.9673690	2.4950050
C	-0.3715420	-1.3414720	-1.3083480
C	-0.3715420	-1.3414720	1.3083480
C	-0.6658880	0.0419190	-0.7080630
C	-0.6658880	0.0419190	0.7080630
C	-1.8780420	0.7796440	-1.1403100
C	-1.8780420	0.7796440	1.1403100
O	-2.4994120	1.3004280	0.0000000
O	-2.3448190	0.9413280	-2.2383710
O	-2.3448190	0.9413280	2.2383710
H	-0.3768600	-1.3474470	-2.4004870
H	-0.3768600	-1.3474470	2.4004870
C	4.2505640	0.3776580	0.7057430
C	4.2505640	0.3776580	-0.7057430
C	1.9819930	1.2290740	0.7117730
C	1.9819930	1.2290740	-0.7117730
C	3.1229880	0.7705270	-1.4059100
C	3.1229880	0.7705270	1.4059100
C	0.7990360	1.7236330	-1.3608190
C	0.7990360	1.7236330	1.3608190
C	-1.3103620	4.7730980	-0.7057610
C	-1.3103620	4.7730980	0.7057610
C	0.0941030	2.7980050	-0.7123660
C	0.0941030	2.7980050	0.7123660
C	-0.6368760	3.7877790	-1.4075290
C	-0.6368760	3.7877790	1.4075290
H	5.1402730	0.0613990	1.2436910
H	5.1402730	0.0613990	-1.2436910
H	3.1184460	0.7633140	-2.4934750
H	3.1184460	0.7633140	2.4934750
H	0.7364400	1.6563760	-2.4453460
H	0.7364400	1.6563760	2.4453460
H	-1.8530280	5.5453130	-1.2441770
H	-1.8530280	5.5453130	1.2441770
H	-0.6555860	3.7724790	2.4940880
H	-0.6555860	3.7724790	-2.4940880

61
2b B3LYP/6-31+G(d) Optimized Geometry

C	2.7902650	-3.0378230	0.6974820
C	2.7902650	-3.0378230	-0.6974820
C	-3.6634490	-3.2589020	-0.6983670
C	-3.6634490	-3.2589020	0.6983670
C	1.7759100	-2.4065970	-1.4320020
C	1.7759100	-2.4065970	1.4320020
C	-2.6617280	-2.5801880	-1.4065710
C	-2.6617280	-2.5801880	1.4065710
C	-1.6592870	-1.9183490	-0.7034210
C	-1.6592870	-1.9183490	0.7034210
C	0.7607110	-1.7742890	-0.7026460
C	0.7607110	-1.7742890	0.7026460
H	3.5935960	-3.5434360	1.2293520
H	3.5935960	-3.5434360	-1.2293520
H	-4.4474350	-3.7804810	-1.2410820
H	-4.4474350	-3.7804810	1.2410820
C	1.7899170	-2.4321420	-2.9437090
H	0.9005190	-2.9271460	-3.3543920
H	1.8227740	-1.4210060	-3.3699240
H	2.6667480	-2.9730530	-3.3138910
C	1.7899170	-2.4321420	2.9437090
H	0.9005190	-2.9271460	3.3543920
H	1.8227740	-1.4210060	3.3699240
H	2.6667480	-2.9730530	3.3138910
H	-2.6724150	-2.5636480	-2.4939180
H	-2.6724150	-2.5636480	2.4939180
C	-0.4891640	-1.1366070	-1.2979270
C	-0.4891640	-1.1366070	1.2979270
C	-0.6517500	0.3448400	-0.7765940
C	-0.6517500	0.3448400	0.7765940
C	-2.0577780	0.8241990	-1.1443040
C	-2.0577780	0.8241990	1.1443040
O	-2.8014140	1.0730070	0.0000000
O	-2.5218210	0.9849940	-2.2392500
O	-2.5218210	0.9849940	2.2392500
H	-0.5041250	-1.1460860	-2.3895090
H	-0.5041250	-1.1460860	2.3895090
C	4.1576510	0.9282120	0.6981300
C	4.1576510	0.9282120	-0.6981300
C	1.7556310	1.1537260	-0.7030290
C	1.7556310	1.1537260	0.7030290
C	2.9519120	1.0413530	-1.4041340
C	2.9519120	1.0413530	1.4041340
C	0.3833010	1.4149500	-1.3020670
C	0.3833010	1.4149500	1.3020670
C	-0.0615810	2.7493390	-0.7038820
C	-0.0615810	2.7493390	0.7038820
C	-0.8179490	5.0387070	-0.6983580
C	-0.8179490	5.0387070	0.6983580
C	-0.4437120	3.8883840	-1.4066760
C	-0.4437120	3.8883840	1.4066760
H	5.0956150	0.8463900	1.2412970
H	5.0956150	0.8463900	-1.2412970
H	2.9541430	1.0561860	-2.4921920
H	2.9541430	1.0561860	2.4921920
H	0.3893780	1.4314580	-2.3954150
H	0.3893780	1.4314580	2.3954150
H	-1.1146720	5.9323660	-1.2410370
H	-1.1146720	5.9323660	1.2410370
H	-0.4572970	3.8835790	2.4940460
H	-0.4572970	3.8835790	-2.4940460

61
3b B3LYP/6-31+G(d) Optimized Geometry

C	-4.1964910	1.0701630	0.6982710
C	-4.1964910	1.0701630	-0.6982710
C	1.2697360	4.4964610	-0.6974300
C	1.2697360	4.4964610	0.6974300
C	-2.9864080	1.0315310	-1.4043040
C	-2.9864080	1.0315310	1.4043040
C	0.7550750	3.4194400	-1.4354630
C	0.7550750	3.4194400	1.4354630
C	0.2324050	2.3444390	-0.7039750
C	0.2324050	2.3444390	0.7039750
C	-1.7853940	0.9979140	-0.7023910
C	-1.7853940	0.9979140	0.7023910
H	-5.1375070	1.1035520	1.2413720
H	-5.1375070	1.1035520	-1.2413720
H	1.6812350	5.3520620	-1.2285560
H	1.6812350	5.3520620	1.2285560
C	0.7730380	3.4376400	-2.9471940
H	-0.2396690	3.3796450	-3.3673620
H	1.2291220	4.3617580	-3.3163710
H	1.3472260	2.5963480	-3.3537940
C	0.7730380	3.4376400	2.9471940
H	-0.2396690	3.3796450	3.3673620
H	1.2291220	4.3617580	3.3163710
H	1.3472260	2.5963480	3.3537940

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H       -2.9867860        1.0355050       -2.4924660
H       -2.9867860        1.0355050        2.4924660
C       -0.3908040        1.0754200       -1.2980350
C       -0.3908040        1.0754200        1.2980350
C        0.4959640       -0.1214920       -0.7768630
C        0.4959640       -0.1214920        0.7768630
C        1.9514370        0.1763820       -1.1433920
C        1.9514370        0.1763820        1.1433920
O        2.7215290        0.3254510        0.0000000
O        2.4324330        0.2793450       -2.2386180
O        2.4324330        0.2793450        2.2386180
H       -0.4003660        1.0826980       -2.3898770
H       -0.4003660        1.0826980        2.3898770
C       -3.3618050       -3.0481060        0.6983120
C       -3.3618050       -3.0481060       -0.6983120
C       -1.1719830       -2.0364500       -0.7028390
C       -1.1719830       -2.0364500        0.7028390
C       -2.2635530       -2.5389050       -1.4042530
C       -2.2635530       -2.5389050        1.4042530
C        0.1440620       -1.5687650       -1.3022010
C        0.1440620       -1.5687650        1.3022010
C        1.2016570       -2.4961560       -0.7039220
C        1.2016570       -2.4961560        0.7039220
C        3.0058810       -4.0956360       -0.6983340
C        3.0058810       -4.0956360        0.6983340
C        2.1044760       -3.2889450       -1.4066410
C        2.1044760       -3.2889450        1.4066410
H       -4.2141310       -3.4482410        1.2413980
H       -4.2141310       -3.4482410       -1.2413980
H       -2.2603910       -2.5463170       -2.4923250
H       -2.2603910       -2.5463170        2.4923250
H        0.1471270       -1.5851850       -2.3955900
H        0.1471270       -1.5851850        2.3955900
H        3.7112290       -4.7195030       -1.2409690
H        3.7112290       -4.7195030        1.2409690
H        2.1135750       -3.2784890        2.4940360
H        2.1135750       -3.2784890       -2.4940360

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1b B3LYP/6-31+G(d) Optimized Geometry
C       -1.0446910        3.4476280        0.6968430
C       -1.0446910        3.4476280       -0.6968430
C        3.9295740       -0.8177230       -0.6974640
C        3.9295740       -0.8177230        0.6974640
C       -0.6711050        2.3118030       -1.4355080
C       -0.6711050        2.3118030        1.4355080
C        2.7345830       -0.6167110       -1.4071820
C        2.7345830       -0.6167110        1.4071820
C        1.5534380       -0.4177020       -0.7030680
C        1.5534380       -0.4177020        0.7030680
C       -0.3014290        1.1794440       -0.7029850
C       -0.3014290        1.1794440        0.7029850
H       -1.3442030        4.3481280        1.2284840
H       -1.3442030        4.3481280       -1.2284840
H        4.8570990       -0.9776580       -1.2406870
H        4.8570990       -0.9776580        1.2406870
H        2.7348460       -0.6207350       -2.4947670
H        2.7348460       -0.6207350        2.4947670
C        0.1612290       -0.1648010       -1.3113130
C        0.1612290       -0.1648010        1.3113130
C       -0.7295480       -1.2005430       -0.6703500
C       -0.7295480       -1.2005430        0.6703500
C       -1.6427650       -2.2605770       -1.1446050
C       -1.6427650       -2.2605770        1.1446050
O       -2.1732620       -2.8779610        0.0000000
O       -1.9434630       -2.6062610       -2.2545740
O       -1.9434630       -2.6062610        2.2545740
H        0.1571860       -0.1835910       -2.4005810
H        0.1571860       -0.1835910        2.4005810
C       -0.6770790        2.3335630       -2.9477250
C       -0.6770790        2.3335630        2.9477250
H       -1.0145450        3.3062450       -3.3189680
H       -1.0145450        3.3062450        3.3189680
H        0.3229590        2.1524790       -3.3624470
H        0.3229590        2.1524790        3.3624470
H       -1.3458390        1.5707840       -3.3660700
H       -1.3458390        1.5707840        3.3660700

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TS2b B3LYP/6-31+G(d) Optimized Geometry
C        2.0893190       -3.5567500        0.6974060
C        2.0893190       -3.5567500       -0.6974060
C       -4.2072130       -2.6824020       -0.6971730
C       -4.2072130       -2.6824020        0.6971730
C        1.2347720       -2.7222310       -1.4317900
C        1.2347720       -2.7222310        1.4317900
C       -3.1131320       -2.1593080       -1.4073910
C       -3.1131320       -2.1593080        1.4073910
C       -2.0301160       -1.6475780       -0.7044190
C       -2.0301160       -1.6475780        0.7044190
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C	0.3782600	-1.8862060	-0.7033150
C	0.3782600	-1.8862060	0.7033150
H	2.7626580	-4.2259650	1.2293120
H	2.7626580	-4.2259650	-1.2293120
H	-5.0606050	-3.0795450	-1.2405950
H	-5.0606050	-3.0795450	1.2405950
C	1.2302660	-2.7642580	-2.9432320
H	0.2759180	-3.1355750	-3.3393250
H	1.3971840	-1.7728220	-3.3829570
H	2.0183040	-3.4275220	-3.3146040
C	1.2302660	-2.7642580	2.9432320
H	0.2759180	-3.1355750	3.3393250
H	1.3971840	-1.7728220	3.3829570
H	2.0183040	-3.4275220	3.3146040
H	-3.1198560	-2.1468890	-2.4949040
H	-3.1198560	-2.1468890	2.4949040
C	-0.7438190	-1.0399670	-1.3041970
C	-0.7438190	-1.0399670	1.3041970
C	-0.7198210	0.3747190	-0.7072310
C	-0.7198210	0.3747190	0.7072310
C	-1.7359540	1.3647950	-1.1404440
C	-1.7359540	1.3647950	1.1404440
O	-2.2271100	2.0104320	0.0000000
O	-2.1537670	1.6277550	-2.2387310
O	-2.1537670	1.6277550	2.2387310
H	-0.7589900	-1.0369640	-2.3945040
H	-0.7589900	-1.0369640	2.3945040
C	4.1463370	-0.3948940	0.7056990
C	4.1463370	-0.3948940	-0.7056990
C	2.1239170	0.9409930	0.7118080
C	2.1239170	0.9409930	-0.7118080
C	3.1350100	0.2405130	-1.4054080
C	3.1350100	0.2405130	1.4054080
C	1.0824570	1.6880320	-1.3610970
C	1.0824570	1.6880320	1.3610970
C	-0.2983560	5.1290460	-0.7057780
C	-0.2983560	5.1290460	0.7057780
C	0.6341570	2.8920570	-0.7123450
C	0.6341570	2.8920570	0.7123450
C	0.1404140	4.0191580	-1.4075010
C	0.1404140	4.0191580	1.4075010
H	4.9436470	-0.9004630	1.2439020
H	4.9436470	-0.9004630	-1.2439020
H	3.1332300	0.2398860	-2.4930570
H	3.1332300	0.2398860	2.4930570
H	1.0078950	1.6380720	-2.4458430
H	1.0078950	1.6380720	2.4458430
H	-0.6572610	6.0020380	-1.2440920
H	-0.6572610	6.0020380	1.2440920
H	0.1174660	4.0076680	2.4940430
H	0.1174660	4.0076680	-2.4940430

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TS3b B3LYP/6-31+G(d) Optimized Geometry

C	-3.8777410	1.9195810	0.6982590
C	-3.8777410	1.9195810	-0.6982590
C	2.0064180	4.3165300	-0.6965720
C	2.0064180	4.3165300	0.6965720
C	-2.7048920	1.6196750	-1.4039800
C	-2.7048920	1.6196750	1.4039800
C	1.3340940	3.3264670	-1.4357370
C	1.3340940	3.3264670	1.4357370
C	0.6594960	2.3446570	-0.7045320
C	0.6594960	2.3446570	0.7045320
C	-1.5383770	1.3282750	-0.7030440
C	-1.5383770	1.3282750	0.7030440
H	-4.7880180	2.1604950	1.2415610
H	-4.7880180	2.1604950	-1.2415610
H	2.5474460	5.0960300	-1.2288210
H	2.5474460	5.0960300	1.2288210
C	1.3617620	3.3344880	-2.9476890
H	1.9636260	4.1701400	-3.3188920
H	1.7936350	2.4088300	-3.3475210
H	0.3553170	3.4390450	-3.3737260
C	1.3617620	3.3344880	2.9476890
H	1.9636260	4.1701400	3.3188920
H	1.7936350	2.4088300	3.3475210
H	0.3553170	3.4390450	3.3737260
H	-2.7017540	1.6334660	-2.4920310
H	-2.7017540	1.6334660	2.4920310
C	-0.1492090	1.1658490	-1.3045520
C	-0.1492090	1.1658490	1.3045520
C	0.5485250	-0.0643680	-0.7072300
C	0.5485250	-0.0643680	0.7072300
C	1.9272540	-0.3965180	-1.1393120
C	1.9272540	-0.3965180	1.1393120
O	2.6777980	-0.7066830	0.0000000
O	2.4233460	-0.4018000	-2.2370670
O	2.4233460	-0.4018000	2.2370670
H	-0.1526830	1.1646710	-2.3951070

H	-0.1526830	1.1646710	2.3951070
C	-4.0324540	-1.8671450	0.7058320
C	-4.0324540	-1.8671450	-0.7058320
C	-1.6128830	-2.0006110	0.7119320
C	-1.6128830	-2.0006110	-0.7119320
C	-2.8390780	-1.9046910	-1.4058850
C	-2.8390780	-1.9046910	1.4058850
C	-0.3364100	-2.1156440	-1.3612050
C	-0.3364100	-2.1156440	1.3612050
C	2.5970230	-4.3832590	-0.7058460
C	2.5970230	-4.3832590	0.7058460
C	0.6617430	-2.9240830	-0.7124340
C	0.6617430	-2.9240830	0.7124340
C	1.6576130	-3.6470960	-1.4075220
C	1.6576130	-3.6470960	1.4075220
H	-4.9760670	-1.8313630	1.2437380
H	-4.9760670	-1.8313630	-1.2437380
H	-2.8369710	-1.8963570	-2.4934640
H	-2.8369710	-1.8963570	2.4934640
H	-0.2974020	-2.0326920	-2.4457790
H	-0.2974020	-2.0326920	2.4457790
H	3.3472760	-4.9559710	-1.2442210
H	3.3472760	-4.9559710	1.2442210
H	1.6703270	-3.6278180	2.4941610
H	1.6703270	-3.6278180	-2.4941610

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2c B3LYP/6-31+G(d) Optimized Geometry

C	1.3171080	-3.6464340	0.7012830
C	1.3171080	-3.6464340	-0.7012830
C	-4.7179990	-1.3737100	-0.6984350
C	-4.7179990	-1.3737100	0.6984350
C	0.6339720	-2.6566840	-1.4129930
C	0.6339720	-2.6566840	1.4129930
C	-3.5337400	-1.1270850	-1.4071940
C	-3.5337400	-1.1270850	1.4071940
C	-2.3555120	-0.8944780	-0.7036680
C	-2.3555120	-0.8944780	0.7036680
C	-0.0672770	-1.6774420	-0.6974610
C	-0.0672770	-1.6774420	0.6974610
H	1.8610630	-4.4291880	1.2180080
H	1.8610630	-4.4291880	-1.2180080
H	-5.6413890	-1.5593890	-1.2409100
H	-5.6413890	-1.5593890	1.2409100
O	0.5888860	-2.5666110	-2.7827030
O	0.5888860	-2.5666110	2.7827030
C	1.2296710	-3.5786020	-3.5462110
H	1.0480150	-3.3224090	-4.5917350
H	2.3115440	-3.5975660	-3.3583160
H	0.8039000	-4.5684920	-3.3339410
C	1.2296710	-3.5786020	3.5462110
H	1.0480150	-3.3224090	4.5917350
H	2.3115440	-3.5975660	3.3583160
H	0.8039000	-4.5684920	3.3339410
H	-3.5351290	-1.1117950	-2.4944850
H	-3.5351290	-1.1117950	2.4944850
C	-0.9759850	-0.6195860	-1.3019290
C	-0.9759850	-0.6195860	1.3019290
C	-0.5560290	0.8092110	-0.7774910
C	-0.5560290	0.8092110	0.7774910
C	-1.6657120	1.7960580	-1.1449000
C	-1.6657120	1.7960580	1.1449000
O	-2.2538570	2.3143020	0.0000000
O	-2.0318400	2.1252520	-2.2392320
O	-2.0318400	2.1252520	2.2392320
H	-0.9819290	-0.6388540	-2.3923290
H	-0.9819290	-0.6388540	2.3923290
C	4.0847440	-0.5529870	0.6982630
C	4.0847440	-0.5529870	-0.6982630
C	1.9727740	0.6119070	-0.7030380
C	1.9727740	0.6119070	0.7030380
C	3.0233110	0.0294600	-1.4049150
C	3.0233110	0.0294600	1.4049150
C	0.8143500	1.3913650	-1.3026710
C	0.8143500	1.3913650	1.3026710
C	0.9274950	2.7927790	-0.7039030
C	0.9274950	2.7927790	0.7039030
C	1.1307210	5.1955370	-0.6983880
C	1.1307210	5.1955370	0.6983880
C	1.0233790	3.9906190	-1.4065290
C	1.0233790	3.9906190	1.4065290
H	4.9135030	-1.0006750	1.2411230
H	4.9135030	-1.0006750	-1.2411230
H	3.0243170	0.0349230	-2.4927600
H	3.0243170	0.0349230	2.4927600
H	0.8260800	1.4023310	-2.3957850
H	0.8260800	1.4023310	2.3957850
H	1.2088160	6.1339300	-1.2411460
H	1.2088160	6.1339300	1.2411460

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H        1.0086440        3.9912790        2.4939060
H        1.0086440        3.9912790       -2.4939060

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3c B3LYP/6-31+G(d) Optimized Geometry
C       -4.3526650        0.2362710        0.6983840
C       -4.3526650        0.2362710       -0.6983840
C        0.6271450        4.3517160       -0.7008530
C        0.6271450        4.3517160        0.7008530
C       -3.1477180        0.3531120       -1.4047700
C       -3.1477180        0.3531120        1.4047700
C        0.2416890        3.2128220       -1.4168910
C        0.2416890        3.2128220        1.4168910
C       -0.1366800        2.0701420       -0.6988830
C       -0.1366800        2.0701420        0.6988830
C       -1.9524590        0.4726440       -0.7026840
C       -1.9524590        0.4726440        0.7026840
H       -5.2904750        0.1498780        1.2413600
H       -5.2904750        0.1498780       -1.2413600
H        0.9278760        5.2561580       -1.2180240
H        0.9278760        5.2561580        1.2180240
O        0.1923500        3.1258780       -2.7822670
O        0.1923500        3.1258780        2.7822670
C        0.7034910        4.2089260       -3.5469850
H        0.1120500        5.1217260       -3.3936560
H        1.7554870        4.4045910       -3.3021190
H        0.6248710        3.8983110       -4.5903010
C        0.7034910        4.2089260        3.5469850
H        0.1120500        5.1217260        3.3936560
H        1.7554870        4.4045910        3.3021190
H        0.6248710        3.8983110        4.5903010
H       -3.1480460        0.3637520       -2.4927120
H       -3.1480460        0.3637520        2.4927120
C       -0.5810650        0.7374150       -1.3020500
C       -0.5810650        0.7374150        1.3020500
C        0.4592320       -0.3284010       -0.7779190
C        0.4592320       -0.3284010        0.7779190
C        1.8640130        0.1573680       -1.1451580
C        1.8640130        0.1573680        1.1451580
O        2.6039460        0.4159150        0.0000000
O        2.3345390        0.3090220       -2.2383920
O        2.3345390        0.3090220        2.2383920
H       -0.5854030        0.7622670       -2.3927160
H       -0.5854030        0.7622670        2.3927160
C       -2.9751540       -3.7419910        0.6983190
C       -2.9751540       -3.7419910       -0.6983190
C       -0.9376740       -2.4505550       -0.7028670
C       -0.9376740       -2.4505550        0.7028670
C       -1.9532970       -3.0928190       -1.4041560
C       -1.9532970       -3.0928190        1.4041560
C        0.3032850       -1.8098110       -1.3024100
C        0.3032850       -1.8098110        1.3024100
C        1.4761960       -2.5863230       -0.7039220
C        1.4761960       -2.5863230        0.7039220
C        3.4850620       -3.9200950       -0.6983940
C        3.4850620       -3.9200950        0.6983940
C        2.4804080       -3.2459600       -1.4064530
C        2.4804080       -3.2459600        1.4064530
H       -3.7680240       -4.2497920        1.2415530
H       -3.7680240       -4.2497920       -1.2415530
H       -1.9495290       -3.0985900       -2.4922230
H       -1.9495290       -3.0985900        2.4922230
H        0.3083120       -1.8264380       -2.3957400
H        0.3083120       -1.8264380        2.3957400
H        4.2705310       -4.4393640       -1.2412540
H        4.2705310       -4.4393640        1.2412540
H        2.4886150       -3.2321260        2.4938060
H        2.4886150       -3.2321260       -2.4938060

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1c B3LYP/6-31+G(d) Optimized Geometry
C       -0.3232740        3.2636720        0.7006900
C       -0.3232740        3.2636720       -0.7006900
C        3.7257850       -1.8953810       -0.6974590
C        3.7257850       -1.8953810        0.6974590
C       -0.1761110        2.0694450       -1.4171660
C       -0.1761110        2.0694450        1.4171660
C        2.5932560       -1.4642800       -1.4076290
C        2.5932560       -1.4642800        1.4076290
C        1.4733790       -1.0402880       -0.7034180
C        1.4733790       -1.0402880        0.7034180
C       -0.0356450        0.8774820       -0.6976400
C       -0.0356450        0.8774820        0.6976400
H       -0.4427650        4.2090990        1.2177680
H       -0.4427650        4.2090990       -1.2177680
H        4.6045480       -2.2327590       -1.2406940
H        4.6045480       -2.2327590        1.2406940
H        2.5931400       -1.4634670       -2.4950910
H        2.5931400       -1.4634670        2.4950910
C        0.1570120       -0.5217040       -1.3146030
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C	0.1570120	-0.5217040	1.3146030
C	-0.9165380	-1.3673630	-0.6706960
C	-0.9165380	-1.3673630	0.6706960
C	-2.0136920	-2.2359680	-1.1451330
C	-2.0136920	-2.2359680	1.1451330
O	-2.6531160	-2.7393480	0.0000000
O	-2.3734170	-2.5227680	-2.2541770
O	-2.3734170	-2.5227680	2.2541770
H	0.1461600	-0.5186210	-2.4032050
H	0.1461600	-0.5186210	2.4032050
O	-0.1583030	1.9692850	-2.7835770
O	-0.1583030	1.9692850	2.7835770
C	-0.3138180	3.1556890	-3.5512060
C	-0.3138180	3.1556890	3.5512060
H	-1.2810550	3.6354070	-3.3516100
H	-1.2810550	3.6354070	3.3516100
H	0.4984000	3.8675600	-3.3532440
H	0.4984000	3.8675600	3.3532440
H	-0.2743200	2.8402140	-4.5951120
H	-0.2743200	2.8402140	4.5951120

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TS2c B3LYP/6-31+G(d) Optimized Geometry

C	1.1892350	-3.6926650	0.7014700
C	1.1892350	-3.6926650	-0.7014700
C	-4.7552140	-1.4974850	-0.6972280
C	-4.7552140	-1.4974850	0.6972280
C	0.5522910	-2.6729460	-1.4124280
C	0.5522910	-2.6729460	1.4124280
C	-3.5762420	-1.2139840	-1.4079410
C	-3.5762420	-1.2139840	1.4079410
C	-2.4112930	-0.9370290	-0.7046950
C	-2.4112930	-0.9370290	0.7046950
C	-0.1093100	-1.6647360	-0.6978830
C	-0.1093100	-1.6647360	0.6978830
H	1.6955510	-4.5001280	1.2185800
H	1.6955510	-4.5001280	-1.2185800
H	-5.6724850	-1.7094200	-1.2405540
H	-5.6724850	-1.7094200	1.2405540
O	0.5068490	-2.5838040	-2.7824970
O	0.5068490	-2.5838040	2.7824970
C	1.0881890	-3.6308780	-3.5454470
H	0.9149010	-3.3692000	-4.5910490
H	2.1687890	-3.7074440	-3.3638010
H	0.6120960	-4.5962490	-3.3270790
C	1.0881890	-3.6308780	3.5454470
H	0.9149010	-3.3692000	4.5910490
H	2.1687890	-3.7074440	3.3638010
H	0.6120960	-4.5962490	3.3270790
H	-3.5776550	-1.2050490	-2.4953800
H	-3.5776550	-1.2050490	2.4953800
C	-1.0269790	-0.6113160	-1.3081770
C	-1.0269790	-0.6113160	1.3081770
C	-0.7059170	0.7651190	-0.7069830
C	-0.7059170	0.7651190	0.7069830
C	-1.4781770	1.9544780	-1.1408900
C	-1.4781770	1.9544780	1.1408900
O	-1.8148120	2.6921810	0.0000000
O	-1.8273670	2.3048140	-2.2386960
O	-1.8273670	2.3048140	2.2386960
H	-1.0290040	-0.6200410	-2.3973990
H	-1.0290040	-0.6200410	2.3973990
C	3.8591280	-1.0706510	0.7059740
C	3.8591280	-1.0706510	-0.7059740
C	2.1909910	0.6860030	0.7119040
C	2.1909910	0.6860030	-0.7119040
C	3.0155940	-0.2261920	-1.4068570
C	3.0155940	-0.2261920	1.4068570
C	1.3455270	1.6478170	-1.3618270
C	1.3455270	1.6478170	1.3618270
C	0.7660320	5.3093660	-0.7059380
C	0.7660320	5.3093660	0.7059380
C	1.1762850	2.9205850	-0.7125550
C	1.1762850	2.9205850	0.7125550
C	0.9456760	4.1296280	-1.4075690
C	0.9456760	4.1296280	1.4075690
H	4.5240230	-1.7420050	1.2432120
H	4.5240230	-1.7420050	-1.2432120
H	3.0042070	-0.2329570	-2.4940920
H	3.0042070	-0.2329570	2.4940920
H	1.2580140	1.6117750	-2.4459420
H	1.2580140	1.6117750	2.4459420
H	0.6103720	6.2404050	-1.2442050
H	0.6103720	6.2404050	1.2442050
H	0.9196870	4.1228210	2.4940670
H	0.9196870	4.1228210	-2.4940670

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TS3c B3LYP/6-31+G(d) Optimized Geometry

C	-4.2454510	0.7859600	0.6981970

C	-4.2454510	0.7859600	-0.6981970
C	0.9863780	4.3843110	-0.7000810
C	0.9863780	4.3843110	0.7000810
C	-3.0357770	0.7419710	-1.4045480
C	-3.0357770	0.7419710	1.4045480
C	0.5324530	3.2682760	-1.4170410
C	0.5324530	3.2682760	1.4170410
C	0.0959610	2.1501980	-0.6992820
C	0.0959610	2.1501980	0.6992820
C	-1.8343560	0.7028650	-0.7035870
C	-1.8343560	0.7028650	0.7035870
H	-5.1861670	0.8292870	1.2414800
H	-5.1861670	0.8292870	-1.2414800
H	1.3455540	5.2668960	-1.2177690
H	1.3455540	5.2668960	1.2177690
O	0.4741600	3.1872100	-2.7835420
O	0.4741600	3.1872100	2.7835420
C	1.0167880	4.2548600	-3.5474680
H	0.4663910	5.1900390	-3.3768690
H	2.0800460	4.4059310	-3.3194340
H	0.9087060	3.9569940	-4.5919150
C	1.0167880	4.2548600	3.5474680
H	0.4663910	5.1900390	3.3768690
H	2.0800460	4.4059310	3.3194340
H	0.9087060	3.9569940	4.5919150
H	-3.0341680	0.7596270	-2.4923580
H	-3.0341680	0.7596270	2.4923580
C	-0.4415450	0.8351830	-1.3081420
C	-0.4415450	0.8351830	1.3081420
C	0.4939760	-0.2253540	-0.7076330
C	0.4939760	-0.2253540	0.7076330
C	1.9118420	-0.2805940	-1.1415510
C	1.9118420	-0.2805940	1.1415510
O	2.7088420	-0.4260480	0.0000000
O	2.4010840	-0.2047150	-2.2390050
O	2.4010840	-0.2047150	2.2390050
H	-0.4355160	0.8520290	-2.3976590
H	-0.4355160	0.8520290	2.3976590
C	-3.6264690	-2.9412940	0.7058280
C	-3.6264690	-2.9412940	-0.7058280
C	-1.2329020	-2.5626340	0.7118560
C	-1.2329020	-2.5626340	-0.7118560
C	-2.4519590	-2.7256930	-1.4057320
C	-2.4519590	-2.7256930	1.4057320
C	0.0400830	-2.4108790	-1.3608410
C	0.0400830	-2.4108790	1.3608410
C	3.3755660	-4.0310670	-0.7057600
C	3.3755660	-4.0310670	0.7057600
C	1.1813710	-3.0017340	-0.7124280
C	1.1813710	-3.0017340	0.7124280
C	2.3045040	-3.5044510	-1.4074960
C	2.3045040	-3.5044510	1.4074960
H	-4.5564330	-3.1044760	1.2439900
H	-4.5564330	-3.1044760	-1.2439900
H	-2.4515100	-2.7154210	-2.4932820
H	-2.4515100	-2.7154210	2.4932820
H	0.0609140	-2.3207220	-2.4453240
H	0.0609140	-2.3207220	2.4453240
H	4.2282820	-4.4358460	-1.2441360
H	4.2282820	-4.4358460	1.2441360
H	2.3138090	-3.4796550	2.4940060
H	2.3138090	-3.4796550	-2.4940060

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1d B3LYP/AVDZ’ Optimized Geometry

C	-2.1528660	3.7541100	0.6982110
C	-2.1528660	3.7541100	-0.6982110
C	3.0029980	-0.3074020	-0.6962590
C	3.0029980	-0.3074020	0.6962590
C	-1.7297500	2.6189460	-1.4101540
C	-1.7297500	2.6189460	1.4101540
C	1.7955790	-0.1624020	-1.3960070
C	1.7955790	-0.1624020	1.3960070
C	0.5948800	-0.0212400	-0.7073880
C	0.5948800	-0.0212400	0.7073880
C	-1.3155840	1.4947740	-0.7033620
C	-1.3155840	1.4947740	0.7033620
H	-2.4847130	4.6402020	1.2434980
H	-2.4847130	4.6402020	-1.2434980
H	3.9401090	-0.4215020	-1.2416620
H	3.9401090	-0.4215020	1.2416620
H	-1.7274760	2.6196290	-2.5025630
H	-1.7274760	2.6196290	2.5025630
Br	1.8487810	-0.1640920	-3.3136030
Br	1.8487810	-0.1640920	3.3136030
C	-0.8085560	0.1748560	-1.3135910
C	-0.8085560	0.1748560	1.3135910
C	-1.6550550	-0.8987220	-0.6710190
C	-1.6550550	-0.8987220	0.6710190

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C       -2.5362260       -1.9898600       -1.1452300
C       -2.5362260       -1.9898600        1.1452300
O       -3.0445310       -2.6236820        0.0000000
O       -2.8273310       -2.3430250       -2.2528270
O       -2.8273310       -2.3430250        2.2528270
H       -0.8110020        0.1654460       -2.4063410
H       -0.8110020        0.1654460        2.4063410

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2d B3LYP/AVDZ' Optimized Geometry
C       -4.0288990       -0.4123110        0.6983310
C       -4.0288990       -0.4123110       -0.6983310
C       -1.2288520        5.4234640       -0.6983790
C       -1.2288520        5.4234640        0.6983790
C       -2.9857930        0.2020380       -1.4055210
C       -2.9857930        0.2020380        1.4055210
C       -1.0917470        4.2217970       -1.4069180
C       -1.0917470        4.2217970        1.4069180
C       -0.9663270        3.0270460       -0.7038070
C       -0.9663270        3.0270460        0.7038070
C       -1.9538360        0.8169370       -0.7031740
C       -1.9538360        0.8169370        0.7031740
H       -4.8421900       -0.8866360        1.2414930
H       -4.8421900       -0.8866360       -1.2414930
H       -1.3303560        6.3595990       -1.2409700
H       -1.3303560        6.3595990        1.2409700
H       -2.9887030        0.2063890       -2.4934060
H       -2.9887030        0.2063890        2.4934060
H       -1.0780930        4.2229760       -2.4942510
H       -1.0780930        4.2229760        2.4942510
C       -0.8174020        1.6290660       -1.3028630
C       -0.8174020        1.6290660        1.3028630
C        0.5682050        1.0840060       -0.7780190
C        0.5682050        1.0840060        0.7780190
C        1.6523110        2.1008300       -1.1447430
C        1.6523110        2.1008300        1.1447430
O        2.2230460        2.6366370        0.0000000
O        2.0104070        2.4353860       -2.2394780
O        2.0104070        2.4353860        2.2394780
H       -0.8297660        1.6403570       -2.3960290
H       -0.8297660        1.6403570        2.3960290
C       -1.2088570       -3.4230940        0.6978540
C       -1.2088570       -3.4230940       -0.6978540
C        0.1548860       -1.4117500       -0.7027150
C        0.1548860       -1.4117500        0.7027150
C       -0.5306460       -2.4114240       -1.3731840
C       -0.5306460       -2.4114240        1.3731840
C        1.0317160       -0.3301870       -1.3059170
C        1.0317160       -0.3301870        1.3059170
C        2.4169370       -0.5686770       -0.7036870
C        2.4169370       -0.5686770        0.7036870
C        4.7929000       -0.9711790       -0.6984390
C        4.7929000       -0.9711790        0.6984390
C        3.6016070       -0.7643370       -1.4075180
C        3.6016070       -0.7643370        1.4075180
H       -1.7273250       -4.1919500        1.2612910
H       -1.7273250       -4.1919500       -1.2612910
Br      -0.5423090       -2.4122620       -3.4357940
Br      -0.5423090       -2.4122620        3.4357940
H        1.0402370       -0.3473430       -2.3971260
H        1.0402370       -0.3473430        2.3971260
H        5.7215220       -1.1269060       -1.2409740
H        5.7215220       -1.1269060        1.2409740
H        3.6028110       -0.7503000        2.4946770
H        3.6028110       -0.7503000       -2.4946770

55
3d B3LYP/AVDZ' Optimized Geometry
C       -3.0647050        3.9929510        0.6983220
C       -3.0647050        3.9929510       -0.6983220
C        3.3752880        4.3521770       -0.6983560
C        3.3752880        4.3521770        0.6983560
C       -2.0281280        3.3678580       -1.4044940
C       -2.0281280        3.3678580        1.4044940
C        2.3938310        3.6456090       -1.4069980
C        2.3938310        3.6456090        1.4069980
C        1.4120670        2.9532960       -0.7038430
C        1.4120670        2.9532960        0.7038430
C       -0.9974790        2.7501550       -0.7028520
C       -0.9974790        2.7501550        0.7028520
H       -3.8682930        4.4836670        1.2413370
H       -3.8682930        4.4836670       -1.2413370
H        4.1428250        4.8977710       -1.2408330
H        4.1428250        4.8977710        1.2408330
H       -2.0238340        3.3756240       -2.4925220
H       -2.0238340        3.3756240        2.4925220
H        2.4019580        3.6341050       -2.4943240
H        2.4019580        3.6341050        2.4943240
C        0.2611430        2.1446620       -1.3026450
C        0.2611430        2.1446620        1.3026450
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C	0.4592010	0.6685580	-0.7778510
C	0.4592010	0.6685580	0.7778510
C	1.8763740	0.2205810	-1.1453770
C	1.8763740	0.2205810	1.1453770
O	2.6217470	-0.0204730	0.0000000
O	2.3444400	0.0737990	-2.2395550
O	2.3444400	0.0737990	2.2395550
H	0.2663690	2.1602930	-2.3959100
H	0.2663690	2.1602930	2.3959100
C	-4.3355300	-0.0051460	0.6983050
C	-4.3355300	-0.0051460	-0.6983050
C	-1.9321930	-0.1948010	-0.7027920
C	-1.9321930	-0.1948010	0.7027920
C	-3.1293770	-0.0997830	-1.4052610
C	-3.1293770	-0.0997830	1.4052610
C	-0.5542420	-0.4220960	-1.3054910
C	-0.5542420	-0.4220960	1.3054910
C	-0.0848370	-1.7442250	-0.7040330
C	-0.0848370	-1.7442250	0.7040330
C	0.6842000	-4.0479370	-0.6975510
C	0.6842000	-4.0479370	0.6975510
C	0.2977330	-2.8938500	-1.3774460
C	0.2977330	-2.8938500	1.3774460
H	-5.2746710	0.0625730	1.2411830
H	-5.2746710	0.0625730	-1.2411830
H	-3.1299180	-0.1090750	-2.4930610
H	-3.1299180	-0.1090750	2.4930610
H	-0.5580340	-0.4438530	-2.3968950
H	-0.5580340	-0.4438530	2.3968950
H	0.9763990	-4.9284570	-1.2603130
H	0.9763990	-4.9284570	1.2603130
Br	0.2864170	-2.9076920	3.4358920
Br	0.2864170	-2.9076920	-3.4358920

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TS2d B3LYP/AVDZ' Optimized Geometry

C	1.1141770	-3.4463620	0.6966440
C	1.1141770	-3.4463620	-0.6966440
C	-4.8179900	-1.1429690	-0.6979710
C	-4.8179900	-1.1429690	0.6979710
C	0.4716510	-2.4142100	-1.3905900
C	0.4716510	-2.4142100	1.3905900
C	-3.6347140	-0.8795670	-1.4104310
C	-3.6347140	-0.8795670	1.4104310
C	-2.4653220	-0.6186580	-0.7047630
C	-2.4653220	-0.6186580	0.7047630
C	-0.1797900	-1.3892490	-0.7080810
C	-0.1797900	-1.3892490	0.7080810
H	1.6093510	-4.2492690	1.2429340
H	1.6093510	-4.2492690	-1.2429340
H	-5.7429020	-1.3430620	-1.2432190
H	-5.7429020	-1.3430620	1.2432190
Br	0.4932390	-2.4721430	-3.3114420
Br	0.4932390	-2.4721430	3.3114420
H	-3.6355640	-0.8740090	-2.5027060
H	-3.6355640	-0.8740090	2.5027060
C	-1.0773440	-0.3121280	-1.3070330
C	-1.0773440	-0.3121280	1.3070330
C	-0.7232580	1.0559650	-0.7076930
C	-0.7232580	1.0559650	0.7076930
C	-1.4809930	2.2574900	-1.1408510
C	-1.4809930	2.2574900	1.1408510
O	-1.8021310	3.0025240	0.0000000
O	-1.8308130	2.6089100	-2.2362300
O	-1.8308130	2.6089100	2.2362300
H	-1.0820760	-0.3168850	-2.4005780
H	-1.0820760	-0.3168850	2.4005780
C	3.8114000	-0.8645630	0.7065270
C	3.8114000	-0.8645630	-0.7065270
C	2.1724940	0.9225880	0.7124760
C	2.1724940	0.9225880	-0.7124760
C	2.9831390	-0.0033310	-1.4086600
C	2.9831390	-0.0033310	1.4086600
C	1.3425270	1.8999370	-1.3636660
C	1.3425270	1.8999370	1.3636660
C	0.8244200	5.5733710	-0.7064560
C	0.8244200	5.5733710	0.7064560
C	1.1919100	3.1758430	-0.7130760
C	1.1919100	3.1758430	0.7130760
C	0.9831800	4.3897060	-1.4092080
C	0.9831800	4.3897060	1.4092080
H	4.4667380	-1.5503510	1.2477830
H	4.4667380	-1.5503510	-1.2477830
H	2.9752680	-0.0097900	-2.5007680
H	2.9752680	-0.0097900	2.5007680
H	1.2603040	1.8670960	-2.4534500
H	1.2603040	1.8670960	2.4534500
H	0.6874520	6.5119930	-1.2473710
H	0.6874520	6.5119930	1.2473710
H	0.9601790	4.3847100	2.5007820

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H        0.9601790        4.3847100       -2.5007820

55
TS3d B3LYP/AVDZ' Optimized Geometry
C        4.2707420       -0.4228390        0.6989640
C        4.2707420       -0.4228390       -0.6989640
C       -0.9104890       -4.0728700       -0.6956570
C       -0.9104890       -4.0728700        0.6956570
C        3.0610620       -0.3808850       -1.4069210
C        3.0610620       -0.3808850        1.4069210
C       -0.4767570       -2.9352210       -1.3955210
C       -0.4767570       -2.9352210        1.3955210
C       -0.0600540       -1.8002570       -0.7092250
C       -0.0600540       -1.8002570        0.7092250
C        1.8588980       -0.3413520       -0.7035340
C        1.8588980       -0.3413520        0.7035340
H        5.2161790       -0.4672360        1.2442120
H        5.2161790       -0.4672360       -1.2442120
H       -1.2446290       -4.9551300       -1.2419130
H       -1.2446290       -4.9551300        1.2419130
H        3.0596180       -0.4005870       -2.4994100
H        3.0596180       -0.4005870        2.4994100
Br      -0.4612840       -3.0062160       -3.3132390
Br      -0.4612840       -3.0062160        3.3132390
C        0.4659970       -0.4746940       -1.3066980
C        0.4659970       -0.4746940        1.3066980
C       -0.4765410        0.5789870       -0.7082660
C       -0.4765410        0.5789870        0.7082660
C       -1.8975120        0.6261280       -1.1416160
C       -1.8975120        0.6261280        1.1416160
O       -2.6946440        0.7722070        0.0000000
O       -2.3852830        0.5411640       -2.2369290
O       -2.3852830        0.5411640        2.2369290
H        0.4636970       -0.4865060       -2.4005940
H        0.4636970       -0.4865060        2.4005940
C        3.6432600        3.2913780        0.7064190
C        3.6432600        3.2913780       -0.7064190
C        1.2480470        2.9108880        0.7123000
C        1.2480470        2.9108880       -0.7123000
C        2.4678860        3.0750210       -1.4073770
C        2.4678860        3.0750210        1.4073770
C       -0.0258930        2.7583790       -1.3625680
C       -0.0258930        2.7583790        1.3625680
C       -3.3657390        4.3757190       -0.7062850
C       -3.3657390        4.3757190        0.7062850
C       -1.1698910        3.3460200       -0.7129720
C       -1.1698910        3.3460200        0.7129720
C       -2.2937990        3.8489890       -1.4092330
C       -2.2937990        3.8489890        1.4092330
H        4.5771770        3.4582610        1.2472160
H        4.5771770        3.4582610       -1.2472160
H        2.4677710        3.0662470       -2.4999420
H        2.4677710        3.0662470        2.4999420
H       -0.0448520        2.6725760       -2.4525600
H       -0.0448520        2.6725760        2.4525600
H       -4.2217110        4.7843870       -1.2472390
H       -4.2217110        4.7843870        1.2472390
H       -2.3027580        3.8270410        2.5007880
H       -2.3027580        3.8270410       -2.5007880


31
1e B3LYP/6-31+G(d) Optimized Geometry
C       -3.8314270       -1.4982650        0.6975880
C       -3.8314270       -1.4982650       -0.6975880
C        0.5831970        3.3525510       -0.6951930
C        0.5831970        3.3525510        0.6951930
C       -2.6700920       -1.1560810       -1.4086970
C       -2.6700920       -1.1560810        1.4086970
C        0.3524570        2.1602920       -1.3952310
C        0.3524570        2.1602920        1.3952310
C        0.1275250        0.9752880       -0.7055810
C        0.1275250        0.9752880        0.7055810
C       -1.5210960       -0.8218510       -0.7028180
C       -1.5210960       -0.8218510        0.7028180
H       -4.7338550       -1.7660400        1.2403640
H       -4.7338550       -1.7660400       -1.2403640
H        0.7625470        4.2721320       -1.2424100
H        0.7625470        4.2721320        1.2424100
H       -2.6704040       -1.1549010       -2.4959400
H       -2.6704040       -1.1549010        2.4959400
Cl       0.3528920        2.1991410       -3.1514360
Cl       0.3528920        2.1991410        3.1514360
C       -0.1678260       -0.4091130       -1.3136640
C       -0.1678260       -0.4091130        1.3136640
C        0.8411910       -1.3302110       -0.6698700
C        0.8411910       -1.3302110        0.6698700
C        1.8616470       -2.2896860       -1.1455550
C        1.8616470       -2.2896860        1.1455550
O        2.4550960       -2.8429940        0.0000000
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O        2.1908210       -2.6060030       -2.2549280
O        2.1908210       -2.6060030        2.2549280
H       -0.1578580       -0.4141260       -2.4022970
H       -0.1578580       -0.4141260        2.4022970

55
2e B3LYP/6-31+G(d) Optimized Geometry
C       -4.1637080        0.0097150        0.6982380
C       -4.1637080        0.0097150       -0.6982380
C       -0.3668120        5.2570410       -0.6984060
C       -0.3668120        5.2570410        0.6984060
C       -3.0291310        0.4316160       -1.4055740
C       -3.0291310        0.4316160        1.4055740
C       -0.4474030        4.0502810       -1.4069970
C       -0.4474030        4.0502810        1.4069970
C       -0.5385760        2.8525290       -0.7038650
C       -0.5385760        2.8525290        0.7038650
C       -1.9047810        0.8543710       -0.7031130
C       -1.9047810        0.8543710        0.7031130
H       -5.0478670       -0.3135890        1.2415850
H       -5.0478670       -0.3135890       -1.2415850
H       -0.2979730        6.1961710       -1.2409550
H       -0.2979730        6.1961710        1.2409550
H       -3.0313510        0.4360210       -2.4932360
H       -3.0313510        0.4360210        2.4932360
H       -0.4330670        4.0487750       -2.4943180
H       -0.4330670        4.0487750        2.4943180
C       -0.6419340        1.4503370       -1.3028180
C       -0.6419340        1.4503370        1.3028180
C        0.6244000        0.6669480       -0.7770740
C        0.6244000        0.6669480        0.7770740
C        1.8723890        1.4737130       -1.1448560
C        1.8723890        1.4737130        1.1448560
O        2.5272410        1.9026540        0.0000000
O        2.2848960        1.7379340       -2.2396390
O        2.2848960        1.7379340        2.2396390
H       -0.6518550        1.4629960       -2.3958930
H       -0.6518550        1.4629960        2.3958930
C       -1.9181260       -3.4609060        0.6958700
C       -1.9181260       -3.4609060       -0.6958700
C       -0.2297650       -1.7217010       -0.7051770
C       -0.2297650       -1.7217010        0.7051770
C       -1.0759710       -2.5867980       -1.3906810
C       -1.0759710       -2.5867980        1.3906810
C        0.8282690       -0.8069920       -1.3011930
C        0.8282690       -0.8069920        1.3011930
C        2.1483190       -1.2907620       -0.7030410
C        2.1483190       -1.2907620        0.7030410
C        4.4096240       -2.1213580       -0.6985110
C        4.4096240       -2.1213580        0.6985110
C        3.2766540       -1.7000860       -1.4079930
C        3.2766540       -1.7000860        1.4079930
H       -2.5682700       -4.1354990        1.2431150
H       -2.5682700       -4.1354990       -1.2431150
Cl      -1.1075400        -2.6118170       -3.1505570
Cl      -1.1075400        -2.6118170        3.1505570
H        0.8357890       -0.8226110       -2.3916420
H        0.8357890       -0.8226110        2.3916420
H        5.2939200       -2.4453900       -1.2406840
H        5.2939200       -2.4453900        1.2406840
H        3.2800370       -1.6877660        2.4951050
H        3.2800370       -1.6877660       -2.4951050

55
3e B3LYP/6-31+G(d) Optimized Geometry
C        3.2458780       -3.4102300        0.6983280
C        3.2458780       -3.4102300       -0.6983280
C       -3.1621600       -4.1730980       -0.6983890
C       -3.1621600       -4.1730980        0.6983890
C        2.1716720       -2.8523650       -1.4044300
C        2.1716720       -2.8523650        1.4044300
C       -2.2255840       -3.4077620       -1.4068850
C       -2.2255840       -3.4077620        1.4068850
C       -1.2879390       -2.6568900       -0.7038400
C       -1.2879390       -2.6568900        0.7038400
C        1.1039920       -2.3011550       -0.7028010
C        1.1039920       -2.3011550        0.7028010
H        4.0790420       -3.8488770        1.2413280
H        4.0790420       -3.8488770       -1.2413280
H       -3.8951240       -4.7641670       -1.2410230
H       -3.8951240       -4.7641670        1.2410230
H        2.1678020       -2.8603320       -2.4924560
H        2.1678020       -2.8603320        2.4924560
H       -2.2346210       -3.3961410       -2.4941850
H       -2.2346210       -3.3961410        2.4941850
C       -0.1902970       -1.7771800       -1.3026140
C       -0.1902970       -1.7771800        1.3026140
C       -0.4834450       -0.3170090       -0.7770070
C       -0.4834450       -0.3170090        0.7770070
C       -1.9272480        0.0367370       -1.1453050
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C	-1.9272480	0.0367370	1.1453050
O	-2.6861670	0.2310660	0.0000000
O	-2.4051800	0.1470760	-2.2393670
O	-2.4051800	0.1470760	2.2393670
H	-0.1947630	-1.7926690	-2.3958850
H	-0.1947630	-1.7926690	2.3958850
C	4.2587390	0.6667830	0.6983830
C	4.2587390	0.6667830	-0.6983830
C	1.8489970	0.6975000	-0.7022050
C	1.8489970	0.6975000	0.7022050
C	3.0491990	0.6820250	-1.4057540
C	3.0491990	0.6820250	1.4057540
C	0.4583920	0.8353040	-1.3007790
C	0.4583920	0.8353040	1.3007790
C	-0.0929550	2.1321450	-0.7063140
C	-0.0929550	2.1321450	0.7063140
C	-0.9829330	4.3850840	-0.6957040
C	-0.9829330	4.3850840	0.6957040
C	-0.5341890	3.2584910	-1.3951700
C	-0.5341890	3.2584910	1.3951700
H	5.2004610	0.6607150	1.2409860
H	5.2004610	0.6607150	-1.2409860
H	3.0490250	0.6919230	-2.4934760
H	3.0490250	0.6919230	2.4934760
H	0.4630070	0.8548590	-2.3915220
H	0.4630070	0.8548590	2.3915220
H	-1.3244120	5.2579880	-1.2421610
H	-1.3244120	5.2579880	1.2421610
Cl	-0.5191190	3.3120910	3.1506350
Cl	-0.5191190	3.3120910	-3.1506350

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TS2e B3LYP/6-31+G(d) Optimized Geometry

C	1.5927160	-3.6214100	0.6957550
C	1.5927160	-3.6214100	-0.6957550
C	-4.5552710	-1.9912510	-0.6973460
C	-4.5552710	-1.9912510	0.6973460
C	0.8412300	-2.6681520	-1.3899560
C	0.8412300	-2.6681520	1.3899560
C	-3.4086610	-1.5999230	-1.4088390
C	-3.4086610	-1.5999230	1.4088390
C	-2.2761660	-1.2128840	-0.7041840
C	-2.2761660	-1.2128840	0.7041840
C	0.0806890	-1.7253780	-0.7059040
C	0.0806890	-1.7253780	0.7059040
H	2.1711580	-4.3578810	1.2437860
H	2.1711580	-4.3578810	-1.2437860
H	-5.4482920	-2.2891890	-1.2402970
H	-5.4482920	-2.2891890	1.2402970
Cl	0.8635060	-2.7039130	-3.1500580
Cl	0.8635060	-2.7039130	3.1500580
H	-3.4106210	-1.5933520	-2.4960790
H	-3.4106210	-1.5933520	2.4960790
C	-0.9301540	-0.7559620	-1.3073280
C	-0.9301540	-0.7559620	1.3073280
C	-0.7315150	0.6428940	-0.7070190
C	-0.7315150	0.6428940	0.7070190
C	-1.6181830	1.7502250	-1.1408650
C	-1.6181830	1.7502250	1.1408650
O	-2.0224870	2.4520200	0.0000000
O	-2.0014410	2.0609080	-2.2386860
O	-2.0014410	2.0609080	2.2386860
H	-0.9357040	-0.7597470	-2.3967200
H	-0.9357040	-0.7597470	2.3967200
C	3.9791180	-0.7664470	0.7059150
C	3.9791180	-0.7664470	-0.7059150
C	2.1601380	0.8337570	0.7119700
C	2.1601380	0.8337570	-0.7119700
C	3.0639460	0.0002830	-1.4071930
C	3.0639460	0.0002830	1.4071930
C	1.2266270	1.7119840	-1.3618730
C	1.2266270	1.7119840	1.3618730
C	0.3005400	5.3012790	-0.7058470
C	0.3005400	5.3012790	0.7058470
C	0.9360960	2.9628650	-0.7125000
C	0.9360960	2.9628650	0.7125000
C	0.5920210	4.1442290	-1.4079230
C	0.5920210	4.1442290	1.4079230
H	4.6996950	-1.3761660	1.2445100
H	4.6996950	-1.3761660	-1.2445100
H	3.0556860	-0.0076500	-2.4943180
H	3.0556860	-0.0076500	2.4943180
H	1.1436120	1.6688340	-2.4461420
H	1.1436120	1.6688340	2.4461420
H	0.0582560	6.2135970	-1.2439810
H	0.0582560	6.2135970	1.2439810
H	0.5690700	4.1360860	2.4944410
H	0.5690700	4.1360860	-2.4944410

55
TS3e B3LYP/6-31+G(d) Optimized Geometry

C	-4.1006880	1.2537950	0.6983310
C	-4.1006880	1.2537950	-0.6983310
C	1.4161100	4.3539990	-0.6947330
C	1.4161100	4.3539990	0.6947330
C	-2.9026360	1.0873490	-1.4053400
C	-2.9026360	1.0873490	1.4053400
C	0.8717760	3.2669130	-1.3948480
C	0.8717760	3.2669130	1.3948480
C	0.3438850	2.1823520	-0.7071780
C	0.3438850	2.1823520	0.7071780
C	-1.7121950	0.9249090	-0.7029640
C	-1.7121950	0.9249090	0.7029640
H	-5.0319190	1.3937860	1.2412120
H	-5.0319190	1.3937860	-1.2412120
H	1.8349040	5.1917610	-1.2424890
H	1.8349040	5.1917610	1.2424890
H	-2.8994620	1.1061320	-2.4929260
H	-2.8994620	1.1061320	2.4929260
Cl	0.8633300	3.3203810	-3.1515120
Cl	0.8633300	3.3203810	3.1515120
C	-0.3126960	0.9178450	-1.3066690
C	-0.3126960	0.9178450	1.3066690
C	0.5192750	-0.2253380	-0.7072190
C	0.5192750	-0.2253380	0.7072190
C	1.9256490	-0.4152700	-1.1415920
C	1.9256490	-0.4152700	1.1415920
O	2.7040820	-0.6369030	0.0000000
O	2.4171160	-0.3832140	-2.2395080
O	2.4171160	-0.3832140	2.2395080
H	-0.3083430	0.9284080	-2.3964110
H	-0.3083430	0.9284080	2.3964110
C	-3.8517760	-2.5119170	0.7058610
C	-3.8517760	-2.5119170	-0.7058610
C	-1.4328510	-2.3736080	0.7118470
C	-1.4328510	-2.3736080	-0.7118470
C	-2.6618290	-2.4146970	-1.4061400
C	-2.6618290	-2.4146970	1.4061400
C	-0.1516820	-2.3528440	-1.3612690
C	-0.1516820	-2.3528440	1.3612690
C	3.0122770	-4.2845190	-0.7058330
C	3.0122770	-4.2845190	0.7058330
C	0.9270120	-3.0502060	-0.7123840
C	0.9270120	-3.0502060	0.7123840
C	1.9969310	-3.6576400	-1.4077910
C	1.9969310	-3.6576400	1.4077910
H	-4.7932220	-2.5835870	1.2438730
H	-4.7932220	-2.5835870	-1.2438730
H	-2.6605370	-2.4068910	-2.4936700
H	-2.6605370	-2.4068910	2.4936700
H	-0.1213970	-2.2659450	-2.4457720
H	-0.1213970	-2.2659450	2.4457720
H	3.8222100	-4.7691660	-1.2440840
H	3.8222100	-4.7691660	1.2440840
H	2.0085240	-3.6343910	2.4942390
H	2.0085240	-3.6343910	-2.4942390

55
2f B3LYP/6-31+G(d) Optimized Geometry

C	-4.1566430	0.8347600	0.6983310
C	-4.1566430	0.8347600	-0.6983310
C	0.7566830	5.0485180	-0.6983790
C	0.7566830	5.0485180	0.6983790
C	-2.9544460	0.9769520	-1.4055210
C	-2.9544460	0.9769520	1.4055210
C	0.3981900	3.8934060	-1.4069180
C	0.3981900	3.8934060	1.4069180
C	0.0317870	2.7493300	-0.7038070
C	0.0317870	2.7493300	0.7038070
C	-1.7622330	1.1241390	-0.7031740
C	-1.7622330	1.1241390	0.7031740
H	-5.0920920	0.7281710	1.2414930
H	-5.0920920	0.7281710	-1.2414930
H	1.0408160	5.9462490	-1.2409700
H	1.0408160	5.9462490	1.2409700
H	-2.9553570	0.9821070	-2.4934060
H	-2.9553570	0.9821070	2.4934060
H	0.4111620	3.8889860	-2.4942510
H	0.4111620	3.8889860	2.4942510
C	-0.3949550	1.4097720	-1.3028630
C	-0.3949550	1.4097720	1.3028630
C	0.6537680	0.3528060	-0.7780190
C	0.6537680	0.3528060	0.7780190
C	2.0555930	0.8468720	-1.1447430
C	2.0555930	0.8468720	1.1447430
O	2.7937930	1.1074280	0.0000000
O	2.5181070	1.0088650	-2.2394780
O	2.5181070	1.0088650	2.2394780

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H       -0.4017240        1.4250860       -2.3960290
H       -0.4017240        1.4250860        2.3960290
C       -2.7880750       -3.0568310        0.6978540
C       -2.7880750       -3.0568310       -0.6978540
C       -0.7297410       -1.7651020       -0.7027150
C       -0.7297410       -1.7651020        0.7027150
C       -1.7598430       -2.4040020       -1.3731840
C       -1.7598430       -2.4040020        1.3731840
C        0.5084380       -1.1282960       -1.3059170
C        0.5084380       -1.1282960        1.3059170
C        1.6802830       -1.9045020       -0.7036870
C        1.6802830       -1.9045020        0.7036870
C        3.6929000       -3.2298620       -0.6984390
C        3.6929000       -3.2298620        0.6984390
C        2.6858120       -2.5607310       -1.4075180
C        2.6858120       -2.5607310        1.4075180
H       -3.5722970       -3.5517490        1.2612910
H       -3.5722970       -3.5517490       -1.2612910
F       -1.7708550       -2.4000720       -2.7357940
F       -1.7708550       -2.4000720        2.7357940
H        0.5093280       -1.1474320       -2.3971260
H        0.5093280       -1.1474320        2.3971260
H        4.4801510       -3.7464140       -1.2409740
H        4.4801510       -3.7464140        1.2409740
H        2.6925680       -2.5483680        2.4946770
H        2.6925680       -2.5483680       -2.4946770

55
3f B3LYP/6-31+G(d) Optimized Geometry
C        3.4030350       -2.9941820        0.6983220
C        3.4030350       -2.9941820       -0.6983220
C       -2.9427500       -4.1489870       -0.6983560
C       -2.9427500       -4.1489870        0.6983560
C        2.2969620       -2.5024120       -1.4044940
C        2.2969620       -2.5024120        1.4044940
C       -2.0564550       -3.3262000       -1.4069980
C       -2.0564550       -3.3262000        1.4069980
C       -1.1680880       -2.5175210       -0.7038430
C       -1.1680880       -2.5175210        0.7038430
C        1.1976880       -2.0172410       -0.7028520
C        1.1976880       -2.0172410        0.7028520
H        4.2612570       -3.3814940        1.2413370
H        4.2612570       -3.3814940       -1.2413370
H       -3.6367300       -4.7855220       -1.2408330
H       -3.6367300       -4.7855220        1.2408330
H        2.2936640       -2.5106510       -2.4925220
H        2.2936640       -2.5106510        2.4925220
H       -2.0659460       -3.3157920       -2.4943240
H       -2.0659460       -3.3157920        2.4943240
C       -0.1262870       -1.5724470       -1.3026450
C       -0.1262870       -1.5724470        1.3026450
C       -0.5058060       -0.1322820       -0.7778510
C       -0.5058060       -0.1322820        0.7778510
C       -1.9675820        0.1365560       -1.1453770
C       -1.9675820        0.1365560        1.1453770
O       -2.7370880        0.2833480        0.0000000
O       -2.4502340        0.2241810       -2.2395550
O       -2.4502340        0.2241810        2.2395550
H       -0.1295350       -1.5886050       -2.3959100
H       -0.1295350       -1.5886050        2.3959100
C        4.1684220        1.1306160        0.6983050
C        4.1684220        1.1306160       -0.6983050
C        1.7601130        1.0208720       -0.7027920
C        1.7601130        1.0208720        0.7027920
C        2.9598420        1.0749990       -1.4052610
C        2.9598420        1.0749990        1.4052610
C        0.3646140        1.0755930       -1.3054910
C        0.3646140        1.0755930        1.3054910
C       -0.2650710        2.3293320       -0.7040330
C       -0.2650710        2.3293320        0.7040330
C       -1.3137620        4.5199390       -0.6975510
C       -1.3137620        4.5199390        0.6975510
C       -0.7872060        3.4226630       -1.3774460
C       -0.7872060        3.4226630        1.3774460
H        5.1087140        1.1798420        1.2411830
H        5.1087140        1.1798420       -1.2411830
H        2.9592260        1.0842870       -2.4930610
H        2.9592260        1.0842870        2.4930610
H        0.3656800        1.0976520       -2.3968950
H        0.3656800        1.0976520        2.3968950
H       -1.7128620        5.3574430       -1.2603130
H       -1.7128620        5.3574430        1.2603130
F       -0.7776940        3.4378010        2.7358920
F       -0.7776940        3.4378010       -2.7358920

31
1f B3LYP/6-31+G(d) Optimized Geometry
C       -3.9319550       -0.7530460        0.6974810
C       -3.9319550       -0.7530460       -0.6974810
C        1.0939490        3.4653250       -0.6970300
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C        1.0939490        3.4653250        0.6970300
C       -2.7350210       -0.5694710       -1.4083510
C       -2.7350210       -0.5694710        1.4083510
C        0.7039400        2.3107250       -1.3773520
C        0.7039400        2.3107250        1.3773520
C        0.3218180        1.1640830       -0.7033240
C        0.3218180        1.1640830        0.7033240
C       -1.5512930       -0.3915750       -0.7034610
C       -1.5512930       -0.3915750        0.7034610
H       -4.8619550       -0.8977960        1.2404470
H       -4.8619550       -0.8977960       -1.2404470
H        1.3925710        4.3433470       -1.2602630
H        1.3925710        4.3433470        1.2602630
H       -2.7354530       -0.5683750       -2.4956490
H       -2.7354530       -0.5683750        2.4956490
F        0.7009050        2.3192010       -2.7365780
F        0.7009050        2.3192010        2.7365780
C       -0.1549160       -0.1624680       -1.3180340
C       -0.1549160       -0.1624680        1.3180340
C        0.7211500       -1.2102990       -0.6702930
C        0.7211500       -1.2102990        0.6702930
C        1.6053280       -2.2968640       -1.1452550
C        1.6053280       -2.2968640        1.1452550
O        2.1194220       -2.9248380        0.0000000
O        1.8907200       -2.6527850       -2.2548330
O        1.8907200       -2.6527850        2.2548330
H       -0.1447640       -0.1668180       -2.4074080
H       -0.1447640       -0.1668180        2.4074080

55
TS2f B3LYP/6-31+G(d) Optimized Geometry
C        2.0823880       -3.5786470        0.6977870
C        2.0823880       -3.5786470       -0.6977870
C       -4.2109440       -2.6804620       -0.6972200
C       -4.2109440       -2.6804620        0.6972200
C        1.2259300       -2.7133840       -1.3731190
C        1.2259300       -2.7133840        1.3731190
C       -3.1180180       -2.1568820       -1.4083730
C       -3.1180180       -2.1568820        1.4083730
C       -2.0380020       -1.6401570       -0.7048010
C       -2.0380020       -1.6401570        0.7048010
C        0.3607140       -1.8633540       -0.7033760
C        0.3607140       -1.8633540        0.7033760
H        2.7347220       -4.2378400        1.2612870
H        2.7347220       -4.2378400       -1.2612870
H       -5.0628320       -3.0806910       -1.2404860
H       -5.0628320       -3.0806910        1.2404860
F        1.2323670       -2.7184990       -2.7361200
F        1.2323670       -2.7184990        2.7361200
H       -3.1215360       -2.1495270       -2.4956780
H       -3.1215360       -2.1495270        2.4956780
C       -0.7556380       -1.0268340       -1.3117820
C       -0.7556380       -1.0268340        1.3117820
C       -0.7254100        0.3850410       -0.7075320
C       -0.7254100        0.3850410        0.7075320
C       -1.7353970        1.3811740       -1.1407330
C       -1.7353970        1.3811740        1.1407330
O       -2.2193030        2.0311120        0.0000000
O       -2.1521150        1.6450010       -2.2386770
O       -2.1521150        1.6450010        2.2386770
H       -0.7578960       -1.0334900       -2.4019660
H       -0.7578960       -1.0334900        2.4019660
C        4.1177790       -0.4577580        0.7059400
C        4.1177790       -0.4577580       -0.7059400
C        2.1212500        0.9154840        0.7120110
C        2.1212500        0.9154840       -0.7120110
C        3.1171410        0.1938430       -1.4068690
C        3.1171410        0.1938430        1.4068690
C        1.0922550        1.6788040       -1.3620330
C        1.0922550        1.6788040        1.3620330
C       -0.2563620        5.1313230       -0.7058310
C       -0.2563620        5.1313230        0.7058310
C        0.6560190        2.8863380       -0.7124790
C        0.6560190        2.8863380        0.7124790
C        0.1722850        4.0177610       -1.4078430
C        0.1722850        4.0177610        1.4078430
H        4.9059760       -0.9771710        1.2444550
H        4.9059760       -0.9771710       -1.2444550
H        3.1100810        0.1854170       -2.4942860
H        3.1100810        0.1854170        2.4942860
H        1.0159770        1.6272880       -2.4465040
H        1.0159770        1.6272880        2.4465040
H       -0.6071790        6.0076340       -1.2439890
H       -0.6071790        6.0076340        1.2439890
H        0.1495680        4.0066800        2.4943530
H        0.1495680        4.0066800       -2.4943530

55
TS3f B3LYP/6-31+G(d) Optimized Geometry
C       -3.8289890        1.9737940        0.6982830
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C	-3.8289890	1.9737940	-0.6982830
C	2.0387280	4.3450920	-0.6966100
C	2.0387280	4.3450920	0.6966100
C	-2.6618590	1.6551820	-1.4049460
C	-2.6618590	1.6551820	1.4049460
C	1.3594210	3.3317760	-1.3773440
C	1.3594210	3.3317760	1.3773440
C	0.6950950	2.3221410	-0.7049580
C	0.6950950	2.3221410	0.7049580
C	-1.5018440	1.3410070	-0.7034630
C	-1.5018440	1.3410070	0.7034630
H	-4.7344460	2.2321060	1.2413820
H	-4.7344460	2.2321060	-1.2413820
H	2.5562020	5.1143900	-1.2604240
H	2.5562020	5.1143900	1.2604240
H	-2.6562520	1.6743990	-2.4925830
H	-2.6562520	1.6743990	2.4925830
F	1.3505320	3.3521670	-2.7367390
F	1.3505320	3.3521670	2.7367390
C	-0.1148360	1.1570030	-1.3110610
C	-0.1148360	1.1570030	1.3110610
C	0.5656030	-0.0819840	-0.7077890
C	0.5656030	-0.0819840	0.7077890
C	1.9374960	-0.4450570	-1.1411530
C	1.9374960	-0.4450570	1.1411530
O	2.6818750	-0.7643910	0.0000000
O	2.4298390	-0.4703450	-2.2389600
O	2.4298390	-0.4703450	2.2389600
H	-0.1077990	1.1688160	-2.4013640
H	-0.1077990	1.1688160	2.4013640
C	-4.0543020	-1.8059240	0.7058370
C	-4.0543020	-1.8059240	-0.7058370
C	-1.6372100	-1.9731950	0.7118800
C	-1.6372100	-1.9731950	-0.7118800
C	-2.8616170	-1.8594150	-1.4061720
C	-2.8616170	-1.8594150	1.4061720
C	-0.3626930	-2.1106580	-1.3612350
C	-0.3626930	-2.1106580	1.3612350
C	2.5258760	-4.4344550	-0.7058020
C	2.5258760	-4.4344550	0.7058020
C	0.6198560	-2.9383900	-0.7123980
C	0.6198560	-2.9383900	0.7123980
C	1.6012570	-3.6801400	-1.4079740
C	1.6012570	-3.6801400	1.4079740
H	-4.9973850	-1.7583800	1.2436860
H	-4.9973850	-1.7583800	-1.2436860
H	-2.8595510	-1.8516090	-2.4937030
H	-2.8595510	-1.8516090	2.4937030
H	-0.3213950	-2.0273060	-2.4456710
H	-0.3213950	-2.0273060	2.4456710
H	3.2648930	-5.0216710	-1.2439730
H	3.2648930	-5.0216710	1.2439730
H	1.6148430	-3.6605790	2.4945010
H	1.6148430	-3.6605790	-2.4945010

M05-2X optimized Cartesian Coordinates

Substituted Benzene Dimers

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24
M05-2X/6-31+G(d) Benzene...Benzene
C     0.98556144    -0.98556144    -2.02500000
C    -0.36074053    -1.34630197    -2.02500000
C     1.34630197     0.36074053    -2.02500000
C    -0.98556144     0.98556144    -2.02500000
C     0.36074053     1.34630197    -2.02500000
C    -1.34630197    -0.36074053    -2.02500000
H     1.75143711    -1.75143711    -2.02500000
H    -0.64107047    -2.39250758    -2.02500000
H    -2.39250758    -0.64107047    -2.02500000
H    -1.75143711     1.75143711    -2.02500000
H     0.64107047     2.39250758    -2.02500000
H     2.39250758     0.64107047    -2.02500000
C     0.98556144    -0.98556144     2.02500000
C     1.34630197     0.36074053     2.02500000
C     0.36074053     1.34630197     2.02500000
C    -0.98556144     0.98556144     2.02500000
C    -1.34630197    -0.36074053     2.02500000
C    -0.36074053    -1.34630197     2.02500000
H     1.75143711    -1.75143711     2.02500000
H     2.39250758     0.64107047     2.02500000
H     0.64107047     2.39250758     2.02500000
H    -1.75143711     1.75143711     2.02500000
H    -2.39250758    -0.64107047     2.02500000
H    -0.64107047    -2.39250758     2.02500000

27
M05-2X/6-31+G(d) Benzene...toluene
C       1.99830194     1.39680916     0.00711381
C       1.31942083     1.56999548    -1.19701495
C       1.30803578     1.53737669     1.20901851
C      -0.74264454     2.02005165     0.00259398
C      -0.04998621     1.84782672     1.20362774
C      -0.03863120     1.88035936    -1.19606094
H       1.82697348     1.40985302     2.15151503
H       1.84726958     1.46800279    -2.13767040
C      -2.22053565     2.32308166    -0.00029184
H      -2.50874272     2.88361325     0.89040859
H      -2.80479608     1.39893570    -0.01558503
H      -2.50037408     2.90758990    -0.87815521
H      -0.58031597     1.95932386     2.14340845
H      -0.56005943     2.01736002    -2.13744925
H       3.05507877     1.15932682     0.00889518
C       1.19271153    -2.44230816    -0.00213543
C       0.50760630    -2.30282355     1.20361255
C      -0.85698141    -2.01901561     1.20100310
C      -1.53646388    -1.87469230    -0.00735434
C      -0.85135864    -2.01417691    -1.21310232
C       0.51322906    -2.29798485    -1.21049287
H       2.25297992    -2.66282354    -0.00010792
H       1.03555608    -2.41496104     2.14249189
H      -1.38930001    -1.91063773     2.13785492
H      -2.59673226    -1.65417692    -0.00938185
H      -1.37930842    -1.90203942    -2.15198166
H       1.04554767    -2.40636273    -2.14734470

25
M05-2X/6-31+G(d) Benzene...phenol
C      -0.75082593    -1.97830694     0.00211294
C      -0.07496521    -1.83581517     1.21300112
C      -0.07112111    -1.83447740    -1.20587506
C       1.97806025    -1.40191339     0.00479676
C       1.29244022    -1.54646834    -1.19776101
C       1.28494658    -1.54857389     1.20701157
H      -0.60192575    -1.94638940    -2.14581347
H       1.81560087    -1.43576180    -2.13977687
H       1.80729635    -1.43844830     2.14956067
H      -0.62753971    -1.95273041     2.13626604
O      -2.08679922    -2.26050340     0.06081505
H      -2.44612490    -2.33620604    -0.83147169
H       3.03702321    -1.17824021     0.00715424
C      -1.55992017     1.83684381     0.00336936
C      -0.87915232     1.98037276     1.21109777
C       0.48455011     2.26841309     1.21243895
C       1.16748469     2.41292448     0.00605172
C       0.48671684     2.26939553    -1.20167669
C      -0.87698559     1.98135520    -1.20301787
H      -2.61950071     1.61303990     0.00232728
H      -1.40978436     1.86808913     2.14844629
H       1.01349861     2.37993338     2.15082955
H       2.22706523     2.63672839     0.00709380
H       1.01734888     2.38167916    -2.13902521
H      -1.40593409     1.86983492    -2.14140847

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M05-2X/6-31+G(d) Benzene...anisole

C	-0.05556317	-1.86154030	-0.25239338
C	0.33528705	-1.66202812	1.07184166
C	0.79072406	-1.47762295	-1.29806258
C	2.42235376	-0.69297672	0.30449447
C	2.01892671	-0.89835902	-1.01760166
C	1.57627967	-1.07695751	1.33686808
H	-0.30259440	-1.95097073	1.89514028
H	1.87399383	-0.92472030	2.36727869
H	2.66688279	-0.60461363	-1.83442973
H	0.46013800	-1.64510699	-2.31508497
O	-1.24016538	-2.42150876	-0.62610690
C	-2.12958190	-2.82589624	0.39922891
H	-2.43350843	-1.97346764	1.01201121
H	-1.67459725	-3.59220230	1.03189944
H	-2.99806807	-3.23927669	-0.10606516
H	3.38151702	-0.24062926	0.52124524
C	-1.73068714	1.71539130	-0.29738154
C	-1.33629739	1.91653066	1.02422848
C	-0.10091972	2.49912372	1.30186256
C	0.74006821	2.88057741	0.25788664
C	0.34567846	2.67943804	-1.06372337
C	-0.88969921	2.09684499	-1.34135746
H	-2.69056087	1.26272343	-0.51309991
H	-1.98973499	1.62014569	1.83538534
H	0.20551641	2.65540661	2.32873780
H	1.69994194	3.33324527	0.47360502
H	0.99911606	2.97582302	-1.87488024
H	-1.19613534	1.94056209	-2.36823270

24

M05-2X/6-31+G(d) Benzene...fluorobenzene

C	0.70908851	2.00325917	0.00000000
C	0.06314069	1.86063520	1.21658000
C	0.06314069	1.86063520	-1.21658000
C	-1.97938639	1.40964937	0.00000000
C	-1.29733710	1.56024447	-1.20644900
C	-1.29733710	1.56024447	1.20644900
F	2.03096993	2.29512791	0.00000000
H	0.61967023	1.98351579	2.13600000
H	0.61967023	1.98351579	-2.13600000
H	-1.82391309	1.44397756	-2.14537100
H	-1.82391309	1.44397756	2.14537100
H	-3.03611913	1.17632492	0.00000000
C	1.58953425	-1.84747914	0.00000000
C	0.90902926	-1.99773326	1.20705841
C	-0.45198071	-2.29824150	1.20705841
C	-1.13248570	-2.44849562	0.00000000
C	-0.45198071	-2.29824150	-1.20705841
C	0.90902926	-1.99773326	-1.20705841
H	2.64702278	-1.61398782	0.00000000
H	1.43777353	-1.88098760	2.14492842
H	-0.98072498	-2.41498716	2.14492842
H	-2.18997423	-2.68198694	0.00000000
H	-0.98072498	-2.41498716	-2.14492842
H	1.43777353	-1.88098760	-2.14492842

24

M05-2X/AVDZ’ Benzene...bromobenzene

C	-0.64483890	1.26226883	0.00000000
C	-1.12739999	0.78862699	1.21544700
C	-1.12739999	0.78862699	-1.21544700
C	-2.62055986	-0.67693458	0.00000000
C	-2.12219950	-0.18778549	-1.20607500
C	-2.12219950	-0.18778549	1.20607500
Br	0.71477591	2.59675367	0.00000000
H	-3.39694307	-1.43896778	0.00000000
H	-0.73125666	1.17744834	2.14993300
H	-0.73125666	1.17744834	-2.14993300
H	-2.50730948	-0.56577742	-2.15106200
H	-2.50730948	-0.56577742	2.15106200
C	2.02910185	-1.43779210	0.00000000
C	1.53174741	-1.92595386	-1.20705841
C	0.53703854	-2.90227738	-1.20705841
C	0.03968410	-3.39043913	0.00000000
C	0.53703854	-2.90227738	1.20705841
C	1.53174741	-1.92595386	1.20705841
H	2.80197879	-0.67920036	0.00000000
H	1.91818588	-1.54665799	-2.14492842
H	0.15060007	-3.28157324	-2.14492842
H	-0.73319284	-4.14903087	0.00000000
H	0.15060007	-3.28157324	2.14492842
H	1.91818588	-1.54665799	2.14492842

24

M05-2X/6-31+G(d) Benzene...chlorobenzene

C	0.03361976	1.85584782	0.00000000
C	-0.57243936	1.54677455	1.21281600
C	-0.57243936	1.54677455	-1.21281600
C	-2.43587344	0.59647505	0.00000000

```
C      -1.81322856     0.91400660    -1.20516800
C      -1.81322856     0.91400660     1.20516800
Cl      1.58712692     2.64809321     0.00000000
H      -3.40034019     0.10462387     0.00000000
H      -0.07859025     1.79862384     2.14214300
H      -0.07859025     1.79862384    -2.14214300
H      -2.29118053     0.67026441    -2.14585700
H      -2.29118053     0.67026441     2.14585700
C       1.81784913    -1.61210840     0.00000000
C       1.19702291    -1.92871249    -1.20705841
C      -0.04462952    -2.56192066    -1.20705841
C      -0.66545574    -2.87852474     0.00000000
C      -0.04462952    -2.56192066     1.20705841
C       1.19702291    -1.92871249     1.20705841
H       2.78259828    -1.12011320     0.00000000
H       1.67939749    -1.68271489    -2.14492842
H      -0.52700409    -2.80791826    -2.14492842
H      -1.63020489    -3.37051994     0.00000000
H      -0.52700409    -2.80791826     2.14492842
H       1.67939749    -1.68271489     2.14492842

25
M05-2X/6-31+G(d) Benzene...cyanobenzene
C      2.39460020     0.67372350     0.00000000
C      1.77567472     0.98778601     1.20898600
C      1.77567472     0.98778601    -1.20898600
C     -0.08143169     1.93014095     0.00000000
C      0.53596888     1.61685223    -1.21523800
C      0.53596888     1.61685223     1.21523800
C     -1.36537242     2.58165337     0.00000000
N     -2.39641699     3.10483822     0.00000000
H      2.25810021     0.74298795     2.14648100
H      2.25810021     0.74298795    -2.14648100
H      0.04365020     1.86667041    -2.14582200
H      0.04365020     1.86667041     2.14582200
H      3.36022077     0.18373687     0.00000000
C      0.65684914    -2.76178892     0.00000000
C      0.03538525    -2.44643835     1.20705841
C     -1.20754251    -1.81573722     1.20705841
C     -1.82900639    -1.50038665     0.00000000
C     -1.20754251    -1.81573722    -1.20705841
C      0.03538525    -2.44643835    -1.20705841
H      1.62258920    -3.25183619     0.00000000
H      0.51825529    -2.69146199     2.14492842
H     -1.69041254    -1.57071358     2.14492842
H     -2.79474646    -1.01033938     0.00000000
H     -1.69041254    -1.57071358    -2.14492842
H      0.51825529    -2.69146199    -2.14492842
```

Maleic anhydride + Benzene

12
Benzene M05-2X/6-31+G(d) Optimized Geometry

C	0.98557655	0.98557655	0.00000000
C	-0.36074606	1.34632261	0.00000000
C	-1.34632261	0.36074606	0.00000000
C	-0.98557655	-0.98557655	0.00000000
C	0.36074606	-1.34632261	0.00000000
C	1.34632261	-0.36074606	0.00000000
H	1.75158165	1.75158165	0.00000000
H	-0.64112338	2.39270503	0.00000000
H	-2.39270503	0.64112338	0.00000000
H	-1.75158165	-1.75158165	0.00000000
H	0.64112338	-2.39270503	0.00000000
H	2.39270503	-0.64112338	0.00000000

9
maleic anhydride M05-2X/6-31+G(d) Optimized Geometry

C	-0.66511601	0.00000000	-1.25825562
C	0.66511601	0.00000000	-1.25825562
C	-1.12517222	0.00000000	0.16203770
H	-1.36057753	0.00000000	-2.08319562
H	1.36057753	0.00000000	-2.08319562
O	0.00000000	0.00000000	0.96858195
O	-2.23387747	0.00000000	0.59829001
C	1.12517222	0.00000000	0.16203770
O	2.23387747	0.00000000	0.59829001

21
Cycloadduct M05-2X/6-31+G(d) Optimized Geometry

C	-0.57263822	2.36825874	-0.66659440
H	-1.00457834	3.14618097	1.28271350
H	-1.00457834	3.14618097	-1.28271350
C	-0.57263822	2.36825874	0.66659440
C	1.43881194	0.93169278	-0.66684070
H	2.31138609	0.75796117	-1.28286490
C	0.06726925	1.13743393	-1.28365590
H	2.31138609	0.75796117	1.28286490
C	-0.80726593	-0.05959287	0.76421420
C	-0.80726593	-0.05959287	-0.76421420
C	1.43881194	0.93169278	0.66684070
C	0.06726925	1.13743393	1.28365590
C	-0.18825407	-1.39015367	1.13979080
H	0.08403621	1.14722267	2.37049640
H	-1.80492398	-0.00184462	1.19906680
C	-0.18825407	-1.39015367	-1.13979080
H	-1.80492398	-0.00184462	-1.19906680
O	0.03429023	-1.82017388	2.23041260
O	0.12805509	-2.10349065	0.00000000
O	0.03429023	-1.82017388	-2.23041260

16
transition state M05-2X/6-31+G(d) Optimized Geometry

H	2.24197736	0.51791155	1.26368833
C	0.16151958	1.27181044	1.31236383
H	2.24197736	0.51791155	-1.26368833
C	-0.97827993	-0.19622085	-0.72212747
C	-0.97827993	-0.19622085	0.72212747
C	1.42233849	0.90987775	-0.67407207
C	0.16151958	1.27181044	-1.31236383
C	-0.19310925	-1.39558777	-1.13399284
H	0.12648862	1.21086734	-2.39458300
H	0.12648862	1.21086734	2.39458300
H	-1.86801850	0.01358290	1.30546519
C	-0.19310925	-1.39558777	1.13399284
H	-1.86801850	0.01358290	-1.30546519
O	0.02799174	-1.82121699	-2.22922430
O	0.35180128	-1.97959278	0.00000000
O	0.02799174	-1.82121699	2.22922430

Reactions in Scheme 1: Anthracene + Substrates 1a-1e

55
2a M05-2X/6-31+G(d) Optimized Geometry

C	-1.98497582	0.69604288	3.82416700
C	-1.98497582	-0.69604288	3.82416700
C	-4.26445542	-0.69607388	-2.32798594
C	-4.26445542	0.69607388	-2.32798594
C	-1.75182380	-1.40074078	2.64100112
C	-1.75182380	1.40074078	2.64100112
C	-3.33985211	-1.40333015	-1.55508832
C	-3.33985211	1.40333015	-1.55508832
C	-2.43315624	-0.70114334	-0.77509375
C	-2.43315624	0.70114334	-0.77509375
C	-1.52251784	-0.69995661	1.46702926
C	-1.52251784	0.69995661	1.46702926
H	-2.16764977	1.23620910	4.74509714
H	-2.16764977	-1.23620910	4.74509714
H	-4.97771873	-1.23581473	-2.93848847
H	-4.97771873	1.23581473	-2.93848847
H	-1.75182765	-2.48529761	2.63829186
H	-1.75182765	2.48529761	2.63829186
H	-3.32080895	-2.48696890	-1.57202374
H	-3.32080895	2.48696890	-1.57202374
C	-1.33490721	-1.30000111	0.09042325
C	-1.33490721	1.30000111	0.09042325
C	0.00000000	-0.77177965	-0.53060207
C	0.00000000	0.77177965	-0.53060207
C	0.00000000	-1.13535965	-2.00933402
C	0.00000000	1.13535965	-2.00933402
O	0.00000000	0.00000000	-2.78987001
O	0.00000000	-2.23100679	-2.48499558
O	0.00000000	2.23100679	-2.48499558
H	-1.34932463	-2.39041175	0.08790304
H	-1.34932463	2.39041175	0.08790304
C	1.98497582	0.69604288	3.82416700
C	1.98497582	-0.69604288	3.82416700
C	1.52251784	-0.69995661	1.46702926
C	1.52251784	0.69995661	1.46702926
C	1.75182380	-1.40074078	2.64100112
C	1.75182380	1.40074078	2.64100112
C	1.33490721	-1.30000111	0.09042325
C	1.33490721	1.30000111	0.09042325
C	2.43315624	-0.70114334	-0.77509375
C	2.43315624	0.70114334	-0.77509375
C	4.26445542	-0.69607388	-2.32798594
C	4.26445542	0.69607388	-2.32798594
C	3.33985211	-1.40333015	-1.55508832
C	3.33985211	1.40333015	-1.55508832
H	2.16764977	1.23620910	4.74509714
H	2.16764977	-1.23620910	4.74509714
H	1.75182765	-2.48529761	2.63829186
H	1.75182765	2.48529761	2.63829186
H	1.34932463	-2.39041175	0.08790304
H	1.34932463	2.39041175	0.08790304
H	4.97771873	-1.23581473	-2.93848847
H	4.97771873	1.23581473	-2.93848847
H	3.32080895	2.48696890	-1.57202374
H	3.32080895	-2.48696890	-1.57202374

31
1a M05-2X/6-31+G(d) Optimized Geometry

C	0.69494540	-3.26431296	2.08667477
C	-0.69494540	-3.26431296	2.08667477
C	-0.69494540	3.26431296	2.08667477
C	0.69494540	3.26431296	2.08667477
C	-1.40353497	-2.23170533	1.46086133
C	1.40353497	-2.23170533	1.46086133
C	-1.40353497	2.23170533	1.46086133
C	1.40353497	2.23170533	1.46086133
C	-0.70084825	1.21347118	0.84062066
C	0.70084825	1.21347118	0.84062066
C	-0.70084825	-1.21347118	0.84062066
C	0.70084825	-1.21347118	0.84062066
H	1.23555675	-4.06752466	2.57165248
H	-1.23555675	-4.06752466	2.57165248
H	-1.23555675	4.06752466	2.57165248
H	1.23555675	4.06752466	2.57165248
H	-2.48743864	-2.23057028	1.46021071
H	2.48743864	-2.23057028	1.46021071
H	-2.48743864	2.23057028	1.46021071
H	2.48743864	2.23057028	1.46021071
C	-1.31251734	0.00000000	0.12840773
C	1.31251734	0.00000000	0.12840773
C	-0.66636294	0.00000000	-1.23009099
C	0.66636294	0.00000000	-1.23009099
C	-1.13743300	0.00000000	-2.63355884
C	1.13743300	0.00000000	-2.63355884
O	0.00000000	0.00000000	-3.43782553
O	-2.24158048	0.00000000	-3.08386513

```
O       2.24158048       0.00000000      -3.08386513
H      -2.39988772       0.00000000       0.11558118
H       2.39988772       0.00000000       0.11558118

55
TS2a M05-2X/6-31+G(d) Optimized Geometry
C      -3.4449160        2.5136380       -0.9544600
C      -3.4447850        2.6174770        0.4334850
C      -3.2730800       -3.7203010        0.8306760
C      -3.2449250       -3.8058210       -0.5551420
C      -2.7032530        1.7227590        1.2093100
C      -2.6938750        1.5190690       -1.5839390
C      -2.6543890       -2.6480310        1.4884840
C      -2.5977170       -2.8205230       -1.3138490
C      -2.0173530       -1.6764010        0.7387480
C      -1.9882530       -1.7633330       -0.6637600
C      -1.9649740        0.7273870        0.5866500
C      -1.9566300        0.6336950       -0.8119290
H      -4.0328930        3.2025810       -1.5486190
H      -4.0310160        3.3888220        0.9180340
H      -3.7677520       -4.4899800        1.4099100
H      -3.7174290       -4.6422020       -1.0549850
H      -2.7168790        1.7946550        2.2911360
H      -2.6989000        1.4254310       -2.6643530
H      -2.6662010       -2.5855090        2.5704470
H      -2.5657920       -2.8908500       -2.3949570
C      -1.2776320       -0.4401950        1.2828100
C      -1.2349770       -0.5961060       -1.3265710
C       0.1171580       -0.6307860        0.7058240
C       0.1413840       -0.6753670       -0.6798930
C       1.0345060       -1.6810920        1.1961290
C       1.0830190       -1.7519160       -1.0656250
O       1.6700240       -2.2424350        0.0918480
O       1.2468640       -2.0685880        2.3092670
O       1.3263210       -2.2077230       -2.1456150
H      -1.3016320       -0.3770780        2.3694530
H      -1.2099880       -0.6708170       -2.4124590
C      -0.3908710        4.1512430       -0.4978870
C      -0.2910090        4.1317270        0.9123230
C       0.9198010        2.1243970       -0.6264530
C       1.0012780        2.0969790        0.7878870
C       0.3669930        3.1073620        1.5475650
C       0.1814310        3.1551920       -1.2520940
C       1.7240780        1.0265360        1.3807170
C       1.5806370        1.0867810       -1.3454230
C       4.8317390       -0.8590820        0.5250220
C       4.7641920       -0.8207140       -0.8869440
C       2.7956610        0.4337260        0.6558090
C       2.7267440        0.4717250       -0.7603940
C       3.8563380       -0.2612320        1.2855730
C       3.7235410       -0.1850800       -1.5207860
H      -0.9332520        4.9526640       -0.9837120
H      -0.7520720        4.9225870        1.4910830
H       0.4339440        3.0753060        2.6292180
H       0.0941060        3.1614160       -2.3326260
H       1.7128080        0.9195750        2.4614820
H       1.4712250        1.0467110       -2.4252700
H       5.6501590       -1.3787360        1.0068440
H       5.5317570       -1.3117580       -1.4715910
H       3.6507040       -0.1825220       -2.6016530
H       3.8842790       -0.3126160        2.3674240


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2b M05-2X/6-31+G(d) Optimized Geometry
C       2.36201206      -3.32137119        0.69587319
C       2.36201206      -3.32137119       -0.69587319
C      -4.15580479      -2.51727872       -0.69607799
C      -4.15580479      -2.51727872        0.69607799
C       1.42455523      -2.58574415       -1.42426235
C       1.42455523      -2.58574415        1.42426235
C      -3.04214068      -2.05625706       -1.40333450
C      -3.04214068      -2.05625706        1.40333450
C      -1.93013518      -1.61635399       -0.70072552
C      -1.93013518      -1.61635399        0.70072552
C       0.48348086      -1.85661223       -0.69910293
C       0.48348086      -1.85661223        0.69910293
H       3.10807443      -3.90116090        1.22853511
H       3.10807443      -3.90116090       -1.22853511
H      -5.02778253      -2.86546174       -1.23579765
H      -5.02778253      -2.86546174        1.23579765
C       1.44334432      -2.57787649       -2.93147926
H       0.51756522      -2.98371653       -3.34770461
H       1.56431860      -1.56281738       -3.32092180
H       2.27160255      -3.18020681       -3.30634374
C       1.44334432      -2.57787649        2.93147926
H       0.51756522      -2.98371653        3.34770461
H       1.56431860      -1.56281738        3.32092180
H       2.27160255      -3.18020681        3.30634374
H      -3.04896396      -2.02991017       -2.48706388
```

H	-3.04896396	-2.02991017	2.48706388
C	-0.65240303	-1.04868389	-1.29680423
C	-0.65240303	-1.04868389	1.29680423
C	-0.57406615	0.42173990	-0.77078490
C	-0.57406615	0.42173990	0.77078490
C	-1.87817275	1.11740570	-1.13539203
C	-1.87817275	1.11740570	1.13539203
O	-2.56845127	1.48282660	0.00000000
O	-2.29736648	1.34215596	-2.23109310
O	-2.29736648	1.34215596	2.23109310
H	-0.67022573	-1.05252562	-2.38587067
H	-0.67022573	-1.05252562	2.38587067
C	4.20200977	0.11240908	0.69576273
C	4.20200977	0.11240908	-0.69576273
C	1.90559289	0.81900137	-0.70030637
C	1.90559289	0.81900137	0.70030637
C	3.04975186	0.46972676	-1.40056076
C	3.04975186	0.46972676	1.40056076
C	0.60357861	1.30460334	-1.30011549
C	0.60357861	1.30460334	1.30011549
C	0.36029709	2.68155290	-0.70117779
C	0.36029709	2.68155290	0.70117779
C	-0.14180927	5.02959500	-0.69605156
C	-0.14180927	5.02959500	0.69605156
C	0.10177100	3.84934403	-1.40327624
C	0.10177100	3.84934403	1.40327624
H	5.10007628	-0.16113724	1.23616815
H	5.10007628	-0.16113724	-1.23616815
H	3.05171309	0.48080669	-2.48513883
H	3.05171309	0.48080669	2.48513883
H	0.60770188	1.31842129	-2.39079024
H	0.60770188	1.31842129	2.39079024
H	-0.34250768	5.94671348	-1.23586829
H	-0.34250768	5.94671348	1.23586829
H	0.07763705	3.84060101	2.48693285
H	0.07763705	3.84060101	-2.48693285

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3b M05-2X/6-31+G(d) Optimized Geometry

C	-4.23596947	0.80035743	0.69606985
C	-4.23596947	0.80035743	-0.69606985
C	1.19105436	4.45128678	-0.69562763
C	1.19105436	4.45128678	0.69562763
C	-3.03084524	0.84991663	-1.40076919
C	-3.03084524	0.84991663	1.40076919
C	0.66837265	3.38143901	-1.42860001
C	0.66837265	3.38143901	1.42860001
C	0.13320673	2.31878629	-0.70091416
C	0.13320673	2.31878629	0.70091416
C	-1.83604924	0.90276700	-0.69957894
C	-1.83604924	0.90276700	0.69957894
H	-5.17421068	0.76243878	1.23615611
H	-5.17421068	0.76243878	-1.23615611
H	1.61226054	5.29726411	-1.22741990
H	1.61226054	5.29726411	1.22741990
C	0.69584814	3.38097177	-2.93589953
H	-0.31241397	3.30624225	-3.35211636
H	1.14368476	4.30321624	-3.30729995
H	1.28293481	2.54149879	-3.31619904
C	0.69584814	3.38097177	2.93589953
H	-0.31241397	3.30624225	3.35211636
H	1.14368476	4.30321624	3.30729995
H	1.28293481	2.54149879	3.31619904
H	-3.02809464	0.84872576	-2.48548639
H	-3.02809464	0.84872576	2.48548639
C	-0.45369062	1.04349363	-1.29691176
C	-0.45369062	1.04349363	1.29691176
C	0.46641017	-0.10523309	-0.77111937
C	0.46641017	-0.10523309	0.77111937
C	1.90132855	0.25173002	-1.13417007
C	1.90132855	0.25173002	1.13417007
O	2.66186064	0.43079650	0.00000000
O	2.36284516	0.37071770	-2.23029253
O	2.36284516	0.37071770	2.23029253
H	-0.45986926	1.04882893	-2.38630789
H	-0.45986926	1.04882893	2.38630789
C	-3.29195343	-3.06202099	0.69604312
C	-3.29195343	-3.06202099	-0.69604312
C	-1.10958577	-2.05829878	-0.69995380
C	-1.10958577	-2.05829878	0.69995380
C	-2.19665490	-2.55744834	-1.40068289
C	-2.19665490	-2.55744834	1.40068289
C	0.18321664	-1.54949608	-1.30002183
C	0.18321664	-1.54949608	1.30002183
C	1.28562765	-2.40944795	-0.70117265
C	1.28562765	-2.40944795	0.70117265
C	3.23151689	-3.81641491	-0.69604313
C	3.23151689	-3.81641491	0.69604313
C	2.25980653	-3.10341905	-1.40322227
C	2.25980653	-3.10341905	1.40322227

H	-4.14425122	-3.45583188	1.23627312
H	-4.14425122	-3.45583188	-1.23627312
H	-2.19421325	-2.55657648	-2.48525352
H	-2.19421325	-2.55657648	2.48525352
H	0.18855354	-1.56282501	-2.39049943
H	0.18855354	-1.56282501	2.39049943
H	3.99491497	-4.36298930	-1.23589928
H	3.99491497	-4.36298930	1.23589928
H	2.27159816	-3.08119629	2.48690909
H	2.27159816	-3.08119629	-2.48690909

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1b M05-2X/6-31+G(d) Optimized Geometry

C	-1.74074123	3.13220591	0.69490745
C	-1.74074123	3.13220591	-0.69490745
C	3.99303734	0.05835949	-0.69490620
C	3.99303734	0.05835949	0.69490620
C	-1.13708831	2.10328574	-1.42802546
C	-1.13708831	2.10328574	1.42802546
C	2.78718990	-0.00864698	-1.40347302
C	2.78718990	-0.00864698	1.40347302
C	1.59695764	-0.07569616	-0.70057415
C	1.59695764	-0.07569616	0.70057415
C	-0.54193916	1.07785027	-0.69992755
C	-0.54193916	1.07785027	0.69992755
H	-2.22013112	3.94603762	1.22734122
H	-2.22013112	3.94603762	-1.22734122
H	4.93006267	0.10751700	-1.23549436
H	4.93006267	0.10751700	1.23549436
H	2.78596726	-0.01072083	-2.48746942
H	2.78596726	-0.01072083	2.48746942
C	0.19096448	-0.12945608	-1.30977140
C	0.19096448	-0.12945608	1.30977140
C	-0.45451126	-1.32470637	-0.66619287
C	-0.45451126	-1.32470637	0.66619287
C	-1.12869296	-2.55486716	-1.13743898
C	-1.12869296	-2.55486716	1.13743898
O	-1.51392439	-3.26158070	0.00000000
O	-1.34820243	-2.94867252	-2.24183165
O	-1.34820243	-2.94867252	2.24183165
H	0.18985180	-0.14911913	-2.39594987
H	0.18985180	-0.14911913	2.39594987
C	-1.13617179	2.11665365	-2.93619609
C	-1.13617179	2.11665365	2.93619609
H	-1.66452219	2.99437803	-3.30901553
H	-1.66452219	2.99437803	3.30901553
H	-0.11790191	2.14659631	-3.33278668
H	-0.11790191	2.14659631	3.33278668
H	-1.62811864	1.23063395	-3.34507612
H	-1.62811864	1.23063395	3.34507612

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TS2b M05-2X/6-31+G(d) Optimized Geometry

C	-3.6547820	-1.7551240	0.8953910
C	-3.6726610	-1.8427380	-0.4933330
C	-2.3289050	4.3352280	-0.8533220
C	-2.2962240	4.4082160	0.5330780
C	-2.7857730	-1.1067320	-1.2832150
C	-2.7423280	-0.9328260	1.5588190
C	-1.9120320	3.1702370	-1.5128430
C	-1.8465610	3.3174540	1.2907620
C	-1.4723670	2.0944080	-0.7637720
C	-1.4392670	2.1682380	0.6387470
C	-1.8771570	-0.2778760	-0.6252840
C	-1.8567180	-0.1968350	0.7722770
H	-4.3638340	-2.3352840	1.4761250
H	-4.3960730	-2.4898690	-0.9776250
H	-2.6684160	5.1855880	-1.4315230
H	-2.6099460	5.3154620	1.0342720
C	-2.8386300	-1.1876720	-2.7870890
H	-3.5545010	-1.9469100	-3.1043490
H	-3.1444820	-0.2343860	-3.2270020
H	-1.8630480	-1.4472810	-3.2055750
C	-2.7366570	-0.8316000	3.0633250
H	-3.4561840	-1.5277810	3.4957680
H	-3.0029620	0.1748930	3.3973260
H	-1.7515660	-1.0648770	3.4769660
H	-1.9237540	3.1164730	-2.5954290
H	-1.8074960	3.3772240	2.3724140
C	-0.9722680	0.7443570	-1.3074210
C	-0.9194670	0.8788370	1.2971100
C	0.4293090	0.6629620	-0.7221250
C	0.4527190	0.7059690	0.6628700
C	1.5332430	1.5177620	-1.2080940
C	1.5751340	1.5897210	1.0538740
O	2.2541110	1.9550540	-0.1000640
O	1.8238240	1.8524980	-2.3206870
O	1.8910700	1.9977430	2.1343730
H	-0.9898910	0.7005870	-2.3938120
H	-0.8812570	0.9506810	2.3814740

C	-0.9861670	-3.9109850	0.5665090
C	-0.8940200	-3.9318380	-0.8440690
C	0.6968040	-2.1785560	0.6579310
C	0.7749080	-2.1891800	-0.7569310
C	-0.0461090	-3.0711500	-1.4972040
C	-0.2212530	-3.0387540	1.3030450
C	1.6849970	-1.2856250	-1.3694080
C	1.5452560	-1.2731160	1.3573950
C	5.0963170	-0.0055840	-0.5491450
C	5.0296380	-0.0087520	0.8632800
C	2.8526140	-0.8937530	-0.6560200
C	2.7845320	-0.8954100	0.7606660
C	4.0223520	-0.4210750	-1.2984030
C	3.8905730	-0.4266960	1.5088510
H	-1.6730780	-4.5823150	1.0664710
H	-1.5055180	-4.6246660	-1.4090850
H	0.0281250	-3.0789410	-2.5787890
H	-0.2949960	-3.0181930	2.3845850
H	1.6898710	-1.1973350	-2.4519760
H	1.4503130	-1.1942690	2.4366430
H	5.9955250	0.3433210	-1.0407730
H	5.8787610	0.3377320	1.4386810
H	3.8233390	-0.3986400	2.5897190
H	4.0547210	-0.3926490	-2.3809870

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TS3b M05-2X/6-31+G(d) Optimized Geometry

C	-2.1530070	3.6576470	-0.9983360
C	-2.1236270	3.7665530	0.3889930
C	-4.1055910	-2.2586660	0.8288590
C	-4.1031940	-2.3597720	-0.5561220
C	-1.7374460	2.6778700	1.1753290
C	-1.7859240	2.4606170	-1.6165210
C	-3.1770510	-1.4568630	1.5081170
C	-3.1722650	-1.6645840	-1.3413080
C	-2.2596220	-0.7605490	0.7303380
C	-2.2564940	-0.8636340	-0.6694770
C	-1.3844020	1.4843600	0.5634800
C	-1.4022130	1.3818350	-0.8336640
H	-2.4654130	4.5020150	-1.6007390
H	-2.4109510	4.6965550	0.8644880
H	-4.8330550	-2.8214430	1.4031970
H	-4.8285400	-3.0004700	-1.0451510
C	-3.1679080	-1.3761440	3.0141800
H	-3.9505030	-2.0088100	3.4339560
H	-2.2090390	-1.7101940	3.4184420
H	-3.3423240	-0.3537400	3.3597790
C	-3.1592620	-1.8014010	-2.8434210
H	-3.9342370	-2.4959250	-3.1689560
H	-2.1959850	-2.1795240	-3.1949310
H	-3.3433710	-0.8411080	-3.3324980
H	-1.7284660	2.7593110	2.2566850
H	-1.8155950	2.3663130	-2.6966250
C	-1.1418660	0.1583700	1.2693470
C	-1.1439560	-0.0245490	-1.3331790
C	0.1029690	-0.5074370	0.7055630
C	0.1158570	-0.5713430	-0.6778790
C	0.5874810	-1.8082520	1.2108430
C	0.6152690	-1.9151390	-1.0474390
O	0.9950890	-2.5672280	0.1170320
O	0.6329350	-2.2382980	2.3283540
O	0.6728050	-2.4433910	-2.1210330
H	-1.1390260	0.2418690	2.3537540
H	-1.1328530	-0.1052960	-2.4177290
C	1.2844150	4.1310700	-0.5506650
C	1.3641100	4.0956790	0.8607280
C	1.8240870	1.7767260	-0.6476690
C	1.8848420	1.7403120	0.7678200
C	1.6300320	2.9162310	1.5116180
C	1.4862690	2.9905190	-1.2898040
C	2.1925980	0.4949280	1.3782450
C	2.0891270	0.5669990	-1.3509320
C	4.4353110	-2.3778150	0.5667680
C	4.3895100	-2.3371190	-0.8462330
C	2.9875950	-0.4464640	0.6675800
C	2.9410870	-0.4051960	-0.7497170
C	3.7329180	-1.4631140	1.3128350
C	3.6435950	-1.3824760	-1.4948710
H	1.0502430	5.0635020	-1.0489000
H	1.1967980	5.0031470	1.4277480
H	1.6760860	2.8764640	2.5941190
H	1.4115620	3.0127510	-2.3710890
H	2.1419220	0.4131420	2.4600560
H	1.9769660	0.5545380	-2.4311840
H	5.0154340	-3.1469260	1.0606680
H	4.9351960	-3.0758770	-1.4195130
H	3.5804260	-1.3681230	-2.5763080
H	3.7386340	-1.5060310	2.3954740

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2c M05-2X/6-31+G(d) Optimized Geometry

C	0.69699033	-3.75279957	0.70003579
C	0.69699033	-3.75279957	-0.70003579
C	-4.90092635	-0.23417716	-0.69625446
C	-4.90092635	-0.23417716	0.69625446
C	0.15212562	-2.68593114	-1.40719041
C	0.15212562	-2.68593114	1.40719041
C	-3.69798598	-0.30492854	-1.40379330
C	-3.69798598	-0.30492854	1.40379330
C	-2.50525412	-0.39193188	-0.70083422
C	-2.50525412	-0.39193188	0.70083422
C	-0.42681468	-1.63611969	-0.69370802
C	-0.42681468	-1.63611969	0.69370802
H	1.14574704	-4.59153456	1.21381979
H	1.14574704	-4.59153456	-1.21381979
H	-5.83773741	-0.16796595	-1.23583223
H	-5.83773741	-0.16796595	1.23583223
O	0.15464718	-2.56902371	-2.76921010
O	0.15464718	-2.56902371	2.76921010
C	0.77917067	-3.60477148	-3.50557611
H	0.69086242	-3.32416146	-4.55191231
H	1.83544306	-3.69089939	-3.23471560
H	0.27587872	-4.56095669	-3.34013181
C	0.77917067	-3.60477148	3.50557611
H	0.69086242	-3.32416146	4.55191231
H	1.83544306	-3.69089939	3.23471560
H	0.27587872	-4.56095669	3.34013181
H	-3.69141048	-0.28101965	-2.48741068
H	-3.69141048	-0.28101965	2.48741068
C	-1.10907112	-0.43081068	-1.30043404
C	-1.10907112	-0.43081068	1.30043404
C	-0.40367342	0.86159531	-0.77129826
C	-0.40367342	0.86159531	0.77129826
C	-1.27684780	2.05361701	-1.13583751
C	-1.27684780	2.05361701	1.13583751
O	-1.74067905	2.68167557	0.00000000
O	-1.55658340	2.44015002	-2.23077910
O	-1.55658340	2.44015002	2.23077910
H	-1.11647247	-0.44557777	-2.38836245
H	-1.11647247	-0.44557777	2.38836245
C	3.75103677	-1.50535928	0.69614808
C	3.75103677	-1.50535928	-0.69614808
C	1.99999792	0.13875688	-0.70024466
C	1.99999792	0.13875688	0.70024466
C	2.87012305	-0.68171269	-1.40198382
C	2.87012305	-0.68171269	1.40198382
C	1.04070677	1.14405464	-1.30025625
C	1.04070677	1.14405464	1.30025625
C	1.42263334	2.48863786	-0.70115273
C	1.42263334	2.48863786	0.70115273
C	1.99650905	4.82045351	-0.69615377
C	1.99650905	4.82045351	0.69615377
C	1.70034597	3.65222874	-1.40335444
C	1.70034597	3.65222874	1.40335444
H	4.43947039	-2.14494784	1.23568068
H	4.43947039	-2.14494784	-1.23568068
H	2.86286688	-0.68172082	-2.48657926
H	2.86286688	-0.68172082	2.48657926
H	1.04986276	1.15169219	-2.39049166
H	1.04986276	1.15169219	2.39049166
H	2.21640153	5.73333773	-1.23584898
H	2.21640153	5.73333773	1.23584898
H	1.67465186	3.65462726	2.48703348
H	1.67465186	3.65462726	-2.48703348

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3c M05-2X/6-31+G(d) Optimized Geometry

C	4.38017246	-0.05296720	0.69616338
C	4.38017246	-0.05296720	-0.69616338
C	-0.68738390	-4.27366644	-0.69955100
C	-0.68738390	-4.27366644	0.69955100
C	3.18916656	-0.24183170	-1.40114132
C	3.18916656	-0.24183170	1.40114132
C	-0.23866133	-3.16302885	-1.41197895
C	-0.23866133	-3.16302885	1.41197895
C	0.21099320	-2.05271162	-0.69547116
C	0.21099320	-2.05271162	0.69547116
C	2.00813159	-0.43083254	-0.69985197
C	2.00813159	-0.43083254	0.69985197
H	5.30804509	0.09183118	1.23619911
H	5.30804509	0.09183118	-1.23619911
H	-1.04602153	-5.15410926	-1.21438694
H	-1.04602153	-5.15410926	1.21438694
O	-0.20362888	-3.06905127	-2.77066822
O	-0.20362888	-3.06905127	2.77066822
C	-0.83679580	-4.09874342	-3.51064895
H	-0.32060668	-5.05292565	-3.37487248
H	-1.88507233	-4.19477808	-3.21691410

H	-0.77502433	-3.79757620	-4.55289246
C	-0.83679580	-4.09874342	3.51064895
H	-0.32060668	-5.05292565	3.37487248
H	-1.88507233	-4.19477808	3.21691410
H	-0.77502433	-3.79757620	4.55289246
H	3.18575310	-0.24586804	-2.48562449
H	3.18575310	-0.24586804	2.48562449
C	0.65199406	-0.72947659	-1.30060489
C	0.65199406	-0.72947659	1.30060489
C	-0.39344160	0.30727376	-0.77179702
C	-0.39344160	0.30727376	0.77179702
C	-1.78021670	-0.20720908	-1.13629742
C	-1.78021670	-0.20720908	1.13629742
O	-2.51150389	-0.48124949	0.00000000
O	-2.23165668	-0.36781707	-2.23029452
O	-2.23165668	-0.36781707	2.23029452
H	0.65091270	-0.75534769	-2.38878443
H	0.65091270	-0.75534769	2.38878443
C	3.01220266	3.66680856	0.69609119
C	3.01220266	3.66680856	-0.69609119
C	0.95726795	2.42249984	-0.69996878
C	0.95726795	2.42249984	0.69996878
C	1.98096500	3.04152822	-1.40065531
C	1.98096500	3.04152822	1.40065531
C	-0.27128573	1.77343437	-1.29997192
C	-0.27128573	1.77343437	1.29997192
C	-1.46124337	2.50745778	-0.70111867
C	-1.46124337	2.50745778	0.70111867
C	-3.54933989	3.69350590	-0.69612765
C	-3.54933989	3.69350590	0.69612765
C	-2.50583531	3.09037729	-1.40324958
C	-2.50583531	3.09037729	1.40324958
H	3.81466479	4.15446335	1.23626380
H	3.81466479	4.15446335	-1.23626380
H	1.97833094	3.04008326	-2.48524864
H	1.97833094	3.04008326	2.48524864
H	-0.27862414	1.78577796	-2.39046885
H	-0.27862414	1.78577796	2.39046885
H	-4.36779365	4.15377345	-1.23583314
H	-4.36779365	4.15377345	1.23583314
H	-2.51483666	3.06646566	2.48695956
H	-2.51483666	3.06646566	-2.48695956

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1c M05-2X/6-31+G(d) Optimized Geometry

C	-0.59874465	3.20795911	0.69919481
C	-0.59874465	3.20795911	-0.69919481
C	3.86027845	-1.53740973	-0.69490211
C	3.86027845	-1.53740973	0.69490211
C	-0.35329952	2.03428897	-1.41178922
C	-0.35329952	2.03428897	1.41178922
C	2.69634723	-1.21497199	-1.40404900
C	2.69634723	-1.21497199	1.40404900
C	1.54718694	-0.89944686	-0.70099840
C	1.54718694	-0.89944686	0.70099840
C	-0.11541555	0.86353113	-0.69429463
C	-0.11541555	0.86353113	0.69429463
H	-0.79432203	4.13823781	1.21387453
H	-0.79432203	4.13823781	-1.21387453
H	4.76408309	-1.78983194	-1.23544709
H	4.76408309	-1.78983194	1.23544709
H	2.69415607	-1.21270188	-2.48780142
H	2.69415607	-1.21270188	2.48780142
C	0.19593310	-0.50440793	-1.31289923
C	0.19593310	-0.50440793	1.31289923
C	-0.79130159	-1.43834372	-0.66649226
C	-0.79130159	-1.43834372	0.66649226
C	-1.80515455	-2.40828028	-1.13794590
C	-1.80515455	-2.40828028	1.13794590
O	-2.38813060	-2.96284094	0.00000000
O	-2.13098618	-2.72300416	-2.24124535
O	-2.13098618	-2.72300416	2.24124535
H	0.18306886	-0.50083414	-2.39818941
H	0.18306886	-0.50083414	2.39818941
O	-0.32605535	1.93589515	-2.77195933
O	-0.32605535	1.93589515	2.77195933
C	-0.58439890	3.11438571	-3.51633657
C	-0.58439890	3.11438571	3.51633657
H	-1.58352542	3.50001320	-3.29906065
H	-1.58352542	3.50001320	3.29906065
H	0.16496784	3.88096595	-3.30375565
H	0.16496784	3.88096595	3.30375565
H	-0.52468102	2.82507107	-4.56173746
H	-0.52468102	2.82507107	4.56173746

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TS2c M05-2X/6-31+G(d) Optimized Geometry

C	1.03217335	-3.70336562	0.70035644
C	1.03217335	-3.70336562	-0.70035644
C	-4.80237437	-1.24473954	-0.69429565

C	-4.80237437	-1.24473954	0.69429565
C	0.44349368	-2.66042194	-1.40660278
C	0.44349368	-2.66042194	1.40660278
C	-3.61284223	-1.02710855	-1.40457259
C	-3.61284223	-1.02710855	1.40457259
C	-2.44133718	-0.81273638	-0.70281823
C	-2.44133718	-0.81273638	0.70281823
C	-0.18269404	-1.63545761	-0.69412699
C	-0.18269404	-1.63545761	0.69412699
H	1.50861946	-4.52624605	1.21500027
H	1.50861946	-4.52624605	-1.21500027
H	-5.72711922	-1.40458557	-1.23510740
H	-5.72711922	-1.40458557	1.23510740
O	0.41957222	-2.55554725	-2.76944372
O	0.41957222	-2.55554725	2.76944372
C	1.06522094	-3.57595317	-3.50831810
H	0.94876526	-3.30801442	-4.55514781
H	2.12888588	-3.62437362	-3.25689059
H	0.59870289	-4.54743546	-3.32515902
C	1.06522094	-3.57595317	3.50831810
H	0.94876526	-3.30801442	4.55514781
H	2.12888588	-3.62437362	3.25689059
H	0.59870289	-4.54743546	3.32515902
H	-3.61142659	-1.01751145	-2.48840986
H	-3.61142659	-1.01751145	2.48840986
C	-1.04996002	-0.55012051	-1.30812960
C	-1.04996002	-0.55012051	1.30812960
C	-0.67653438	0.79073195	-0.69282417
C	-0.67653438	0.79073195	0.69282417
C	-1.32242718	2.04697395	-1.13195481
C	-1.32242718	2.04697395	1.13195481
O	-1.58544034	2.80970436	0.00000000
O	-1.63006724	2.41600329	-2.22879214
O	-1.63006724	2.41600329	2.22879214
H	-1.04787880	-0.55458124	-2.39444020
H	-1.04787880	-0.55458124	2.39444020
C	3.58694251	-1.42531072	0.70731720
C	3.58694251	-1.42531072	-0.70731720
C	2.19711758	0.54924211	0.70883304
C	2.19711758	0.54924211	-0.70883304
C	2.88396148	-0.47324729	-1.40462393
C	2.88396148	-0.47324729	1.40462393
C	1.47515667	1.58355289	-1.36636309
C	1.47515667	1.58355289	1.36636309
C	0.86251590	5.21042327	-0.70726871
C	0.86251590	5.21042327	0.70726871
C	1.31981770	2.83796903	-0.70933539
C	1.31981770	2.83796903	0.70933539
C	1.06725116	4.04514776	-1.40527643
C	1.06725116	4.04514776	1.40527643
H	4.13631116	-2.19233592	1.24008967
H	4.13631116	-2.19233592	-1.24008967
H	2.86169256	-0.48092878	-2.48860095
H	2.86169256	-0.48092878	2.48860095
H	1.38180904	1.55229020	-2.44789170
H	1.38180904	1.55229020	2.44789170
H	0.68204009	6.13493501	-1.24126144
H	0.68204009	6.13493501	1.24126144
H	1.03594873	4.03291976	2.48823854
H	1.03594873	4.03291976	-2.48823854

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TS3c M05-2X/6-31+G(d) Optimized Geometry

C	0.7987110	4.2481810	0.2810980
C	0.8498150	4.1202070	-1.1038500
C	4.3300550	-1.1273260	-0.5669900
C	4.3119180	-0.9981810	0.8234630
C	0.8055630	2.8553790	-1.6943950
C	0.7138290	3.1143160	1.0937930
C	3.2373100	-0.7197300	-1.3361220
C	3.2006520	-0.4585290	1.4756840
C	2.1257130	-0.1991700	-0.6802720
C	2.1085020	-0.0688160	0.7062220
C	0.7187430	1.7320780	-0.8858790
C	0.6806900	1.8570570	0.5099140
H	0.8362950	5.2311800	0.7349720
H	0.9293720	5.0032940	-1.7262860
H	5.2079420	-1.5517650	-1.0334790
H	5.1765250	-1.3270350	1.3827000
O	3.1731840	-0.7903590	-2.6970830
O	3.1007700	-0.2773710	2.8241310
C	4.2452840	-1.4294980	-3.3673850
H	5.1792450	-0.8789070	-3.2260690
H	4.3630670	-2.4583180	-3.0176170
H	3.9794630	-1.4307280	-4.4209010
C	4.1544090	-0.7778150	3.6281500
H	5.0927310	-0.2606540	3.4102850
H	4.2787030	-1.8534330	3.4788890
H	3.8624300	-0.5837460	4.6565520
H	0.8588450	2.7463280	-2.7719350

H	0.6928440	3.2134160	2.1732490
C	0.8345960	0.2953070	-1.3567760
C	0.7971940	0.5291200	1.2478510
C	-0.2406850	-0.5413660	-0.6753300
C	-0.2373470	-0.4476890	0.7078970
C	-0.4009220	-1.9740200	-1.0167870
C	-0.3854020	-1.8180370	1.2431400
O	-0.5909000	-2.6762210	0.1656470
O	-0.3535340	-2.5230690	-2.0795050
O	-0.3340420	-2.2253690	2.3681260
H	0.8601690	0.1805280	-2.4370850
H	0.7990920	0.6232670	2.3304680
C	-2.6439780	3.6934690	0.7966410
C	-2.5834980	3.7208660	-0.6157710
C	-2.5292200	1.2829990	0.7500800
C	-2.4883720	1.3060690	-0.6661600
C	-2.4823090	2.5530180	-1.3328240
C	-2.5862550	2.4985570	1.4708160
C	-2.4381750	0.0545910	-1.3451040
C	-2.5008890	0.0118900	1.3846900
C	-3.9505490	-3.3161750	-0.7649340
C	-3.9736750	-3.3400030	0.6487470
C	-3.0197870	-1.0866980	-0.7180570
C	-3.0441610	-1.1110450	0.6999290
C	-3.4661880	-2.2203880	-1.4383440
C	-3.5108220	-2.2670570	1.3711020
H	-2.7174400	4.6240740	1.3459430
H	-2.6042430	4.6720960	-1.1327360
H	-2.4205070	2.5728420	-2.4149410
H	-2.6127010	2.4691000	2.5542930
H	-2.3316360	0.0491460	-2.4259400
H	-2.4212290	-0.0339530	2.4668220
H	-4.3024950	-4.1769670	-1.3193640
H	-4.3431020	-4.2184780	1.1624620
H	-3.4962290	-2.2896190	2.4542350
H	-3.4154460	-2.2119240	-2.5204510

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1d M05-2X/AVDZ' Optimized Geometry

C	-2.0480800	3.7753880	0.6956060
C	-2.0480800	3.7753880	-0.6956060
C	2.9851210	-0.3547420	-0.6935100
C	2.9851210	-0.3547420	0.6935100
C	-1.6576640	2.6334100	-1.4062550
C	-1.6576640	2.6334100	1.4062550
C	1.7825110	-0.1923120	-1.3879520
C	1.7825110	-0.1923120	1.3879520
C	0.5884750	-0.0381090	-0.7040580
C	0.5884750	-0.0381090	0.7040580
C	-1.2771440	1.5035860	-0.7005870
C	-1.2771440	1.5035860	0.7005870
H	-2.3539160	4.6680530	1.2382400
H	-2.3539160	4.6680530	-1.2382400
H	3.9146830	-0.4803140	-1.2433700
H	3.9146830	-0.4803140	1.2433700
H	-1.6533760	2.6320590	-2.4953190
H	-1.6533760	2.6320590	2.4953190
Br	1.8287490	-0.1853220	-3.2874950
Br	1.8287490	-0.1853220	3.2874950
C	-0.8018160	0.1800440	-1.3119920
C	-0.8018160	0.1800440	1.3119920
C	-1.6630530	-0.8715510	-0.6668080
C	-1.6630530	-0.8715510	0.6668080
C	-2.5650940	-1.9504300	-1.1375500
C	-2.5650940	-1.9504300	1.1375500
O	-3.0788650	-2.5685570	0.0000000
O	-2.8564440	-2.2926160	-2.2396580
O	-2.8564440	-2.2926160	2.2396580
H	-0.8061270	0.1699330	-2.4016940
H	-0.8061270	0.1699330	2.4016940

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2d M05-2X/AVDZ' Optimized Geometry

C	-4.0288990	-0.4123110	0.6983310
C	-4.0288990	-0.4123110	-0.6983310
C	-1.2288520	5.4234640	-0.6983790
C	-1.2288520	5.4234640	0.6983790
C	-2.9857930	0.2020380	-1.4055210
C	-2.9857930	0.2020380	1.4055210
C	-1.0917470	4.2217970	-1.4069180
C	-1.0917470	4.2217970	1.4069180
C	-0.9663270	3.0270460	-0.7038070
C	-0.9663270	3.0270460	0.7038070
C	-1.9538360	0.8169370	-0.7031740
C	-1.9538360	0.8169370	0.7031740
H	-4.8421900	-0.8866360	1.2414930
H	-4.8421900	-0.8866360	-1.2414930
H	-1.3303560	6.3595990	-1.2409700
H	-1.3303560	6.3595990	1.2409700

H	-2.9887030	0.2063890	-2.4934060
H	-2.9887030	0.2063890	2.4934060
H	-1.0780930	4.2229760	-2.4942510
H	-1.0780930	4.2229760	2.4942510
C	-0.8174020	1.6290660	-1.3028630
C	-0.8174020	1.6290660	1.3028630
C	0.5682050	1.0840060	-0.7780190
C	0.5682050	1.0840060	0.7780190
C	1.6523110	2.1008300	-1.1447430
C	1.6523110	2.1008300	1.1447430
O	2.2230460	2.6366370	0.0000000
O	2.0104070	2.4353860	-2.2394780
O	2.0104070	2.4353860	2.2394780
H	-0.8297660	1.6403570	-2.3960290
H	-0.8297660	1.6403570	2.3960290
C	-1.2088570	-3.4230940	0.6978540
C	-1.2088570	-3.4230940	-0.6978540
C	0.1548860	-1.4117500	-0.7027150
C	0.1548860	-1.4117500	0.7027150
C	-0.5306460	-2.4114240	-1.3731840
C	-0.5306460	-2.4114240	1.3731840
C	1.0317160	-0.3301870	-1.3059170
C	1.0317160	-0.3301870	1.3059170
C	2.4169370	-0.5686770	-0.7036870
C	2.4169370	-0.5686770	0.7036870
C	4.7929000	-0.9711790	-0.6984390
C	4.7929000	-0.9711790	0.6984390
C	3.6016070	-0.7643370	-1.4075180
C	3.6016070	-0.7643370	1.4075180
H	-1.7273250	-4.1919500	1.2612910
H	-1.7273250	-4.1919500	-1.2612910
Br	-0.5423090	-2.4122620	-3.4357940
Br	-0.5423090	-2.4122620	3.4357940
H	1.0402370	-0.3473430	-2.3971260
H	1.0402370	-0.3473430	2.3971260
H	5.7215220	-1.1269060	-1.2409740
H	5.7215220	-1.1269060	1.2409740
H	3.6028110	-0.7503000	2.4946770
H	3.6028110	-0.7503000	-2.4946770

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3d M05-2X/AVDZ' Optimized Geometry

C	-3.0647050	3.9929510	0.6983220
C	-3.0647050	3.9929510	-0.6983220
C	3.3752880	4.3521770	-0.6983560
C	3.3752880	4.3521770	0.6983560
C	-2.0281280	3.3678580	-1.4044940
C	-2.0281280	3.3678580	1.4044940
C	2.3938310	3.6456090	-1.4069980
C	2.3938310	3.6456090	1.4069980
C	1.4120670	2.9532960	-0.7038430
C	1.4120670	2.9532960	0.7038430
C	-0.9974790	2.7501550	-0.7028520
C	-0.9974790	2.7501550	0.7028520
H	-3.8682930	4.4836670	1.2413370
H	-3.8682930	4.4836670	-1.2413370
H	4.1428250	4.8977710	-1.2408330
H	4.1428250	4.8977710	1.2408330
H	-2.0238340	3.3756240	-2.4925220
H	-2.0238340	3.3756240	2.4925220
H	2.4019580	3.6341050	-2.4943240
H	2.4019580	3.6341050	2.4943240
C	0.2611430	2.1446620	-1.3026450
C	0.2611430	2.1446620	1.3026450
C	0.4592010	0.6685580	-0.7778510
C	0.4592010	0.6685580	0.7778510
C	1.8763740	0.2205810	-1.1453770
C	1.8763740	0.2205810	1.1453770
O	2.6217470	-0.0204730	0.0000000
O	2.3444400	0.0737990	-2.2395550
O	2.3444400	0.0737990	2.2395550
H	0.2663690	2.1602930	-2.3959100
H	0.2663690	2.1602930	2.3959100
C	-4.3355300	-0.0051460	0.6983050
C	-4.3355300	-0.0051460	-0.6983050
C	-1.9321930	-0.1948010	-0.7027920
C	-1.9321930	-0.1948010	0.7027920
C	-3.1293770	-0.0997830	-1.4052610
C	-3.1293770	-0.0997830	1.4052610
C	-0.5542420	-0.4220960	-1.3054910
C	-0.5542420	-0.4220960	1.3054910
C	-0.0848370	-1.7442250	-0.7040330
C	-0.0848370	-1.7442250	0.7040330
C	0.6842000	-4.0479370	-0.6975510
C	0.6842000	-4.0479370	0.6975510
C	0.2977330	-2.8938500	-1.3774460
C	0.2977330	-2.8938500	1.3774460
H	-5.2746710	0.0625730	1.2411830
H	-5.2746710	0.0625730	-1.2411830
H	-3.1299180	-0.1090750	-2.4930610

H	-3.1299180	-0.1090750	2.4930610
H	-0.5580340	-0.4438530	-2.3968950
H	-0.5580340	-0.4438530	2.3968950
H	0.9763990	-4.9284570	-1.2603130
H	0.9763990	-4.9284570	1.2603130
Br	0.2864170	-2.9076920	3.4358920
Br	0.2864170	-2.9076920	-3.4358920

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TS2d M05-2X/AVDZ' Optimized Geometry

C	0.9750250	-3.4666710	0.6942770
C	0.9750250	-3.4666710	-0.6942770
C	-4.8329520	-0.9382720	-0.6950020
C	-4.8329520	-0.9382720	0.6950020
C	0.3840230	-2.4070370	-1.3818660
C	0.3840230	-2.4070370	1.3818660
C	-3.6432560	-0.7261490	-1.4069040
C	-3.6432560	-0.7261490	1.4069040
C	-2.4706010	-0.5148500	-0.7024520
C	-2.4706010	-0.5148500	0.7024520
C	-0.2252900	-1.3611360	-0.7043560
C	-0.2252900	-1.3611360	0.7043560
H	1.4344930	-4.2833780	1.2455860
H	1.4344930	-4.2833780	-1.2455860
H	-5.7630460	-1.0974010	-1.2375910
H	-5.7630460	-1.0974010	1.2375910
Br	0.4315940	-2.4341160	-3.2843620
Br	0.4315940	-2.4341160	3.2843620
H	-3.6412130	-0.7192510	-2.4959250
H	-3.6412130	-0.7192510	2.4959250
C	-1.0793410	-0.2585350	-1.3070770
C	-1.0793410	-0.2585350	1.3070770
C	-0.6847490	1.0758650	-0.6932420
C	-0.6847490	1.0758650	0.6932420
C	-1.3236210	2.3385160	-1.1316070
C	-1.3236210	2.3385160	1.1316070
O	-1.5784920	3.1043090	0.0000000
O	-1.6326190	2.7067080	-2.2262510
O	-1.6326190	2.7067080	2.2262510
H	-1.0828270	-0.2573500	-2.3977690
H	-1.0828270	-0.2573500	2.3977690
C	3.5652370	-1.1865200	0.7076860
C	3.5652370	-1.1865200	-0.7076860
C	2.1889710	0.7999250	0.7092060
C	2.1889710	0.7999250	-0.7092060
C	2.8706850	-0.2263880	-1.4059890
C	2.8706850	-0.2263880	1.4059890
C	1.4791940	1.8435380	-1.3681520
C	1.4791940	1.8435380	1.3681520
C	0.8998560	5.4774220	-0.7075230
C	0.8998560	5.4774220	0.7075230
C	1.3315030	3.0989930	-0.7097710
C	1.3315030	3.0989930	0.7097710
C	1.0922430	4.3091400	-1.4067530
C	1.0922430	4.3091400	1.4067530
H	4.1130890	-1.9585290	1.2457970
H	4.1130890	-1.9585290	-1.2457970
H	2.8571820	-0.2313050	-2.4950760
H	2.8571820	-0.2313050	2.4950760
H	1.3938570	1.8152860	-2.4558610
H	1.3938570	1.8152860	2.4558610
H	0.7311800	6.4088060	-1.2445450
H	0.7311800	6.4088060	1.2445450
H	1.0648600	4.2992300	2.4950100
H	1.0648600	4.2992300	-2.4950100

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TS3d M05-2X/AVDZ' Optimized Geometry

C	-0.4771550	3.7903390	-2.0477340
C	-0.4245370	4.2384050	-0.7295380
C	-4.0133480	-0.6710250	1.0089320
C	-4.0362120	-1.1190500	-0.3020690
C	-0.3453630	3.3259150	0.3266660
C	-0.4422070	2.4221190	-2.3285260
C	-2.8729840	-0.0254530	1.5027530
C	-2.9191150	-0.9221010	-1.1232720
C	-1.7634220	0.1617860	0.6990760
C	-1.7864080	-0.2951930	-0.6372480
C	-0.3167020	1.9657910	0.0494610
C	-0.3583110	1.5183680	-1.2779410
H	-0.5550030	4.5082280	-2.8626190
H	-0.4593620	5.3057580	-0.5173340
H	-4.8741110	-0.8184210	1.6564730
H	-4.9148610	-1.6231910	-0.6966550
H	-0.3261770	3.6752380	1.3583100
H	-0.5001520	2.0636640	-3.3557180
Br	-2.8954190	0.5940020	3.2998250
Br	-3.0046830	-1.5326820	-2.9218120
C	-0.4376450	0.8477890	1.0758450
C	-0.4848950	0.0125050	-1.3996640

C	0.5802670	-0.2434760	0.7815020
C	0.5770570	-0.6607520	-0.5418400
C	0.7035120	-1.4549780	1.6244270
C	0.7094070	-2.1384330	-0.5344200
O	0.8931430	-2.5456000	0.7800790
O	0.6396260	-1.5829340	2.8112790
O	0.6423050	-2.9192210	-1.4366880
H	-0.4274890	1.1978390	2.1091260
H	-0.5086580	-0.3476420	-2.4292430
C	2.9807500	3.4534220	-1.5143740
C	3.0358070	3.7685520	-0.1361510
C	2.8502110	1.0986070	-0.9778590
C	2.8881970	1.4187110	0.4027400
C	2.9604820	2.7727800	0.8083510
C	2.8655810	2.1468810	-1.9284620
C	2.8437850	0.3388010	1.3276100
C	2.7850410	-0.2800530	-1.3351450
C	4.2662600	-3.1151160	1.4297510
C	4.2434340	-3.4343630	0.0516440
C	3.3686770	-0.9261910	0.9363570
C	3.3447990	-1.2460060	-0.4462210
C	3.8194820	-1.8916220	1.8701110
C	3.7751900	-2.5271060	-0.8701140
H	3.0221560	4.2542840	-2.2503930
H	3.1245760	4.8084260	0.1737510
H	2.9869770	3.0084270	1.8716900
H	2.8122700	1.9036990	-2.9890320
H	2.7702100	0.5606280	2.3936960
H	2.6850350	-0.5451510	-2.3890530
H	4.6264400	-3.8511260	2.1458670
H	4.5862460	-4.4131480	-0.2784510
H	3.7286590	-2.7811120	-1.9276880
H	3.8084380	-1.6496530	2.9315620

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1e M05-2X/6-31+G(d) Optimized Geometry

C	-3.8497800	-1.3810000	0.6950800
C	-3.8497800	-1.3810000	-0.6950800
C	0.6499790	3.3232480	-0.6929030
C	0.6499790	3.3232480	0.6929030
C	-2.6824210	-1.0758820	-1.4049480
C	-2.6824210	-1.0758820	1.4049480
C	0.3971590	2.1390420	-1.3902100
C	0.3971590	2.1390420	1.3902100
C	0.1518850	0.9638200	-0.7023100
C	0.1518850	0.9638200	0.7023100
C	-1.5288390	-0.7793510	-0.7002240
C	-1.5288390	-0.7793510	0.7002240
H	-4.7573570	-1.6193800	1.2350850
H	-4.7573570	-1.6193800	-1.2350850
H	0.8447830	4.2345850	-1.2420190
H	0.8447830	4.2345850	1.2420190
H	-2.6807830	-1.0724780	-2.4885400
H	-2.6807830	-1.0724780	2.4885400
Cl	0.3926560	2.1716650	-3.1302610
Cl	0.3926560	2.1716650	3.1302610
C	-0.1724770	-0.4049800	-1.3120680
C	-0.1724770	-0.4049800	1.3120680
C	0.8085710	-1.3445100	-0.6657580
C	0.8085710	-1.3445100	0.6657580
C	1.8109450	-2.3283430	-1.1384740
C	1.8109450	-2.3283430	1.1384740
O	2.3855130	-2.8886440	0.0000000
O	2.1285160	-2.6458000	-2.2422780
O	2.1285160	-2.6458000	2.2422780
H	-0.1621090	-0.4123260	-2.3975370
H	-0.1621090	-0.4123260	2.3975370

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2e M05-2X/6-31+G(d) Optimized Geometry

C	-4.0042180	-0.8480450	0.6960580
C	-4.0042180	-0.8480450	-0.6960580
C	-1.1350340	5.0719400	-0.6961160
C	-1.1350340	5.0719400	0.6961160
C	-2.9951130	-0.1880340	-1.4024690
C	-2.9951130	-0.1880340	1.4024690
C	-1.0573870	3.8696230	-1.4035550
C	-1.0573870	3.8696230	1.4035550
C	-0.9966820	2.6751400	-0.7010180
C	-0.9966820	2.6751400	0.7010180
C	-1.9952480	0.4677290	-0.7003600
C	-1.9952480	0.4677290	0.7003600
H	-4.7908750	-1.3601370	1.2364840
H	-4.7908750	-1.3601370	-1.2364840
H	-1.1852580	6.0094240	-1.2356010
H	-1.1852580	6.0094240	1.2356010
H	-2.9912430	-0.1892710	-2.4867010
H	-2.9912430	-0.1892710	2.4867010
H	-1.0332480	3.8672660	-2.4871150
H	-1.0332480	3.8672660	2.4871150

C	-0.8703310	1.2834100	-1.3009640
C	-0.8703310	1.2834100	1.3009640
C	0.4957640	0.7381700	-0.7710020
C	0.4957640	0.7381700	0.7710020
C	1.5786250	1.7447820	-1.1358830
C	1.5786250	1.7447820	1.1358830
O	2.1484160	2.2776470	0.0000000
O	1.9276790	2.0663640	-2.2312610
O	1.9276790	2.0663640	2.2312610
H	-0.8780500	1.2932860	-2.3913680
H	-0.8780500	1.2932860	2.3913680
C	-1.3891810	-3.6590780	0.6936170
C	-1.3891810	-3.6590780	-0.6936170
C	0.0607420	-1.7280030	-0.7015340
C	0.0607420	-1.7280030	0.7015340
C	-0.6708950	-2.6850490	-1.3848790
C	-0.6708950	-2.6850490	1.3848790
C	0.9501570	-0.6598410	-1.2998550
C	0.9501570	-0.6598410	1.2998550
C	2.3282120	-0.8904790	-0.7003140
C	2.3282120	-0.8904790	0.7003140
C	4.7062990	-1.2055850	-0.6962580
C	4.7062990	-1.2055850	0.6962580
C	3.5136180	-1.0400820	-1.4047030
C	3.5136180	-1.0400820	1.4047030
H	-1.9507730	-4.4023610	1.2436740
H	-1.9507730	-4.4023610	-1.2436740
Cl	-0.7301350	-2.6780630	-3.1270270
Cl	-0.7301350	-2.6780630	3.1270270
H	0.9612800	-0.6693430	-2.3878900
H	0.9612800	-0.6693430	2.3878900
H	5.6376380	-1.3254110	-1.2353580
H	5.6376380	-1.3254110	1.2353580
H	3.5117650	-1.0174780	2.4881400
H	3.5117650	-1.0174780	-2.4881400

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3e M05-2X/6-31+G(d) Optimized Geometry

C	3.1269250	-3.4529370	0.6960650
C	3.1269250	-3.4529370	-0.6960650
C	-3.4191650	-3.8531230	-0.6961040
C	-3.4191650	-3.8531230	0.6961040
C	2.0620140	-2.8872780	-1.4009340
C	2.0620140	-2.8872780	1.4009340
C	-2.4131660	-3.1900090	-1.4035230
C	-2.4131660	-3.1900090	1.4035230
C	-1.4051380	-2.5463910	-0.7010280
C	-1.4051380	-2.5463910	0.7010280
C	1.0053990	-2.3266020	-0.6998980
C	1.0053990	-2.3266020	0.6998980
H	3.9547820	-3.8954870	1.2361570
H	3.9547820	-3.8954870	-1.2361570
H	-4.2089320	-4.3606600	-1.2356610
H	-4.2089320	-4.3606600	1.2356610
H	2.0590000	-2.8871310	-2.4853910
H	2.0590000	-2.8871310	2.4853910
H	-2.4234950	-3.1672630	-2.4870700
H	-2.4234950	-3.1672630	2.4870700
C	-0.2576590	-1.7476240	-1.3003530
C	-0.2576590	-1.7476240	1.3003530
C	-0.4639740	-0.2910380	-0.7710300
C	-0.4639740	-0.2910380	0.7710300
C	-1.8783400	0.1416510	-1.1363730
C	-1.8783400	0.1416510	1.1363730
O	-2.6236790	0.3739660	0.0000000
O	-2.3330260	0.2795480	-2.2311680
O	-2.3330260	0.2795480	2.2311680
H	-0.2644700	-1.7597470	-2.3907780
H	-0.2644700	-1.7597470	2.3907780
C	4.2833030	0.3294200	0.6961870
C	4.2833030	0.3294200	-0.6961870
C	1.8961920	0.5765650	-0.6992800
C	1.8961920	0.5765650	0.6992800
C	3.0848460	0.4543460	-1.4021060
C	3.0848460	0.4543460	1.4021060
C	0.5241050	0.7976460	-1.2995700
C	0.5241050	0.7976460	1.2995700
C	0.0275050	2.1060570	-0.7029780
C	0.0275050	2.1060570	0.7029780
C	-0.8529680	4.3523350	-0.6934860
C	-0.8529680	4.3523350	0.6934860
C	-0.4126060	3.2265500	-1.3908060
C	-0.4126060	3.2265500	1.3908060
H	5.2176090	0.2354190	1.2357590
H	5.2176090	0.2354190	-1.2357590
H	3.0815340	0.4580500	-2.4863630
H	3.0815340	0.4580500	2.4863630
H	0.5262250	0.8137440	-2.3879140
H	0.5262250	0.8137440	2.3879140
H	-1.1919630	5.2208420	-1.2421180

H	-1.1919630	5.2208420	1.2421180
Cl	-0.4138230	3.2630930	3.1294010
Cl	-0.4138230	3.2630930	-3.1294010

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TS2e M05-2X/6-31+G(d) Optimized Geometry

C	1.3727430	-3.6775710	0.6936020
C	1.3727430	-3.6775710	-0.6936020
C	-4.6357020	-1.6947150	-0.6944900
C	-4.6357020	-1.6947150	0.6944900
C	0.6909920	-2.6778870	-1.3843910
C	0.6909920	-2.6778870	1.3843910
C	-3.4705880	-1.3754030	-1.4054920
C	-3.4705880	-1.3754030	1.4054920
C	-2.3229540	-1.0592010	-0.7021380
C	-2.3229540	-1.0592010	0.7021380
C	-0.0088780	-1.6952830	-0.7024190
C	-0.0088780	-1.6952830	0.7024190
H	1.9017400	-4.4441020	1.2443190
H	1.9017400	-4.4441020	-1.2443190
H	-5.5426770	-1.9356330	-1.2346590
H	-5.5426770	-1.9356330	1.2346590
Cl	0.7313690	-2.6897240	-3.1269980
Cl	0.7313690	-2.6897240	3.1269980
H	-3.4696870	-1.3672670	-2.4891460
H	-3.4696870	-1.3672670	2.4891460
C	-0.9603050	-0.6768170	-1.3072550
C	-0.9603050	-0.6768170	1.3072550
C	-0.6908510	0.6874100	-0.6923140
C	-0.6908510	0.6874100	0.6923140
C	-1.4375190	1.8867640	-1.1322420
C	-1.4375190	1.8867640	1.1322420
O	-1.7610990	2.6248430	0.0000000
O	-1.7737920	2.2272410	-2.2293200
O	-1.7737920	2.2272410	2.2293200
H	-0.9643700	-0.6741170	-2.3937080
H	-0.9643700	-0.6741170	2.3937080
C	3.7355880	-1.1873940	0.7071920
C	3.7355880	-1.1873940	-0.7071920
C	2.1936730	0.6711930	0.7088310
C	2.1936730	0.6711930	-0.7088310
C	2.9607170	-0.2920750	-1.4047440
C	2.9607170	-0.2920750	1.4047440
C	1.3935680	1.6462650	-1.3666690
C	1.3935680	1.6462650	1.3666690
C	0.4797750	5.2079530	-0.7071480
C	0.4797750	5.2079530	0.7071480
C	1.1348970	2.8829510	-0.7093410
C	1.1348970	2.8829510	0.7093410
C	0.7824430	4.0641970	-1.4056360
C	0.7824430	4.0641970	1.4056360
H	4.3429350	-1.9072970	1.2420610
H	4.3429350	-1.9072970	-1.2420610
H	2.9461280	-0.2988600	-2.4885730
H	2.9461280	-0.2988600	2.4885730
H	1.3051990	1.6088540	-2.4485400
H	1.3051990	1.6088540	2.4485400
H	0.2227710	6.1140460	-1.2409840
H	0.2227710	6.1140460	1.2409840
H	0.7538260	4.0500720	2.4885000
H	0.7538260	4.0500720	-2.4885000

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TS3e M05-2X/6-31+G(d) Optimized Geometry

C	-1.4031330	3.9416140	-1.1005300
C	-1.3602200	4.0780230	0.2841850
C	-4.2448630	-1.5097250	0.8478970
C	-4.2554970	-1.6435530	-0.5297790
C	-1.1297340	2.9663900	1.0984820
C	-1.2056040	2.6916950	-1.6904830
C	-3.1791130	-0.8566190	1.4774440
C	-3.2009570	-1.1246820	-1.2896310
C	-2.1316770	-0.3520260	0.7312150
C	-2.1420900	-0.4886120	-0.6708530
C	-0.9409510	1.7228480	0.5143400
C	-0.9719910	1.5911250	-0.8797550
H	-1.5977100	4.8063090	-1.7232000
H	-1.5193490	5.0492750	0.7365480
H	-5.0536460	-1.9084350	1.4455900
H	-5.0724540	-2.1490570	-1.0271150
H	-1.1161200	3.0695240	2.1775960
H	-1.2531140	2.5748140	-2.7673860
Cl	-3.2038780	-0.6894250	3.2101750
Cl	-3.2521150	-1.2959310	-3.0214180
C	-0.8892950	0.3921540	1.2544690
C	-0.9153080	0.1498170	-1.3474850
C	0.2440640	-0.4624710	0.7096290
C	0.2491480	-0.5585830	-0.6712360
C	0.5533350	-1.8052170	1.2472360
C	0.5730540	-1.9635060	-1.0125960

O	0.8517280	-2.6350480	0.1698440
O	0.5512320	-2.2099980	2.3736070
O	0.5777120	-2.5143630	-2.0747600
H	-0.8862040	0.4932820	2.3365130
H	-0.9257300	0.0355690	-2.4282090
C	2.0617000	3.9484670	-0.6322160
C	2.1296490	3.9313600	0.7803470
C	2.2656970	1.5404850	-0.6789470
C	2.3133110	1.5252710	0.7375200
C	2.2231430	2.7401310	1.4565860
C	2.1044070	2.7763020	-1.3476370
C	2.4432640	0.2623740	1.3746240
C	2.3674740	0.2924450	-1.3566800
C	4.2779270	-2.9041370	0.6387090
C	4.2464570	-2.8865890	-0.7753160
C	3.1057870	-0.7931380	0.6891000
C	3.0732420	-0.7750430	-0.7291560
C	3.7018390	-1.8879080	1.3611060
C	3.6408900	-1.8536580	-1.4493310
H	1.9646940	4.8943260	-1.1503780
H	2.0906180	4.8650330	1.3277890
H	2.2586890	2.7164520	2.5399290
H	2.0396820	2.7868970	-2.4297130
H	2.3756020	0.2101840	2.4573530
H	2.2601780	0.2728110	-2.4373260
H	4.7456180	-3.7345400	1.1521550
H	4.6903380	-3.7040670	-1.3291150
H	3.5866520	-1.8532300	-2.5312720
H	3.6950280	-1.9090450	2.4443030

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2f M05-2X/6-31+G(d) Optimized Geometry

C	-4.15921429	-0.44939937	0.69604728
C	-4.15921429	-0.44939937	-0.69604728
C	-0.48564766	5.01307632	-0.69610626
C	-0.48564766	5.01307632	0.69610626
C	-3.06752047	0.06283130	-1.40230512
C	-3.06752047	0.06283130	1.40230512
C	-0.57934085	3.81182559	-1.40355671
C	-0.57934085	3.81182559	1.40355671
C	-0.68903479	2.62094056	-0.70104218
C	-0.68903479	2.62094056	0.70104218
C	-1.98722697	0.57561946	-0.70038234
C	-1.98722697	0.57561946	0.70038234
H	-5.00934448	-0.84778714	1.23636376
H	-5.00934448	-0.84778714	-1.23636376
H	-0.40223491	5.94824809	-1.23577955
H	-0.40223491	5.94824809	1.23577955
H	-3.06292601	0.05905755	-2.48676635
H	-3.06292601	0.05905755	2.48676635
H	-0.55537488	3.80617137	-2.48720260
H	-0.55537488	3.80617137	2.48720260
C	-0.75915394	1.22527070	-1.30077402
C	-0.75915394	1.22527070	1.30077402
C	0.51838981	0.49388273	-0.77202556
C	0.51838981	0.49388273	0.77202556
C	1.72905459	1.34340371	-1.13576096
C	1.72905459	1.34340371	1.13576096
O	2.36569240	1.79357881	0.00000000
O	2.11897666	1.61420992	-2.23118974
O	2.11897666	1.61420992	2.23118974
H	-0.76532789	1.23723541	-2.39104437
H	-0.76532789	1.23723541	2.39104437
C	-1.96076147	-3.59329800	0.69568073
C	-1.96076147	-3.59329800	-0.69568073
C	-0.24571379	-1.88547828	-0.69929880
C	-0.24571379	-1.88547828	0.69929880
C	-1.10744109	-2.73003287	-1.36776446
C	-1.10744109	-2.73003287	1.36776446
C	0.77750044	-0.95372170	-1.30484729
C	0.77750044	-0.95372170	1.30484729
C	2.11231801	-1.36489424	-0.70106257
C	2.11231801	-1.36489424	0.70106257
C	4.43161557	-1.98178371	-0.69612892
C	4.43161557	-1.98178371	0.69612892
C	3.26959031	-1.66477022	-1.40417524
C	3.26959031	-1.66477022	1.40417524
H	-2.61691307	-4.24208336	1.26022596
H	-2.61691307	-4.24208336	-1.26022596
F	-1.13085609	-2.70803894	-2.72213127
F	-1.13085609	-2.70803894	2.72213127
H	0.78314970	-0.96851760	-2.39339800
H	0.78314970	-0.96851760	2.39339800
H	5.34002734	-2.21918501	-1.23568270
H	5.34002734	-2.21918501	1.23568270
H	3.27156433	-1.64133877	2.48769507
H	3.27156433	-1.64133877	-2.48769507

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3f M05-2X/6-31+G(d) Optimized Geometry
C       3.21813169      -3.13889846       0.69605644
C       3.21813169      -3.13889846      -0.69605644
C      -3.31491406      -3.74929585      -0.69606614
C      -3.31491406      -3.74929585       0.69606614
C       2.13570867      -2.60746516      -1.40092839
C       2.13570867      -2.60746516       1.40092839
C      -2.32908655      -3.05642477      -1.40357786
C      -2.32908655      -3.05642477       1.40357786
C      -1.34083734      -2.38303484      -0.70112457
C      -1.34083734      -2.38303484       0.70112457
C       1.06116221      -2.08208796      -0.69997145
C       1.06116221      -2.08208796       0.69997145
H       4.05998616      -3.55453512       1.23622004
H       4.05998616      -3.55453512      -1.23622004
H      -4.08933532      -4.28014369      -1.23576095
H      -4.08933532      -4.28014369       1.23576095
H       2.13268010      -2.60774383      -2.48545848
H       2.13268010      -2.60774383       2.48545848
H      -2.34065879      -3.03352033      -2.48718993
H      -2.34065879      -3.03352033       2.48718993
C      -0.22059065      -1.54628937      -1.30043126
C      -0.22059065      -1.54628937       1.30043126
C      -0.47756548      -0.09695373      -0.77202867
C      -0.47756548      -0.09695373       0.77202867
C      -1.90680332       0.28463279      -1.13621846
C      -1.90680332       0.28463279       1.13621846
O      -2.66020139       0.48785056       0.00000000
O      -2.36519267       0.41037317      -2.23102303
O      -2.36519267       0.41037317       2.23102303
H      -0.22696206      -1.55896243      -2.39078161
H      -0.22696206      -1.55896243       2.39078161
C       4.24268155       0.69599784       0.69608056
C       4.24268155       0.69599784      -0.69608056
C       1.84739252       0.85865211      -0.69994769
C       1.84739252       0.85865211       0.69994769
C       3.04010655       0.77724558      -1.40167006
C       3.04010655       0.77724558       1.40167006
C       0.46898145       1.02906633      -1.30435901
C       0.46898145       1.02906633       1.30435901
C      -0.07889424       2.31053792      -0.70096975
C      -0.07889424       2.31053792       0.70096975
C      -1.08529751       4.51056233      -0.69535117
C      -1.08529751       4.51056233       0.69535117
C      -0.58243459       3.40648652      -1.37259873
C      -0.58243459       3.40648652       1.37259873
H       5.17965018       0.63474728       1.23599610
H       5.17965018       0.63474728      -1.23599610
H       3.03712398       0.77953023      -2.48602251
H       3.03712398       0.77953023       2.48602251
H       0.46782807       1.05011589      -2.39302293
H       0.46782807       1.05011589       2.39302293
H      -1.46988243       5.34978844      -1.25911293
H      -1.46988243       5.34978844       1.25911293
F      -0.58219946       3.41070907       2.72275682
F      -0.58219946       3.41070907      -2.72275682

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1f M05-2X/6-31+G(d) Optimized Geometry
C      -3.96683752      -0.36968180       0.69491725
C      -3.96683752      -0.36968180      -0.69491725
C       1.40782875       3.33282181      -0.69465214
C       1.40782875       3.33282181       0.69465214
C      -2.76183674      -0.30205938      -1.40456493
C      -2.76183674      -0.30205938       1.40456493
C       0.91268368       2.22305911      -1.37181489
C       0.91268368       2.22305911       1.37181489
C       0.42714930       1.12236752      -0.70026222
C       0.42714930       1.12236752       0.70026222
C      -1.57212583      -0.23931311      -0.70088612
C      -1.57212583      -0.23931311       0.70088612
H      -4.90354009      -0.42408803       1.23535667
H      -4.90354009      -0.42408803      -1.23535667
H       1.78537843       4.17465040      -1.25922251
H       1.78537843       4.17465040       1.25922251
H      -2.76015388      -0.30054223      -2.48826767
H      -2.76015388      -0.30054223       2.48826767
F       0.90827746       2.22747568      -2.72310745
F       0.90827746       2.22747568       2.72310745
C      -0.16817900      -0.14578968      -1.31644310
C      -0.16817900      -0.14578968       1.31644310
C       0.60006781      -1.26574464      -0.66615976
C       0.60006781      -1.26574464       0.66615976
C       1.37933226      -2.43420676      -1.13803117
C       1.37933226      -2.43420676       1.13803117
O       1.82693252      -3.10041377       0.00000000
O       1.62555322      -2.80960327      -2.24197574
O       1.62555322      -2.80960327       2.24197574
H      -0.15739591      -0.15076534      -2.40255558
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H      -0.15739591      -0.15076534       2.40255558

55
TS2f M05-2X/6-31+G(d) Optimized Geometry
C      -1.72592905       3.72739237       0.69577442
C      -1.72592905       3.72739237      -0.69577442
C       4.42764800       2.21958256      -0.69430110
C       4.42764800       2.21958256       0.69430110
C      -0.96499744       2.78198225      -1.36724402
C      -0.96499744       2.78198225       1.36724402
C       3.28949134       1.81314240      -1.40498933
C       3.28949134       1.81314240       1.40498933
C       2.16832769       1.41192432      -0.70280678
C       2.16832769       1.41192432       0.70280678
C      -0.18866509       1.85601051      -0.70003939
C      -0.18866509       1.85601051       0.70003939
H      -2.30857779       4.44249619       1.26107781
H      -2.30857779       4.44249619      -1.26107781
H       5.31396657       2.52757740      -1.23499852
H       5.31396657       2.52757740       1.23499852
F      -0.97804434       2.77383643      -2.72206044
F      -0.97804434       2.77383643       2.72206044
H       3.29026797       1.80407140      -2.48873309
H       3.29026797       1.80407140       2.48873309
C       0.83975532       0.92393089      -1.31169330
C       0.83975532       0.92393089       1.31169330
C       0.68244749      -0.45731558      -0.69268085
C       0.68244749      -0.45731558       0.69268085
C       1.52391016      -1.59223843      -1.13182840
C       1.52391016      -1.59223843       1.13182840
O       1.90502873      -2.30253762       0.00000000
O       1.88847920      -1.90270898      -2.22888349
O       1.88847920      -1.90270898       2.22888349
H       0.84039764       0.92540963      -2.39872361
H       0.84039764       0.92540963       2.39872361
C      -3.88648304       1.04508273       0.70732765
C      -3.88648304       1.04508273      -0.70732765
C      -2.19429209      -0.67780330       0.70889365
C      -2.19429209      -0.67780330      -0.70889365
C      -3.03700101       0.22053988      -1.40481012
C      -3.03700101       0.22053988       1.40481012
C      -1.31888870      -1.58569563      -1.36686272
C      -1.31888870      -1.58569563       1.36686272
C      -0.12839628      -5.06487034      -0.70728007
C      -0.12839628      -5.06487034       0.70728007
C      -0.96184938      -2.79753524      -0.70942654
C      -0.96184938      -2.79753524       0.70942654
C      -0.51820386      -3.94802723      -1.40568845
C      -0.51820386      -3.94802723       1.40568845
H      -4.55308784       1.71120317       1.24137658
H      -4.55308784       1.71120317      -1.24137658
H      -3.01986813       0.23115527      -2.48889387
H      -3.01986813       0.23115527       2.48889387
H      -1.23431879      -1.54222330      -2.44876457
H      -1.23431879      -1.54222330       2.44876457
H       0.19753106      -5.94867452      -1.24109996
H       0.19753106      -5.94867452       1.24109996
H      -0.49103098      -3.93184112       2.48867272
H      -0.49103098      -3.93184112      -2.48867272

55
TS3f M05-2X/6-31+G(d) Optimized Geometry
C      -2.1852790        3.6138720       -0.9772620
C      -2.1555290        3.7161230        0.4105080
C      -4.1578640       -2.2650140        0.8196110
C      -4.1566690       -2.3592940       -0.5651410
C      -1.7559120        2.6288720        1.1917990
C      -1.8055350        2.4248120       -1.6028090
C      -3.1967960       -1.4748700        1.4466190
C      -3.1947490       -1.6609820       -1.2917040
C      -2.2403510       -0.7926300        0.7293340
C      -2.2382490       -0.8891370       -0.6718580
C      -1.3869520        1.4440760        0.5729460
C      -1.4056990        1.3482890       -0.8254580
H      -2.5101950        4.4567910       -1.5748600
H      -2.4551490        4.6395330        0.8909590
H      -4.8852990       -2.7929840        1.4211240
H      -4.8830370       -2.9641270       -1.0907870
H      -1.7511080        2.7030620        2.2733540
H      -1.8398590        2.3335810       -2.6826780
F      -3.2135730       -1.3754990        2.7946420
F      -3.2095200       -1.7448790       -2.6408670
C      -1.1291200        0.1169000        1.2780430
C      -1.1332750       -0.0539130       -1.3381100
C       0.1214720       -0.5335530        0.7037580
C       0.1326390       -0.5902930       -0.6818170
C       0.6382030       -1.8267120        1.2019970
C       0.6659550       -1.9196720       -1.0610780
O       1.0527400       -2.5715460        0.1014310
O       0.7086460       -2.2567800        2.3168100
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O	0.7498780	-2.4344200	-2.1380250
H	-1.1388250	0.1835260	2.3632410
H	-1.1366010	-0.1411300	-2.4218880
C	1.2454230	4.1404740	-0.5443450
C	1.3214820	4.1029270	0.8670480
C	1.8006710	1.7904820	-0.6445130
C	1.8579400	1.7518300	0.7707920
C	1.5926770	2.9237260	1.5166600
C	1.4559290	3.0026120	-1.2855740
C	2.1783780	0.5076580	1.3788500
C	2.0826360	0.5848010	-1.3494060
C	4.4836430	-2.3155960	0.5678040
C	4.4417710	-2.2720650	-0.8449500
C	2.9960110	-0.4159000	0.6687550
C	2.9530540	-0.3719900	-0.7483120
C	3.7594420	-1.4181400	1.3144260
C	3.6777650	-1.3318940	-1.4941140
H	1.0085280	5.0728440	-1.0414350
H	1.1484060	5.0085050	1.4352900
H	1.6365270	2.8822440	2.5991440
H	1.3851910	3.0268840	-2.3670620
H	2.1249600	0.4216210	2.4602020
H	1.9731340	0.5721690	-2.4299290
H	5.0783390	-3.0735330	1.0615450
H	5.0049560	-2.9975360	-1.4181700
H	3.6172380	-1.3165580	-2.5755900
H	3.7618280	-1.4643100	2.3968480

Butadiene + Substrates 1a-1e

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butadiene M05-2X/6-31+G(d) Optimized Geometry

C	0.12080402	-1.84072224	0.00000000
H	1.19457957	-1.99421140	0.00000000
H	-0.50579205	-2.72333159	0.00000000
C	-0.40212927	-0.61018215	0.00000000
H	-1.48092673	-0.48029605	0.00000000
C	0.40212927	0.61018215	0.00000000
H	1.48092673	0.48029605	0.00000000
C	-0.12080402	1.84072224	0.00000000
H	-1.19457957	1.99421140	0.00000000
H	0.50579205	2.72333159	0.00000000

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TS4a M05-2X/6-31+G(d) Optimized Geometry

C	-3.91063371	-0.94173378	-0.69576289
C	-3.91063371	-0.94173378	0.69576289
C	2.05886004	-3.69577291	0.69463743
C	2.05886004	-3.69577291	-0.69463743
C	-2.70921211	-0.82466754	1.40191237
C	-2.70921211	-0.82466754	-1.40191237
C	1.36479212	-2.70681398	1.40364216
C	1.36479212	-2.70681398	-1.40364216
C	0.68250346	-1.72929889	0.70177977
C	0.68250346	-1.72929889	-0.70177977
C	-1.51808771	-0.70827329	0.70127539
C	-1.51808771	-0.70827329	-0.70127539
H	-4.84435133	-1.03523876	-1.23630316
H	-4.84435133	-1.03523876	1.23630316
H	2.60347535	-4.45987052	1.23531105
H	2.60347535	-4.45987052	-1.23531105
H	-2.70732796	-0.82521730	2.48626341
H	-2.70732796	-0.82521730	-2.48626341
C	-0.12716161	-0.57608191	1.30861706
C	-0.12716161	-0.57608191	-1.30861706
C	0.48304846	0.66673340	0.68701808
C	0.48304846	0.66673340	-0.68701808
C	1.66604780	1.42407511	1.13727218
C	1.66604780	1.42407511	-1.13727218
O	2.23599793	1.99620960	0.00000000
O	2.13914182	1.56830686	2.22652249
O	2.13914182	1.56830686	-2.22652249
H	-0.12302049	-0.57225416	2.39720581
H	-0.12302049	-0.57225416	-2.39720581
C	-0.91787379	2.44132717	1.44360783
C	-0.91787379	2.44132717	-1.44360783
C	-0.40223221	3.47589816	0.71164412
C	-0.40223221	3.47589816	-0.71164412
H	-0.77245847	2.40774533	2.51732854
H	-0.77245847	2.40774533	-2.51732854
H	0.20091652	4.22421036	1.21426782
H	0.20091652	4.22421036	-1.21426782
H	1.36931061	-2.70185565	2.48759125
H	1.36931061	-2.70185565	-2.48759125
H	-1.67632870	1.78377914	1.03946179
H	-1.67632870	1.78377914	-1.03946179

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TS4b M05-2X/6-31+G(d) Optimized Geometry

C	2.63010452	2.68570403	-0.69568129
C	2.63010452	2.68570403	0.69568129
C	-3.87543705	1.85572239	0.69465437
C	-3.87543705	1.85572239	-0.69465437
C	-2.76312030	1.38341157	1.40359976
C	-2.76312030	1.38341157	-1.40359976
C	-1.66667056	0.91587943	0.70135917
C	-1.66667056	0.91587943	-0.70135917
C	0.74281050	1.23019599	0.70044044
C	0.74281050	1.23019599	-0.70044044
H	3.37735485	3.26354372	-1.22822844
H	3.37735485	3.26354372	1.22822844
H	-4.74193510	2.21590128	1.23531404
H	-4.74193510	2.21590128	-1.23531404
C	-0.36677430	0.37266135	1.30565833
C	-0.36677430	0.37266135	-1.30565833
C	-0.21416929	-1.00376760	0.68693398
C	-0.21416929	-1.00376760	-0.68693398
C	-0.79884716	-2.28064004	1.13740606
C	-0.79884716	-2.28064004	-1.13740606
O	-0.96663069	-3.07090032	0.00000000
O	-1.11880078	-2.65848854	2.22639259
O	-1.11880078	-2.65848854	-2.22639259
H	-0.37749866	0.36063263	2.39294069
H	-0.37749866	0.36063263	-2.39294069
C	1.91986942	-1.72865751	1.44397789
C	1.91986942	-1.72865751	-1.44397789
C	2.05705393	-2.87655993	0.71131145
C	2.05705393	-2.87655993	-0.71131145

H	1.77768514	-1.78507727	2.51723106
H	1.77768514	-1.78507727	-2.51723106
H	1.96148841	-3.83306171	1.21373848
H	1.96148841	-3.83306171	-1.21373848
H	-2.76468705	1.37589837	2.48768592
H	-2.76468705	1.37589837	-2.48768592
C	1.68520332	1.95794187	1.42617283
C	1.68520332	1.95794187	-1.42617283
C	1.69344622	1.96436061	2.93427946
H	0.76070100	2.36947233	3.33494961
H	1.81695535	0.95618863	3.33902034
H	2.51366328	2.57735984	3.30869839
C	1.69344622	1.96436061	-2.93427946
H	1.81695535	0.95618863	-3.33902034
H	0.76070100	2.36947233	-3.33494961
H	2.51366328	2.57735984	-3.30869839
H	2.19750650	-0.76248992	1.04216200
H	2.19750650	-0.76248992	-1.04216200

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TS5b M05-2X/6-31+G(d) Optimized Geometry

C	-4.08922783	0.30418257	-0.69575056
C	-4.08922783	0.30418257	0.69575056
C	1.03212241	-3.81696414	0.69463783
C	1.03212241	-3.81696414	-0.69463783
C	-2.89582505	0.12115219	1.40189068
C	-2.89582505	0.12115219	-1.40189068
C	0.60149785	-2.70350738	1.42816589
C	0.60149785	-2.70350738	-1.42816589
C	0.17159331	-1.59905040	0.70078539
C	0.17159331	-1.59905040	-0.70078539
C	-1.71336459	-0.06244245	0.70089442
C	-1.71336459	-0.06244245	-0.70089442
H	-5.01698082	0.44517692	-1.23631074
H	-5.01698082	0.44517692	1.23631074
H	1.38245184	-4.69409538	1.22741474
H	1.38245184	-4.69409538	-1.22741474
H	-2.89372506	0.12242132	2.48635888
H	-2.89372506	0.12242132	-2.48635888
C	-0.33325799	-0.27786315	1.30581015
C	-0.33325799	-0.27786315	-1.30581015
C	0.56754221	0.77258072	0.68593451
C	0.56754221	0.77258072	-0.68593451
C	1.90309170	1.20407295	1.13637329
C	1.90309170	1.20407295	-1.13637329
O	2.60003846	1.61576326	0.00000000
O	2.39904212	1.21534146	2.22539998
O	2.39904212	1.21534146	-2.22539998
H	-0.33230659	-0.26564700	2.39320891
H	-0.33230659	-0.26564700	-2.39320891
C	-0.34362089	2.85208972	1.44568992
C	-0.34362089	2.85208972	-1.44568992
C	0.41619291	3.72025713	0.71236806
C	0.41619291	3.72025713	-0.71236806
H	-0.21186487	2.78496118	2.51958574
H	-0.21186487	2.78496118	-2.51958574
H	1.18814322	4.29357654	1.21418386
H	1.18814322	4.29357654	-1.21418386
C	0.62326662	-2.70520802	-2.93632940
H	1.25177954	-1.89941839	-3.32396554
H	1.01942723	-3.64983068	-3.30999361
H	-0.38066051	-2.57707289	-3.34995612
C	0.62326662	-2.70520802	2.93632940
H	1.01942723	-3.64983068	3.30999361
H	1.25177954	-1.89941839	3.32396554
H	-0.38066051	-2.57707289	3.34995612
H	-1.23908881	2.39906744	1.04074565
H	-1.23908881	2.39906744	-1.04074565

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TS4c M05-2X/6-31+G(d) Optimized Geometry

C	0.43989430	-3.43677358	0.69997129
C	0.43989430	-3.43677358	-0.69997129
C	-4.25114540	1.17487565	-0.69467330
C	-4.25114540	1.17487565	0.69467330
C	-3.08156516	0.87133104	-1.40395866
C	-3.08156516	0.87133104	1.40395866
C	-1.92721206	0.57525143	-0.70163914
C	-1.92721206	0.57525143	0.70163914
C	-0.20005567	-1.12583056	-0.69481135
C	-0.20005567	-1.12583056	0.69481135
H	0.69185503	-4.35346247	1.21445001
H	0.69185503	-4.35346247	-1.21445001
H	-5.15795375	1.41661042	-1.23536787
H	-5.15795375	1.41661042	1.23536787
C	-0.56447933	0.21956044	-1.30913520
C	-0.56447933	0.21956044	1.30913520
C	0.38964598	1.22322502	-0.68699669
C	0.38964598	1.22322502	0.68699669
C	0.70232872	2.59224624	-1.13778916

C	0.70232872	2.59224624	1.13778916
O	1.04746225	3.32248454	0.00000000
O	0.68077424	3.08767160	-2.22645254
O	0.68077424	3.08767160	2.22645254
H	-0.55928865	0.21394394	-2.39546281
H	-0.55928865	0.21394394	2.39546281
C	2.52494361	0.49718432	-1.44509506
C	2.52494361	0.49718432	1.44509506
C	3.33048680	1.32535987	-0.71172372
C	3.33048680	1.32535987	0.71172372
H	2.44051261	0.62360043	-2.51820747
H	2.44051261	0.62360043	2.51820747
H	3.83542398	2.14362808	-1.21375069
H	3.83542398	2.14362808	1.21375069
H	-3.07771655	0.87462152	-2.48784390
H	-3.07771655	0.87462152	2.48784390
C	0.12458117	-2.28018561	-1.40993375
C	0.12458117	-2.28018561	1.40993375
O	0.11980583	-2.17504945	2.77064934
O	0.11980583	-2.17504945	-2.77064934
C	0.43819296	-3.33848158	3.51571543
H	0.37432000	-3.04934168	4.56114929
H	-0.27767792	-4.13884283	3.31155752
H	1.45202891	-3.67991661	3.29067846
C	0.43819296	-3.33848158	-3.51571543
H	-0.27767792	-4.13884283	-3.31155752
H	0.37432000	-3.04934168	-4.56114929
H	1.45202891	-3.67991661	-3.29067846
H	2.15469839	-0.43598493	-1.04093089
H	2.15469839	-0.43598493	1.04093089

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TS5c M05-2X/6-31+G(d) Optimized Geometry

C	4.06166269	-1.07089764	-0.69576721
C	4.06166269	-1.07089764	0.69576721
C	-0.51534269	3.62061295	0.69881586
C	-0.51534269	3.62061295	-0.69881586
C	2.89679172	-0.75331559	1.40243819
C	2.89679172	-0.75331559	-1.40243819
C	-0.22358971	2.45666355	1.41188323
C	-0.22358971	2.45666355	-1.41188323
C	0.05145828	1.29440322	0.69525839
C	0.05145828	1.29440322	-0.69525839
C	1.74259984	-0.43855491	0.70135866
C	1.74259984	-0.43855491	-0.70135866
H	4.96751640	-1.31498589	-1.23608091
H	4.96751640	-1.31498589	1.23608091
H	-0.74836976	4.54194880	1.21327596
H	-0.74836976	4.54194880	-1.21327596
H	2.89426904	-0.75053008	2.48626813
H	2.89426904	-0.75053008	-2.48626813
C	0.39462121	-0.06850856	1.30883127
C	0.39462121	-0.06850856	-1.30883127
C	-0.61583933	-1.01633072	0.68724178
C	-0.61583933	-1.01633072	-0.68724178
C	-1.98864188	-1.31358886	1.13827842
C	-1.98864188	-1.31358886	-1.13827842
O	-2.72312892	-1.64795372	0.00000000
O	-2.48453580	-1.28931348	2.22665525
O	-2.48453580	-1.28931348	-2.22665525
H	0.38592638	-0.05850738	2.39492939
H	0.38592638	-0.05850738	-2.39492939
C	0.07259749	-3.16650030	1.44385135
C	0.07259749	-3.16650030	-1.44385135
C	-0.77070941	-3.95715786	0.71145762
C	-0.77070941	-3.95715786	-0.71145762
H	-0.05452282	-3.08192549	2.51666531
H	-0.05452282	-3.08192549	-2.51666531
H	-1.59777722	-4.44631137	1.21366863
H	-1.59777722	-4.44631137	-1.21366863
O	-0.18454465	2.36357792	-2.77233123
O	-0.18454465	2.36357792	2.77233123
C	-0.54468547	3.51541130	-3.51517855
H	-0.48611858	3.22585808	-4.56039239
H	-1.56469562	3.82683164	-3.27748542
H	0.14989890	4.33702231	-3.32274161
C	-0.54468547	3.51541130	3.51517855
H	-1.56469562	3.82683164	3.27748542
H	-0.48611858	3.22585808	4.56039239
H	0.14989890	4.33702231	3.32274161
H	1.01406271	-2.81683731	-1.04234948
H	1.01406271	-2.81683731	1.04234948

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TS4d M05-2X/AVDZ’ Optimized Geometry

C	-3.1852212	-0.4417468	0.6941511
C	-3.1852212	-0.4417468	-0.6941511
C	1.4014628	4.2681437	-0.6953063
C	1.4014628	4.2681437	0.6953063

C	1.1146906	3.0950032	-1.4061909
C	1.1146906	3.0950032	1.4061909
C	0.8369840	1.9357055	-0.7014075
C	0.8369840	1.9357055	0.7014075
C	-0.8488227	0.1976736	-0.7049276
C	-0.8488227	0.1976736	0.7049276
H	-4.0895688	-0.6898832	1.2445749
H	-4.0895688	-0.6898832	-1.2445749
H	1.6301254	5.1838090	-1.2379097
H	1.6301254	5.1838090	1.2379097
C	0.4996577	0.5691281	-1.3081542
C	0.4996577	0.5691281	1.3081542
C	1.5049797	-0.3829872	-0.6873144
C	1.5049797	-0.3829872	0.6873144
C	2.8786050	-0.6809054	-1.1393575
C	2.8786050	-0.6809054	1.1393575
O	3.6136761	-1.0135338	0.0000000
O	3.3723364	-0.6524082	-2.2258427
O	3.3723364	-0.6524082	2.2258427
H	0.5019511	0.5680162	-2.3987298
H	0.5019511	0.5680162	2.3987298
C	0.8012805	-2.5319047	-1.4460138
C	0.8012805	-2.5319047	1.4460138
C	1.6484481	-3.3178268	-0.7116969
C	1.6484481	-3.3178268	0.7116969
H	0.9204879	-2.4540435	-2.5268593
H	0.9204879	-2.4540435	2.5268593
H	2.4772045	-3.8148864	-1.2168751
H	2.4772045	-3.8148864	1.2168751
H	1.1164241	3.0917463	-2.4954624
H	1.1164241	3.0917463	2.4954624
C	-2.0131987	-0.1257186	-1.3853867
C	-2.0131987	-0.1257186	1.3853867
Br	-2.0480086	-0.1696450	-3.2864964
Br	-2.0480086	-0.1696450	3.2864964
H	-0.1424408	-2.1818429	-1.0332102
H	-0.1424408	-2.1818429	1.0332102

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TS5d M05-2X/AVDZ’ Optimized Geometry

C	-4.0783892	-1.3352690	-0.6963953
C	-4.0783892	-1.3352690	0.6963953
C	0.5120648	3.3334800	0.6931448
C	0.5120648	3.3334800	-0.6931448
C	-2.9098432	-1.0344276	1.4046984
C	-2.9098432	-1.0344276	-1.4046984
C	0.2232850	2.1534704	1.3873163
C	0.2232850	2.1534704	-1.3873163
C	-0.0499724	0.9810875	0.7050922
C	-0.0499724	0.9810875	-0.7050922
C	-1.7500570	-0.7398533	0.7011263
C	-1.7500570	-0.7398533	-0.7011263
H	-4.9936995	-1.5656116	-1.2389253
H	-4.9936995	-1.5656116	1.2389253
H	0.7358272	4.2440135	1.2437320
H	0.7358272	4.2440135	-1.2437320
H	-2.9084501	-1.0285174	2.4942270
H	-2.9084501	-1.0285174	-2.4942270
C	-0.3985664	-0.3854699	1.3078998
C	-0.3985664	-0.3854699	-1.3078998
C	0.6111831	-1.3329600	0.6873732
C	0.6111831	-1.3329600	-0.6873732
C	1.9844296	-1.6350906	1.1397537
C	1.9844296	-1.6350906	-1.1397537
O	2.7180585	-1.9708173	0.0000000
O	2.4783886	-1.6075064	2.2257818
O	2.4783886	-1.6075064	-2.2257818
H	-0.3928518	-0.3829879	2.3985739
H	-0.3928518	-0.3829879	-2.3985739
C	-0.0926434	-3.4797338	1.4444030
C	-0.0926434	-3.4797338	-1.4444030
C	0.7519277	-4.2697441	0.7117666
C	0.7519277	-4.2697441	-0.7117666
H	0.0321903	-3.4027151	2.5248853
H	0.0321903	-3.4027151	-2.5248853
H	1.5782121	-4.7703881	1.2172691
H	1.5782121	-4.7703881	-1.2172691
Br	0.2136939	2.2042447	3.2879657
Br	0.2136939	2.2042447	-3.2879657
H	-1.0344439	-3.1231332	1.0332532
H	-1.0344439	-3.1231332	-1.0332532

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TS4e M05-2X/6-31+G(d) Optimized Geometry

C	0.8327282	3.4762568	-0.6933419
C	0.8327282	3.4762568	0.6933419
C	-4.3164701	-0.6259092	0.6948139
C	-4.3164701	-0.6259092	-0.6948139
C	-3.1221481	-0.4493874	1.4049657

C	-3.1221481	-0.4493874	-1.4049657
C	-1.9432830	-0.2804446	0.7010256
C	-1.9432830	-0.2804446	-0.7010256
C	-0.0460016	1.2261942	0.7029850
C	-0.0460016	1.2261942	-0.7029850
H	1.1715200	4.3445634	-1.2428035
H	1.1715200	4.3445634	1.2428035
H	-5.2440742	-0.7686383	1.2350215
H	-5.2440742	-0.7686383	-1.2350215
C	-0.5498698	-0.0773823	1.3082148
C	-0.5498698	-0.0773823	-1.3082148
C	0.2971072	-1.1717757	0.6864429
C	0.2971072	-1.1717757	-0.6864429
C	0.4525915	-2.5677629	1.1379599
C	0.4525915	-2.5677629	-1.1379599
O	0.7133931	-3.3308534	0.0000000
O	0.3725711	-3.0548638	2.2268110
O	0.3725711	-3.0548638	-2.2268110
H	-0.5479650	-0.0822561	2.3947204
H	-0.5479650	-0.0822561	-2.3947204
C	2.5054390	-0.6866992	1.4460922
C	2.5054390	-0.6866992	-1.4460922
C	3.2042460	-1.6057864	0.7115887
C	3.2042460	-1.6057864	-0.7115887
H	2.4114960	-0.7990888	2.5199869
H	2.4114960	-0.7990888	-2.5199869
H	3.6092321	-2.4776547	1.2137010
H	3.6092321	-2.4776547	-1.2137010
H	-3.1192076	-0.4526073	2.4887593
H	-3.1192076	-0.4526073	-2.4887593
C	0.3953878	2.3471278	1.3880455
C	0.3953878	2.3471278	-1.3880455
Cl	0.4336378	2.3650953	3.1284791
Cl	0.4336378	2.3650953	-3.1284791
H	2.2543591	0.2849338	1.0409771
H	2.2543591	0.2849338	-1.0409771

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TS5e M05-2X/6-31+G(d) Optimized Geometry

C	4.0823716	0.7295482	-0.6958963
C	4.0823716	0.7295482	0.6958963
C	-0.7510919	-3.6856579	0.6923915
C	-0.7510919	-3.6856579	-0.6923915
C	2.9003929	0.4886733	1.4033441
C	2.9003929	0.4886733	-1.4033441

C	-0.3991329	-2.5259631	1.3900577
C	-0.3991329	-2.5259631	-1.3900577
C	-0.0629132	-1.3740439	0.7033362
C	-0.0629132	-1.3740439	-0.7033362
C	1.7284025	0.2527181	0.7006722
C	1.7284025	0.2527181	-0.7006722
H	5.0028662	0.9128339	-1.2359663
H	5.0028662	0.9128339	1.2359663
H	-1.0231424	-4.5768877	1.2421767
H	-1.0231424	-4.5768877	-1.2421767
H	2.8984043	0.4845232	2.4874949
H	2.8984043	0.4845232	-2.4874949
C	0.3597198	-0.0292486	1.3081396
C	0.3597198	-0.0292486	-1.3081396
C	-0.5957426	0.9717495	0.6864365
C	-0.5957426	0.9717495	-0.6864365
C	-1.9497987	1.3468919	1.1384686
C	-1.9497987	1.3468919	-1.1384686
O	-2.6627314	1.7228847	0.0000000
O	-2.4428565	1.3481012	2.2274703
O	-2.4428565	1.3481012	-2.2274703
H	0.3534590	-0.0285021	2.3948036
H	0.3534590	-0.0285021	-2.3948036
C	0.2228099	3.0785679	1.4442661
C	0.2228099	3.0785679	-1.4442661
C	-0.5762021	3.9133493	0.7116187
C	-0.5762021	3.9133493	-0.7116187
H	0.0934725	3.0037939	2.5179579
H	0.0934725	3.0037939	-2.5179579
H	-1.3735617	4.4499449	1.2142053
H	-1.3735617	4.4499449	-1.2142053
Cl	-0.3926490	-2.5627888	3.1298084
Cl	-0.3926490	-2.5627888	-3.1298084
H	1.1419671	2.6752303	1.0399957
H	1.1419671	2.6752303	-1.0399957

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TS4f M05-2X/6-31+G(d) Optimized Geometry

C	-1.98812465	3.22733943	0.69545683
C	-1.98812465	3.22733943	-0.69545683
C	4.18308941	0.96286699	-0.69465214
C	4.18308941	0.96286699	0.69465214
C	2.99437393	0.74975417	-1.40451799
C	2.99437393	0.74975417	1.40451799

C	1.82252920	0.53481058	-0.70176483
C	1.82252920	0.53481058	0.70176483
C	-0.45226954	1.35470063	-0.70068693
C	-0.45226954	1.35470063	0.70068693
H	-2.57198754	3.94181494	1.26003966
H	-2.57198754	3.94181494	-1.26003966
H	5.10768664	1.12280249	-1.23513324
H	5.10768664	1.12280249	1.23513324
C	0.43673314	0.28339743	-1.31287214
C	0.43673314	0.28339743	1.31287214
C	-0.01189765	-1.02491320	-0.68677917
C	-0.01189765	-1.02491320	0.68677917
C	0.28825851	-2.39732521	-1.13789067
C	0.28825851	-2.39732521	1.13789067
O	0.28743672	-3.20369459	0.00000000
O	0.51914517	-2.83302394	-2.22706645
O	0.51914517	-2.83302394	2.22706645
H	0.43278523	0.28229131	-2.39991099
H	0.43278523	0.28229131	2.39991099
C	-2.26041075	-1.28420731	-1.44620072
C	-2.26041075	-1.28420731	1.44620072
C	-2.62464618	-2.37942396	-0.71172921
C	-2.62464618	-2.37942396	0.71172921
H	-2.13561421	-1.36103539	-2.52004042
H	-2.13561421	-1.36103539	2.52004042
H	-2.72683439	-3.33532821	-1.21383132
H	-2.72683439	-3.33532821	1.21383132
H	2.99311420	0.74541452	-2.48829899
H	2.99311420	0.74541452	2.48829899
C	-1.21864508	2.28709354	-1.37004760
C	-1.21864508	2.28709354	1.37004760
F	-1.22876663	2.28113282	-2.72242527
F	-1.22876663	2.28113282	2.72242527
H	-2.33408984	-0.28378856	-1.04054278
H	-2.33408984	-0.28378856	1.04054278

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TS5f M05-2X/6-31+G(d) Optimized Geometry

C	-4.06999674	0.25486542	-0.69577452
C	-4.06999674	0.25486542	0.69577452
C	1.03500741	-3.85433521	0.69430523
C	1.03500741	-3.85433521	-0.69430523
C	-2.87532747	0.08573825	1.40282820
C	-2.87532747	0.08573825	-1.40282820
C	0.60920569	-2.71527592	1.37188850
C	0.60920569	-2.71527592	-1.37188850
C	0.19928770	-1.58444013	0.70115968
C	0.19928770	-1.58444013	-0.70115968
C	-1.69070251	-0.07935561	0.70128769
C	-1.69070251	-0.07935561	-0.70128769
H	-4.99963692	0.38278361	-1.23617216
H	-4.99963692	0.38278361	1.23617216
H	1.36030663	-4.71758247	1.25913940
H	1.36030663	-4.71758247	-1.25913940
H	-2.87336933	0.08261891	2.48698525
H	-2.87336933	0.08261891	-2.48698525
C	-0.30721833	-0.27493103	1.31254526
C	-0.30721833	-0.27493103	-1.31254526
C	0.58003942	0.78693077	0.68699434
C	0.58003942	0.78693077	-0.68699434
C	1.90535259	1.25395225	1.13836972
C	1.90535259	1.25395225	-1.13836972
O	2.59120388	1.67698115	0.00000000
O	2.39716459	1.28961548	2.22732542
O	2.39716459	1.28961548	-2.22732542
H	-0.29881838	-0.27917309	2.39966168
H	-0.29881838	-0.27917309	-2.39966168
C	-0.37511685	2.83538998	1.44378842
C	-0.37511685	2.83538998	-1.44378842
C	0.36717262	3.72156486	0.71147904
C	0.36717262	3.72156486	-0.71147904
H	-0.24205671	2.77003134	2.51764612
H	-0.24205671	2.77003134	-2.51764612
H	1.12700628	4.30991546	1.21428685
H	1.12700628	4.30991546	-1.21428685
F	0.59736478	-2.72504389	2.72334749
F	0.59736478	-2.72504389	-2.72334749
H	-1.26571972	2.37287401	1.03910001
H	-1.26571972	2.37287401	-1.03910001

M06-2X optimized Cartesian Coordinates

Substituted Benzene Dimers

24
M06-2X/6-31+G(d) Benzene...benzene

C	0.98616698	0.98616698	-1.87500000
C	-0.36096217	1.34712915	-1.87500000
C	-1.34712915	0.36096217	-1.87500000
C	-0.98616698	-0.98616698	-1.87500000
C	0.36096217	-1.34712915	-1.87500000
C	1.34712915	-0.36096217	-1.87500000
H	1.75424527	1.75424527	-1.87500000
H	-0.64209833	2.39634360	-1.87500000
H	-2.39634360	0.64209833	-1.87500000
H	-1.75424527	-1.75424527	-1.87500000
H	0.64209833	-2.39634360	-1.87500000
H	2.39634360	-0.64209833	-1.87500000
C	0.98616698	0.98616698	1.87500000
C	-0.36096217	1.34712915	1.87500000
C	-1.34712915	0.36096217	1.87500000
C	-0.98616698	-0.98616698	1.87500000
C	0.36096217	-1.34712915	1.87500000
C	1.34712915	-0.36096217	1.87500000
H	1.75424527	1.75424527	1.87500000
H	-0.64209833	2.39634360	1.87500000
H	-2.39634360	0.64209833	1.87500000
H	-1.75424527	-1.75424527	1.87500000
H	0.64209833	-2.39634360	1.87500000
H	2.39634360	-0.64209833	1.87500000

27
M06-2X/6-31+G(d) Benzene...toluene

C	-2.02328231	1.26140127	0.00000000
C	-1.33860446	1.41922228	1.20396100
C	0.01928458	1.73366976	1.20062500
C	0.71672821	1.89824468	0.00000000
C	0.01928458	1.73366976	-1.20062500
C	-1.33860446	1.41922228	-1.20396100
H	-1.86127300	1.29405044	2.14823300
H	0.54786687	1.85181209	2.14425200
H	0.54786687	1.85181209	-2.14425200
H	-1.86127300	1.29405044	-2.14823300
H	-3.08070872	1.01328212	0.00000000
C	2.17848389	2.27217061	0.00000000
H	2.30158564	3.36143636	0.00000000
H	2.68778483	1.88176113	0.88597800
H	2.68778483	1.88176113	-0.88597800
C	1.56167329	-1.69506895	0.00000000
C	0.88358170	-1.85771995	1.20780300
C	-0.47259954	-2.18302147	1.20780300
C	-1.15069113	-2.34567246	0.00000000
C	-0.47259954	-2.18302147	-1.20780300
C	0.88358170	-1.85771995	-1.20780300
H	2.61793781	-1.44170720	0.00000000
H	1.41171493	-1.73103884	2.14850300
H	-1.00073277	-2.30970258	2.14850300
H	-2.20695565	-2.59903422	0.00000000
H	-1.00073277	-2.30970258	-2.14850300
H	1.41171493	-1.73103884	-2.14850300

25
M06-2X/6-31+G(d) Benzene...phenol

C	-1.99685297	-1.25561850	0.00618317
C	-1.31660291	-1.41952488	-1.19794502
C	0.03870802	-1.74668832	-1.20714487
C	0.71716038	-1.91076728	0.00056685
C	0.04500740	-1.74881753	1.21281175
C	-1.30684042	-1.42248667	1.20848689
H	-1.83884147	-1.29322151	-2.14198115
H	0.56692887	-1.87396126	-2.15000979
H	0.59601379	-1.88206067	2.13836950
H	-1.82630381	-1.29732847	2.15423601
H	-3.05182172	-1.00095479	0.00952947
O	2.04239170	-2.23068711	0.06083741
H	2.40193057	-2.31725326	-0.83329634
C	-1.12405238	2.33996754	0.00792311
C	-0.44881599	2.17727276	-1.20147318
C	0.90688979	1.85001250	-1.20466433
C	1.58736111	1.68544655	0.00153881
C	0.91212471	1.84814133	1.21093511
C	-0.44358106	2.17540159	1.21412626
H	-2.17994714	2.59485500	0.01040914
H	-0.97880377	2.30544560	-2.14092728
H	1.43279870	1.72329741	-2.14660546
H	2.64325586	1.43055909	-0.00094721
H	1.44211250	1.71996849	2.15038921
H	-0.96948997	2.30211668	2.15606738

28
M06-2X/6-31+G(d) Benzene...anisole

C	-2.41349322	-0.34883022	-0.30581264
C	-1.60730355	-0.81027680	-1.33941977
C	-0.42774568	-1.51214585	-1.07422721
C	-0.05760092	-1.75105344	0.25067281
C	-0.86492036	-1.28913613	1.29743429
C	-2.03243331	-0.59416432	1.01699654
H	-1.88935980	-0.62787370	-2.37241473
H	0.18274942	-1.86094702	-1.89910934
H	-0.55208069	-1.48955454	2.31727831
H	-2.65149618	-0.24020955	1.83625682
H	-3.32725471	0.19505000	-0.52237642
O	1.06645034	-2.42170098	0.62358196
C	1.91175931	-2.90648566	-0.39716818
H	1.38782887	-3.62742459	-1.03642518
H	2.29968438	-2.08621257	-1.01326214
H	2.73927813	-3.40368252	0.10830032
C	-0.55011687	2.78929134	-0.25514667
C	0.25119400	2.33090835	-1.30053511
C	1.42582216	1.63178407	-1.02390550
C	1.79913946	1.39104279	0.29811056
C	0.99782858	1.84942578	1.34349900
C	-0.17679957	2.54855006	1.06686939
H	-1.46497903	3.33380605	-0.47059825
H	-0.03956659	2.51841115	-2.33018984
H	2.04992459	1.27477166	-1.83810964
H	2.71400161	0.84652808	0.51356214
H	1.28858917	1.66192298	2.37315373
H	-0.80090201	2.90556247	1.88107353

24
M06-2X/6-31+G(d) Benzene...fluorobenzene

C	0.02349647	-1.75125368	-1.21686000
C	-1.32577359	-1.40087952	-1.20719300
C	-2.00201050	-1.22527646	0.00000000
C	-1.32577359	-1.40087952	1.20719300
C	0.02349647	-1.75125368	1.21686000
C	0.66699614	-1.91835563	0.00000000
H	0.57581138	-1.89467706	-2.13939200
H	-1.84837304	-1.26517255	-2.14912700
H	-3.05238475	-0.95251861	0.00000000
H	-1.84837304	-1.26517255	2.14912700
H	0.57581138	-1.89467706	2.13939200
F	1.97261397	-2.25739432	0.00000000
C	-1.07651429	2.35710794	0.00000000
C	-0.40157340	2.18184144	-1.20780300
C	0.94830644	1.83130893	-1.20780300
C	1.62324733	1.65604242	0.00000000
C	0.94830644	1.83130893	1.20780300
C	-0.40157340	2.18184144	1.20780300
H	-2.12787096	2.63012090	0.00000000
H	-0.92725270	2.31834817	-2.14850300
H	1.47398574	1.69480220	-2.14850300
H	2.67460400	1.38302946	0.00000000
H	1.47398574	1.69480220	2.14850300
H	-0.92725270	2.31834817	2.14850300

24
M06-2X/6-31+G(d) Benzene...chlorobenzene

C	-0.06048859	1.76314706	0.00000000
C	-0.63976502	1.40639398	1.21281600
C	-0.63976502	1.40639398	-1.21281600
C	-2.42085108	0.30949465	0.00000000
C	-1.82572184	0.67601083	-1.20516800
C	-1.82572184	0.67601083	1.20516800
Cl	1.42436669	2.67760976	0.00000000
H	-3.34269656	-0.25823294	0.00000000
H	-0.16773986	1.69709531	2.14214300
H	-0.16773986	1.69709531	-2.14214300
H	-2.28255238	0.39466726	-2.14585700
H	-2.28255238	0.39466726	2.14585700
C	1.86542304	-1.33742696	0.00000000
C	1.27203208	-1.70287260	-1.20705841
C	0.08525018	-2.43376388	-1.20705841
C	-0.50814077	-2.79920953	0.00000000
C	0.08525018	-2.43376388	1.20705841
C	1.27203208	-1.70287260	1.20705841
H	2.78753843	-0.76953314	0.00000000
H	1.73308978	-1.41892569	-2.14492842
H	-0.37580752	-2.71771079	-2.14492842
H	-1.43025617	-3.36710335	0.00000000
H	-0.37580752	-2.71771079	2.14492842
H	1.73308978	-1.41892569	2.14492842

24
M06-2X/AVDZ’ Benzene...bromobenzene

C	0.66318361	-1.19488651	0.00000000
C	1.12341543	-0.69951948	1.21544700
C	1.12341543	-0.69951948	-1.21544700

C	2.54748313	0.83326499	0.00000000
C	2.07218313	0.32167944	-1.20607500
C	2.07218313	0.32167944	1.20607500
Br	-0.63351850	-2.59058198	0.00000000
H	3.28794119	1.63025141	0.00000000
H	0.74560261	-1.10617544	2.14993300
H	0.74560261	-1.10617544	-2.14993300
H	2.43947312	0.71700923	-2.15106200
H	2.43947312	0.71700923	2.15106200
C	-2.02239861	1.27704317	0.00000000
C	-1.54805797	1.78759611	-1.20705841
C	-0.59937671	2.80870199	-1.20705841
C	-0.12503608	3.31925492	0.00000000
C	-0.59937671	2.80870199	1.20705841
C	-1.54805797	1.78759611	1.20705841
H	-2.75951264	0.48365607	0.00000000
H	-1.91661499	1.39090256	-2.14492842
H	-0.23081969	3.20539554	-2.14492842
H	0.61207795	4.11264203	0.00000000
H	-0.23081969	3.20539554	2.14492842
H	-1.91661499	1.39090256	2.14492842
H	1.74522590	1.34414754	2.14850300
H	-0.37793159	2.62748611	2.14850300
H	-1.43950949	3.26915488	0.00000000
H	-0.37793159	2.62748611	-2.14850300
H	1.74522590	1.34414754	-2.14850300

25

M06-2X/6-31+G(d) Benzene...cyanobenzene

C	-0.01521980	-1.85672514	0.00000000
C	-0.60908272	-1.49776581	-1.21559900
C	-0.60908272	-1.49776581	1.21559900
C	-2.39421709	-0.41874468	0.00000000
C	-1.79960534	-0.77815664	1.20950400
C	-1.79960534	-0.77815664	-1.20950400
C	1.21802652	-2.60215856	0.00000000
N	2.20872118	-3.20098209	0.00000000
H	-0.13557563	-1.78397628	-2.14911700
H	-0.13557563	-1.78397628	2.14911700
H	-3.32336883	0.14287934	0.00000000
H	-2.26349485	-0.49775950	2.14982200
H	-2.26349485	-0.49775950	-2.14982200
C	1.87720191	1.26437489	0.00000000
C	1.28042410	1.62509612	1.20780300
C	0.08687021	2.34653753	1.20780300
C	-0.50990760	2.70725876	0.00000000
C	0.08687021	2.34653753	-1.20780300
C	1.28042410	1.62509612	-1.20780300
H	2.80680380	0.70247877	0.00000000

Maleic Anhydride + Benzene

12
Benzene M06-2X/6-31+G(d) Optimized Geometry

C	0.98616659	0.98616659	0.00000000
C	-0.36096202	1.34712862	0.00000000
C	-1.34712862	0.36096202	0.00000000
C	-0.98616659	-0.98616659	0.00000000
C	0.36096202	-1.34712862	0.00000000
C	1.34712862	-0.36096202	0.00000000
H	1.75424475	1.75424475	0.00000000
H	-0.64209814	2.39634289	0.00000000
H	-2.39634289	0.64209814	0.00000000
H	-1.75424475	-1.75424475	0.00000000
H	0.64209814	-2.39634289	0.00000000
H	2.39634289	-0.64209814	0.00000000

9
maleic anhydride M06-2X/6-31+G(d) Optimized Geometry

C	-0.66552383	0.00000000	-1.25944978
C	0.66552383	0.00000000	-1.25944978
C	-1.12437511	0.00000000	0.16298082
H	-1.36369792	0.00000000	-2.08599078
H	1.36369792	0.00000000	-2.08599078
O	0.00000000	0.00000000	0.96639906
O	-2.23203096	0.00000000	0.60242764
C	1.12437511	0.00000000	0.16298082
O	2.23203096	0.00000000	0.60242764

21
Cycloadduct M06-2X/6-31+G(d) Optimized Geometry

C	-0.57301622	2.37041812	0.66687106
H	-1.00601598	3.14959539	-1.28571540
H	-1.00601598	3.14959539	1.28571540
C	-0.57301622	2.37041812	-0.66687106
C	1.44065214	0.93451385	0.66713208
H	2.31494854	0.76094789	1.28594246
C	0.06763189	1.13887550	1.28429128
H	2.31494854	0.76094789	-1.28594246
C	-0.80694891	-0.06070733	-0.76489251
C	-0.80694891	-0.06070733	0.76489251
C	1.44065214	0.93451385	-0.66713208
C	0.06763189	1.13887550	-1.28429128
C	-0.18915061	-1.39491427	-1.13908629
H	0.08358251	1.14892465	-2.37451175
H	0.08358251	1.14892465	2.37451175
H	-1.80711921	-0.00216101	1.20176239
C	-0.18915061	-1.39491427	1.13908629
H	-1.80711921	-0.00216101	-1.20176239
O	0.03428491	-1.82707667	-2.22832759
O	0.12584941	-2.10563220	0.00000000
O	0.03428491	-1.82707667	2.22832759

21
transition state M06-2X/6-31+G(d) Optimized Geometry

C	0.57772639	2.36072644	0.67867452
H	1.22164100	3.01030283	-1.26331744
H	1.22164100	3.01030283	1.26331744
C	0.57772639	2.36072644	-0.67867452
C	-1.41348357	0.91981975	0.67960467
H	-2.22370787	0.49224847	1.26170069
C	-0.19557265	1.33091117	1.32745304
H	-2.22370787	0.49224847	-1.26170069
C	1.01975682	-0.24657378	-0.70551386
C	1.01975682	-0.24657378	0.70551386
C	-1.41348357	0.91981975	-0.67960467
C	-0.19557265	1.33091117	-1.32745304
C	0.18783886	-1.40395117	-1.13102763
H	-0.14236190	1.24601504	-2.40997211
H	-0.14236190	1.24601504	2.40997211
H	1.86340200	0.02681446	1.32529493
C	0.18783886	-1.40395117	1.13102763
H	1.86340200	0.02681446	-1.32529493
O	-0.04037017	-1.82321332	-2.22716086
O	-0.37041735	-1.97567055	0.00000000
O	-0.04037017	-1.82321332	2.22716086

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