Supporting Information

Regioselectivity enhancement in synthesis of [70]fullerene derivatives by introduction of a branched structure

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General methods

^{1}H NMR and ^{13}C NMR spectra were recorded with a 600 MHz instrument in deuterated chloroform with tetramethylsilane as an internal reference. Mass spectra were obtained with matrix-assisted laser desorption ionization time-of-flight (MALDI–TOF) mass spectrometry using sinapinic acid as a matrix. High-performance liquid chromatography (HPLC) analysis was performed with a COSMOSIL Buckyprep-D column (4.6 mm I.D. × 250 mm) using toluene as an eluent at 1.0 mL/min flow rate, 320 nm detection, at 30 ºC. [6,6]-Phenyl-C_{61}-butylic acid methyl ester ([60]PCBM)[1], [6,6]-Phenyl-C_{71}-butylic acid methyl ester ([70]PCBM)[2] and methyl 4-benzoylvalerate[3] were synthesized in accordance with the methods described in the literatures. All the other solvents and materials are commercially available and were used as received.

Synthesis and characterization

Methyl 4-benzoylvalerate p-tosylhydrazone (**1b**). A mixture of 1.0 g (4.5 mmol) of methyl 4-benzoylvalerate and 1.5 g (9.1 mmol) of *p*-toluenesulfonyl hydrazide was dissolved in methanol (3.0 mL). 0.9 mL of conc. HCl was added to the solution and stirred for 18 h at 60 ºC. After cooling to room temperature, the crude product was extracted with ethyl acetate from $NaHCO_3$ aqueous solution. After silica column separation using ethyl acetate/hexane (1:3) as an eluent, recrystallization from methanol gave the white crystal of **1b** (0.5 g, 27%). ^{1}H NMR: *δH* (600 MHz; $CDCl_3$; Me_4Si) 7.76 (d, 2 H, *J* = 8.3 Hz, Ar), 7.43 (m, 3 H, Ar), 7.32 (d, 2 H, *J* = 8.3 Hz, Ar), 7.26 (s, 1 H, NH), 6.99 (dd, 2 H, *J* = 7.6, 1.4 Hz, Ar), 3.65, (s, 3 H, OCH_3), 2.61 (qt, 1 H, *J* = 6.9, 6.9 Hz, CH), 2.44 (s, 3 H, $ArCH_3$), 2.13 (m, 2 H, CH_2), 1.86 (dt, 1 H, *J* = 8.3, 14.5 Hz, CH_2), 1.62 (dt, 1 H, *J* = 6.9, 14.4 Hz, CH_2), 1.01 (d, 3 H, *J* = 6.9 Hz, CCH_3). ^{13}C NMR: *δC* (151 MHz; $CDCl_3$; Me_4Si) 173.71, 160.60, 144.02, 135.18, 131.92, 129.78, 129.58, 129.50, 127.88, 126.95, 51.50, 40.87, 31.37, 28.41, 21.56, 17.96. FT-IR (KBr): ν_{max}/cm^{-1} 3197, 2952, 1737, 1342, 1165, 671, 549. HRMS (MALDI-TOF, positive): *m/z* calcd for $C_{20}H_{25}N_2O_4S$ $[M+H]^+$ 389.1535; found 389.1531.

1-(3-(Methoxycarbonyl)-1-methylpropyl)-1-phenyl-[6,6]-[70]-methanofullerene ([70]PCMBM, **2b**). To a solution of **1b** (25 mg, 0.065 mmol) in 1.0 mL of 1,2-dichlorobenzene, 2.0 M THF solution of sodium *tert*-butoxide (0.036 mL, 0.071 mmol) was added under argon atmosphere and stirred for 30 min at room temperature. Then the mixture was added to a solution of C_{70} (50 mg, 0.059 mmol) in 6 mL of 1,2-dichlorobenzene, and stirred for 2 h at 90 ºC. The reaction mixture was irradiated with a 375 W incandescent lamp and stirred for 2 h. The mixture was concentrated and purified by silica gel column (Toluene) and recycle preparative gel permeation chromatography (chloroform). The obtained product was centrifuged with methanol to afford **2b** as a brown powder (33 mg, 54%). 99.26% purity in HPLC analysis. ^{1}H NMR (α-diastereomers): *δH* (600 MHz; $CDCl_3$; Me_4Si) 8.02, 7.99 (d, 1 H, *J* = 7.6 Hz, Ar), 7.73, 7.69 (1 H, Ar), 7.56 (1 H, Ar), 7.44 (2 H, Ar), 3.77, 3.61 (s, 3 H, OCH_3), 2.72, 2.65, 1.82, 1.73 (m, 2 H, CH_2), 2.56, 2.48, 2.31 (m, 2 H, CH_2), 2.48 (m, 1 H, CH), 1.51, 1.33 (d, 3 H, *J* = 6.9 Hz, CCH_3). ^{13}C NMR (α-diastereomers): *δC* (151 MHz; $CDCl_3$; Me_4Si) 173.70, 173.54, 156.07, 155.97, 155.18, 152.14, 152.10, 151.89, 151.46, 151.20, 151.13, 150.88, 150.83, 150.58, 150.52, 149.42, 149.39, 149.19, 149.14, 148.63, 148.55, 148.52, 148.46, 148.42, 148.33, 148.02, 147.93, 147.88, 147.56, 147.53, 147.41, 147.35, 147.04, 146.85, 146.29, 146.19, 146.10, 145.92, 145.81, 145.61, 144.79, 144.66, 144.51, 144.12, 144.05, 143.92, 143.84, 143.74, 143.61, 143.31, 143.21, 142.63, 142.46, 141.89, 141.84, 141.54, 141.50, 141.32, 140.97, 140.84, 140.27, 140.21, 139.26, 139.15, 139.08, 139.01, 137.83, 137.69, 134.02, 133.82, 133.72, 133.66, 133.35, 133.25, 132.95, 132.83, 130.91, 130.75, 130.66, 130.44, 128.27, 128.00, 127.88, 127.84, 127.72, 72.42, 71.67, 70.38, 69.55, 51.85, 51.70, 40.92, 40.85, 34.47, 34.45, 32.46, 32.30, 29.69, 28.87, 28.79, 16.55. FT-IR (KBr): ν_{max}/cm^{-1} 2924, 2852, 1737, 1428, 1256, 1076, 795. HRMS (MALDI-TOF, negative): *m/z* calcd for $C_{83}H_{16}O_2$ $[M]^-$ 1044.1150; found 1044.1193.

Computational details for density functional theory calculations

NMR calculations. ^{1}H NMR shielding tensors were calculated using the GIAO method on Q-Chem 4.0.1[4] with BP86/6–31G** on the optimized geometry at BP86/6–31G. The chemical shifts of protons were obtained by subtracting the shielding tensors from the tensor of tetramethylsilane calculated at the same theoretical level. The average values were applied to the chemically identical protons.

Calculations for reaction models. All ground state structures of models were optimized at the theoretical level of BP86/6–31G using Q-Chem or ORCA 3.0.3[5]. Frequency calculations were conducted on ORCA at BP86/6–31G* (instead of 6–31G** to minimize the calculation cost), and the Gibbs free enthalpies were obtained. The optimized structures that were located at the minimum on the potential surface were confirmed by the absence of imaginary frequencies. Transition state (TS) structures between reactants and products were obtained by using the climbing image nudged elastic band (CI–NEB) method implemented in the atomistic simulation environment (ASE[6]) using ORCA as a calculator with a PM3 semi-empirical method. The TS structures were further optimized at BP86/6–31G on ORCA and were confirmed by a single imaginary frequency at BP86/6–31G*. Unrestricted triplet calculations were performed for the photo-isomerization process in Fig. 5. ^{3}TS1s were obtained at UBP86/6–31G//UBP86/6–31G* and ^{3}TS2s at UBP86/6–31G* with a slow convergence strategy. The alpha spin density, single occupied molecular orbital (SOMO), and SOMO–1 of the triplet intermediate (^{3}IM-Pr), were calculated at BP86/6–31G* on Q-Chem. According to the reaction coordinates (minimum energy path), we confirmed reliability of the procedure in identifying TSs using the CI–NEB method as follows. The saddle point geometries of forward and reverse directions were generated using the imaginary vibrational mode at TSs. The geometries were optimized at BP86/6–31G and confirmed their connections to the corresponding reactants, intermediates and products, as shown in Fig. S1.

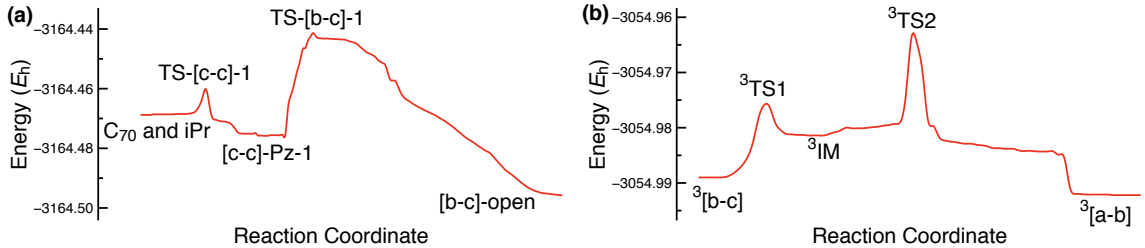
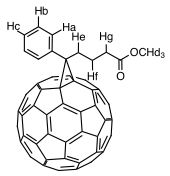


Fig. S1 Reaction coordinates for **(a)** the pathway from C_{70} and iPr to [b-c]-open PCiPr via [c-c]-Pz-PCiPr-1 intermediate, and **(b)** the pathway of the photo-isomerization process from the triplet ^{3}[b-c]-PCiPr to ^{3}[a-b]-PCiPr via the ^{3}IM-iPr biradical intermediate.

Calibration of level of theory for NMR calculations of [60]PCBM

^{1}H NMR chemical shifts of [60]PCBM were calculated at various conditions on the optimized geometries at BP86/6–31G, 6–31G* and 6–31G** (Table S1). The root mean square displacements (RMSD) from the experimental shifts were evaluated. BP86/6–31G//BP86/6–31G** calculations gave the best result (RMSD: 0.08 ppm).

Table S1 Calculated and experimental ^{1}H NMR chemical shifts (ppm) of [60]PCBM. The protons are labeled as depicted.

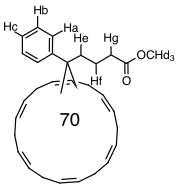
Proton label	Level of theory[a)]	Ha	Hb	Hc	Hd	He	Hf	Hg	RMSD[b)] (*)
	BP86/6–31G//HF/6–31G	8.62	8.04	7.98	4.11	2.59	2.55	2.65	0.45 (0.43)
	BP86/6–31G//B97–2/6–31G	8.01	7.49	7.42	3.88	2.79	2.47	2.64	0.15 (0.20)
	BP86/6–31G//B97–2/6–31G (PCM)	8.41	8.75	9.11	3.64	4.32	2.78	2.48	0.98 (0.04)
	BP86/6–31G//BP86/6–31G	7.87	7.40	7.35	3.85	2.94	2.55	2.69	0.18 (0.17)
	BP86/6–31G//B3LYP/6–31G	7.94	7.42	7.35	3.87	2.77	2.48	2.64	0.16 (0.19)
	BP86/6–31G//HCTH/6–31G	7.82	7.34	7.27	3.80	2.90	2.52	2.66	0.19 (0.12)
	BP86/6–31G//BOP/6–31G	7.76	7.30	7.25	3.82	2.86	2.51	2.64	0.20 (0.14)
	BP86/6–31G//PBEOP/6–31G	7.76	7.31	7.25	3.83	2.88	2.51	2.64	0.20 (0.15)
	BP86/6–31G//B97–2/6–31G**	8.09	7.57	7.49	3.64	2.68	2.31	2.36	0.13 (0.04)
	BP86/6–31G//BP86/6–31G**	8.00	7.52	7.46	3.66	2.86	2.38	2.46	0.08 (0.02)
	BP86/6–31G//BP86/6–311G**	8.11	7.76	7.75	3.83	3.02	2.32	2.49	0.17 (0.15)
	BP86/6–31G//BP86/DZ**	8.38	7.98	8.00	3.95	2.98	2.44	2.49	0.34 (0.27)
	BP86/6–31G//B3LYP/6–31G**	8.00	7.47	7.40	3.64	2.64	2.30	2.35	0.14 (0.04)
	BP86/6–31G*//BP86/6–31G**	8.05	7.55	7.49	3.61	2.94	2.38	2.42	0.10 (0.07)
	BP86/6–31G**//BP86/6–31G**	8.08	7.57	7.50	3.61	2.96	2.40	2.43	0.11 (0.07)
	BP86/6–31G*//BP86/6–31G*	7.85	7.37	7.32	3.52	2.91	2.41	2.41	0.15 (0.16)
	Experimental	7.93	7.55	7.48	3.68	2.91	2.19	2.53	-

[a)] Geometry optimization//NMR calculation. [b)] RMSD: root mean square displacement from experimental values. * RMSD for Hd protons. PCM: polarizable continuum method.

Validation of NMR calculation using experimental chemical shifts of [70]PCBM

^{1}H NMR calculations at the BP86/6–31G//BP86/6–31G** level of theory were validated by [70]PCBM isomers. The structures of α, β1, and β2 are shown in Scheme 1. The complete assignments of the chemical shifts to the isomers that are isolated by means of HPLC technique are reported in literature.[7] The validation results are summarized in Table S2 and Fig. S2.

Table S2 Calculated[a)] and experimental ^{1}H NMR chemical shifts (ppm) of [70]PCBM isomers. The protons are labeled as denoted.

Proton label	Isomers	Ha	Hb	Hc	Hd	He	Hf	Hg	RMSD[b)]
	α (calculated)	7.83	7.51	7.49	3.74	2.27	2.20	2.55	0.09
	α (experimental)	7.91	7.53	7.43	3.68	2.45	2.15	2.49	-
	β1 (calculated)	7.38	7.18	7.19	3.81	2.39	2.07	2.36	0.07
	β1 (experimental)	7.41	7.20	7.22	3.74	2.41	2.02	2.20	-
	β2 (calculated)	7.71	7.49	7.48	3.53	2.07	1.85	2.23	0.06
	β2 (experimental)	7.78	7.56	7.50	3.51	2.02	1.80	2.12	-

[a)] BP86/6–31G//BP86/6–31G**. [b)] RMSD: root mean square displacement from experimental values.

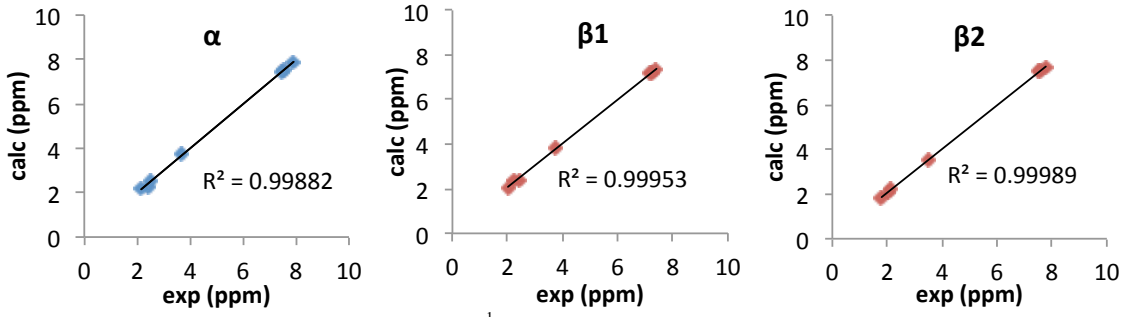


Fig. S2 Correlations of calculated and experimental ^{1}H NMR chemical shifts of α-, β1-, and β2-[70]PCBM (left to right).

Assignments of ^{1}H NMR chemical shifts to [70]PCMBM isomers

The experimental ^{1}H NMR chemical shifts of [70]PCMBM were assigned to two α-diastereomers by using the predicted values at BP86/6–31G//BP86/6–31G** (Table S3). The predicted chemical shifts of β1-, and β2-[70]PCMBM are also summarized. Experimental chemical shifts of the methyl ester protons of α- and β-[70]PCMBM isomers are assigned as shown in Fig. 1 (b) in the main text. The three-dimensional structures of the two α-diastereomers (α1 and α2) are described in Fig. S3.

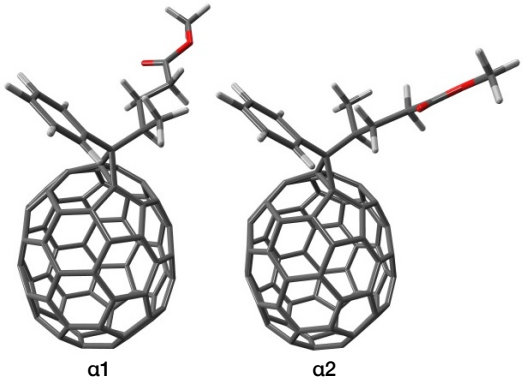
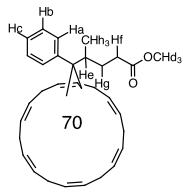


Fig. S3 Three-dimensional structures of α-[70]PCMBM diastereomers (α1 and α2).

Table S3 Calculated[a] and experimental ^{1}H NMR chemical shifts (ppm) of [70]PCMBM isomers. The protons are labeled as denoted. Apostrophes on the labels describe the protons that exhibit different shifts due to the stereo environment.

Proton label	Isomers	Ha	Ha'	Hb	Hb'	Hc	Hd	He	Hf	Hf'	Hg	Hg'	Hh	RMSD[b]
	α1 (calc.)	7.85	7.59	7.48	7.36	7.43	3.70	2.19	2.44	2.12	2.70	1.56	1.11	0.15
	α1 (exp.)	8.02	7.69	7.56	7.44	7.44	3.77	2.48	2.56	2.31	2.72	1.73	1.33	-
	α2 (calc.)	7.85	7.81	7.48	7.46	7.45	3.64	2.28	2.16	2.53	2.52	1.77	1.22	0.15
	α2 (exp.)	7.99	7.73	7.56	7.44	7.44	3.61	2.48	2.48	2.57	2.65	1.82	1.51	-
	β1 (calc.)	7.37	7.47	7.20	7.17	7.21	3.68	2.44	2.51	2.31	1.67	2.50	1.19	-
	β2 (calc.)	7.82	7.67	7.43	7.47	7.44	3.55	2.05	1.83	2.26	2.45	1.45	0.92	-

[a] BP86/6–31G//BP86/6–31G**. [b] RMSD: root mean square displacement from experimental values.

References

1 J. C. Hummelen, B. Knight, F. LePeq and F. Wudl, *J. Org. Chem.*, 1995, **60**, 532–538.

2 M. M. Wienk, J. M. Kroon, W. J. H. Verhees, J. Knol, J. C. Hummelen, P. A. van Hal and R. A. J. Janssen, *Angew. Chem. Int. Ed. Engl.*, 2003, **42**, 3371–3375.

3 S. P. France, S. Hussain, A. M. Hill, L. J. Hepworth, R. M. Howard, K. R. Mulholland, S. L. Flitsch and N. J. Turner, *ACS Catal.*, 2016, **6**, 3753–3759.

4 Y. Shao, Z. Gan, E. Epifanovsky, A. T. B. Gilbert, M. Wormit, J. Kussmann, A. W. Lange, A. Behn, J. Deng, X. Feng, D. Ghosh, M. Goldey, P. R. Horn, L. D. Jacobson, I. Kaliman, R. Z. Khaliullin, T. Kuś, A. Landau, J. Liu, E. I. Proynov, Y. M. Rhee, R. M. Richard, M. A. Rohrdanz, R. P. Steele, E. J. Sundstrom, H. L. Woodcock III, P. M. Zimmerman, D. Zuev, B. Albrecht, E. Alguire, B. Austin, G. J. O. Beran, Y. A. Bernard, E. Berquist, K. Brandhorst, K. B. Bravaya, S. T. Brown, D. Casanova, C.-M. Chang, Y. Chen, S. H. Chien, K. D. Closser, D. L. Crittenden, M. Diedenhofen, R. A. DiStasio Jr, H. Do, A. D. Dutoi, R. G. Edgar, S. Fatehi, L. Fusti-Molnar, A. Ghysels, A. Golubeva-Zadorozhnaya, J. Gomes, M. W. D. Hanson-Heine, P. H. P. Harbach, A. W. Hauser, E. G. Hohenstein, Z. C. Holden, T.-C. Jagau, H. Ji, B. Kaduk, K. Khistyaev, J. Kim, J. Kim, R. A. King, P. Klunzinger, D. Kosenkov, T. Kowalczyk, C. M. Krauter, K. U. Lao, A. D. Laurent, K. V. Lawler, S. V. Levchenko, C. Y. Lin, F. Liu, E. Livshits, R. C. Lochan, A. Luenser, P. Manohar, S. F. Manzer, S.-P. Mao, N. Mardirossian, A. V. Marenich, S. A. Maurer, N. J. Mayhall, E. Neuscamman, C. M. Oana, R. Olivares-Amaya, D. P. O'Neill, J. A. Parkhill, T. M. Perrine, R. Peverati, A. Prociuk, D. R. Rehn, E. Rosta, N. J. Russ, S. M. Sharada, S. Sharma, D. W. Small, A. Sodt, T. Stein, D. Stück, Y.-C. Su, A. J. W. Thom, T. Tsuchimochi, V. Vanovschi, L. Vogt, O. Vydrov, T. Wang, M. A. Watson, J. Wenzel, A. White, C. F. Williams, J. Yang, S. Yeganeh, S. R. Yost, Z.-Q. You, I. Y. Zhang, X. Zhang, Y. Zhao, B. R. Brooks, G. K. L. Chan, D. M. Chipman, C. J. Cramer, W. A. Goddard III, M. S. Gordon, W. J. Hehre, A. Klamt, H. F. Schaefer III, M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Warshel, X. Xu, A. Aspuru-Guzik, R. Baer, A. T. Bell, N. A. Besley, J.-D. Chai, A. Dreuw, B. D. Dunietz, T. R. Furlani, S. R. Gwaltney, C.-P. Hsu, Y. Jung, J. Kong, D. S. Lambrecht, W. Liang, C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik, T. Van Voorhis, J. M. Herbert, A. I. Krylov, P. M. W. Gill and M. Head-Gordon, *Mol. Phys.*, 2014, **113**, 184–215.

5 F. Neese, *WIREs Comput Mol Sci*, 2011, **2**, 73–78.

6 A. H. Larsen, J. J. Mortensen, J. Blomqvist, I. E. Castelli, R. Christensen, M. Dułak, J. Friis, M. N. Groves, B. Hammer, C. Hargus, E. D. Hermes, P. C. Jennings, P. B. Jensen, J. Kermode, J. R. Kitchin, E. L. Kolsbjerg, J. Kubal, K. Kaasbjerg, S. Lysgaard, J. B. Maronsson, T. Maxson, T. Olsen, L. Pastewka, A. Peterson, C. Rostgaard, J. Schiøtz, O. Schütt, M. Strange, K. S. Thygesen, T. Vegge, L. Vilhelmsen, M. Walter, Z. Zeng and K. W. Jacobsen, *J. Phys.: Condens. Matter*, 2017, **29**, 273002.

7 T. Umeyama, T. Miyata, A. C. Jakowetz, S. Shibata, K. Kurotobi, T. Higashino, T. Koganezawa, M. Tsujimoto, S. Gélinas, W. Matsuda, S. Seki, R. H. Friend and H. Imahori, *Chem. Sci.*, 2017, **8**, 181–188.

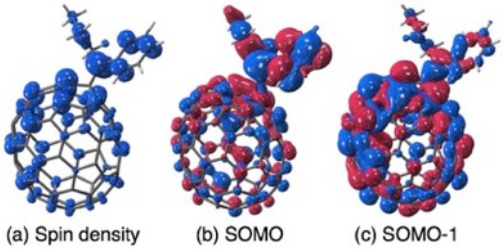


Fig. S4 Biradical nature of triplet intermediate (^{3}IM-Pr) on the pathway from ^{3}[b-c]-PCPr to ^{3}[a-b]-PCPr. **(a)** Alpha spin density map calculated at BP86/6–31G*. **(b)**, **(c)** SOMO and SOMO-1 orbitals.

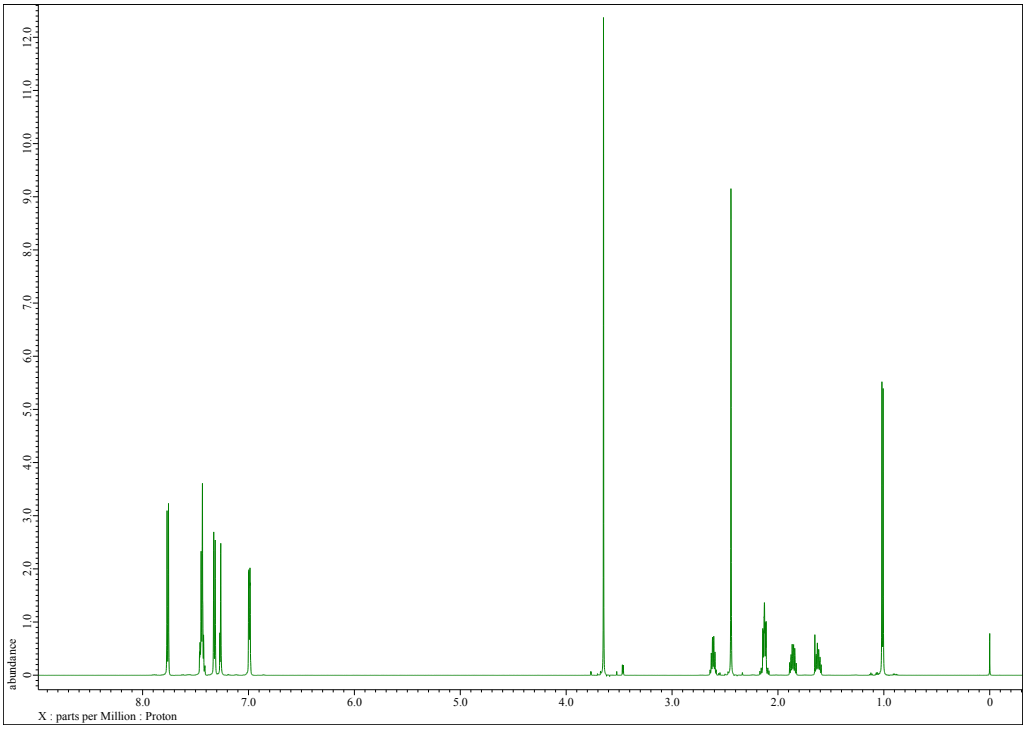


Fig. S5 ^{1}H NMR spectrum of **1b** (600 MHz, $CDCl_3$).

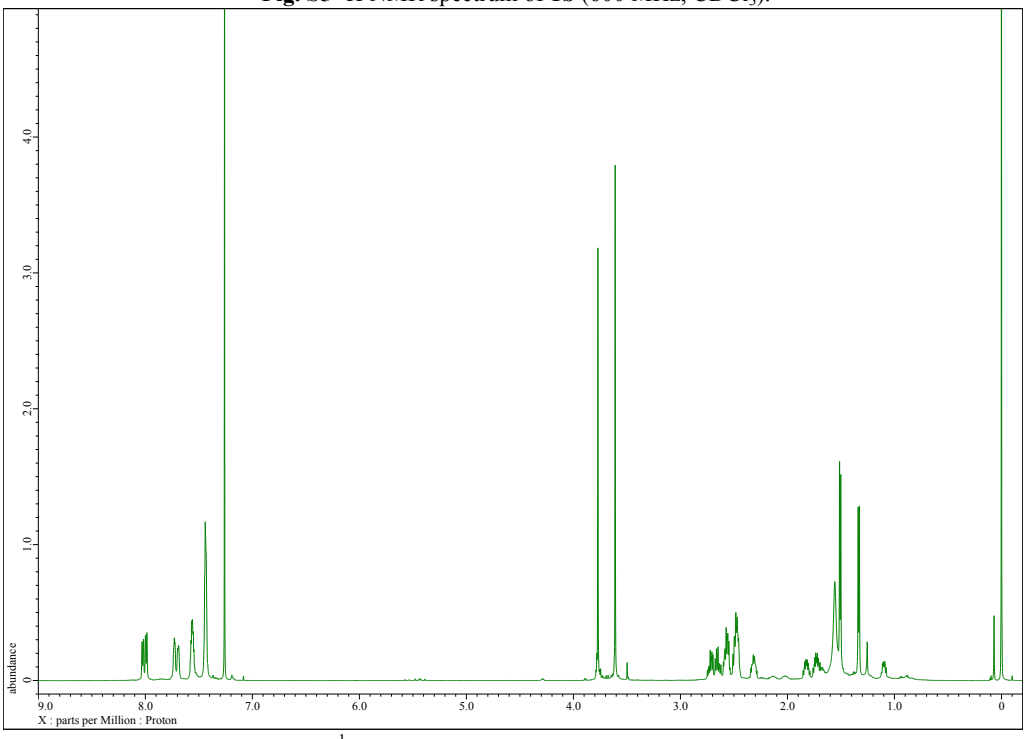


Fig. S6 ^{1}H NMR spectrum of **2b** (600 MHz, $CDCl_3$).

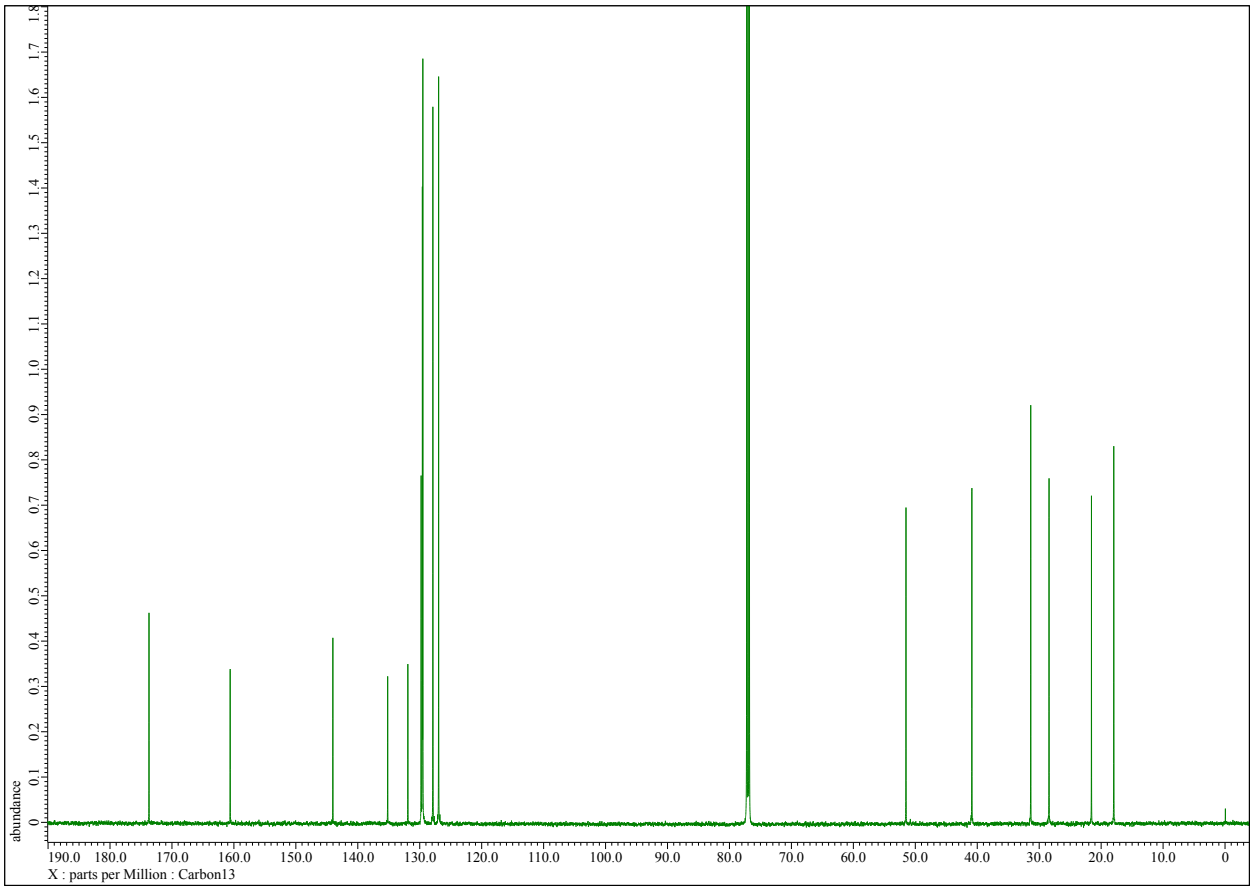


Fig. S7 ^{13}C NMR spectrum of **1b** (151 MHz, $CDCl_3$).

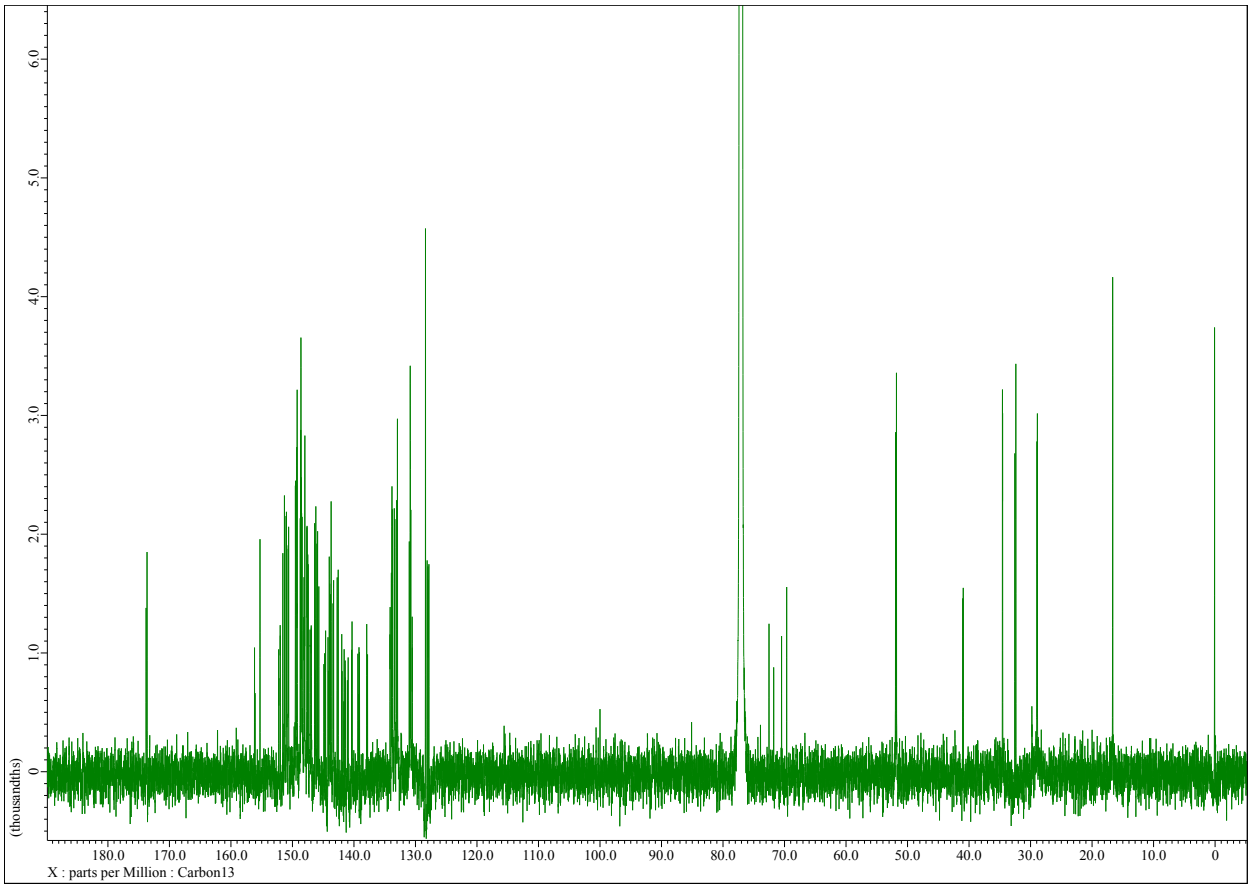


Fig. S8 ^{13}C NMR spectrum of **2b** (151 MHz, $CDCl_3$).

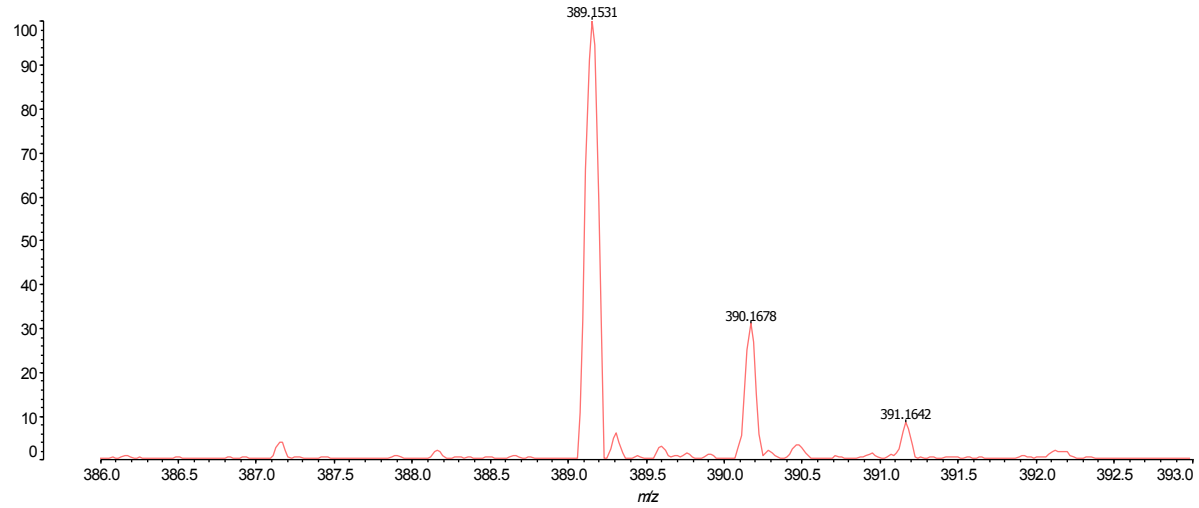


Fig. S9 MALDI–TOF–HRMS spectrum of **1b** (positive, matrix: Sinapinic Acid (SA)).

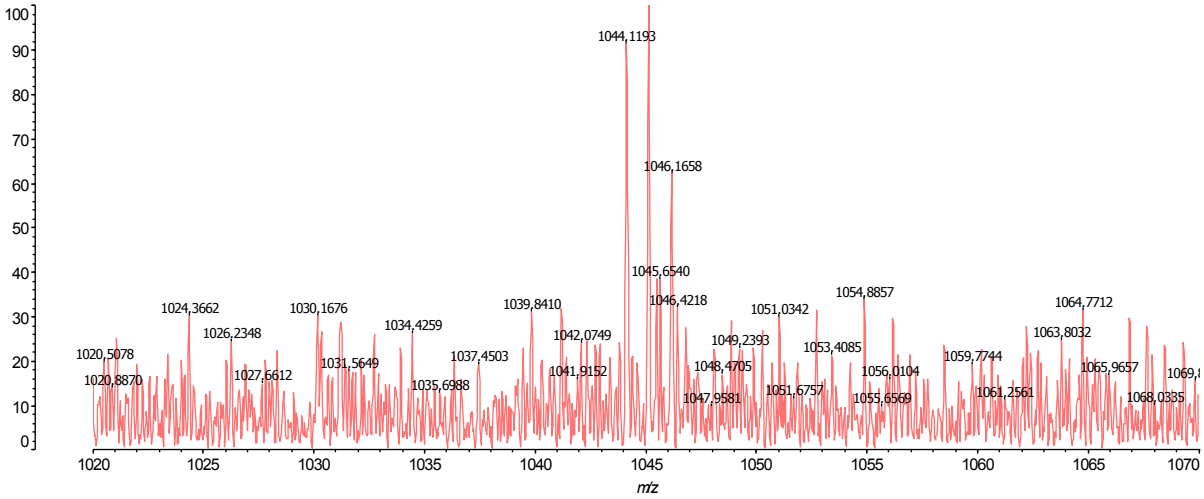
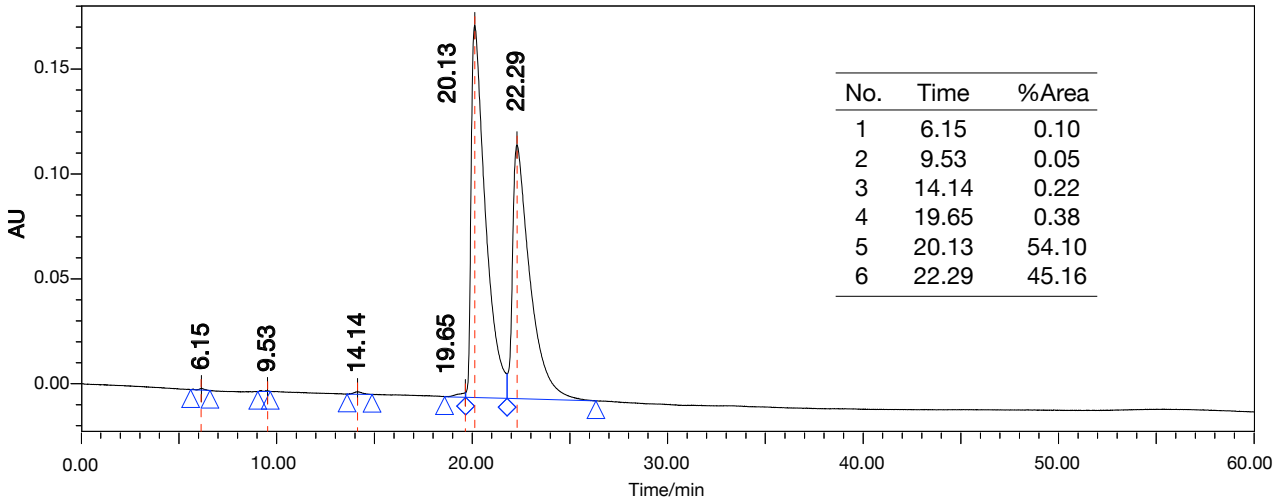


Fig. S10 MALDI–TOF–HRMS spectrum of **2b** (negative, without matrix).



No.	Time	%Area
1	6.15	0.10
2	9.53	0.05
3	14.14	0.22
4	19.65	0.38
5	20.13	54.10
6	22.29	45.16

Fig. S11 HPLC chromatogram of **2b** (Buckyprep-D column (4.6 mm I.D. × 250 mm), 30 ºC, Toluene 1.0 mL/min, UV 320 nm).

Table S4 Computational data: Cartesian coordinates optimized at BP86/6–31G, Gibbs free enthalpies and number of imaginary frequencies calculated at BP86/6–31G*.

Rows: Name / Gibbs free enthalpy (Eh) / Number of imaginary frequency (cm^{-1}) / Cartesian coordinates (Angstrom) (Atom, x, y, z)

[60]PCBM -2901.882866 0	α-[70]PCBM -3282.967722 0	β1-[70]PCBM -3282.96231 0	β2-[70]PCBM -3282.963047 0	α1-[70]PCMBM -3322.250464 0
C -3.752000 2.719000 -0.238000	C 0.428940 1.990050 -2.273140	C -2.545840 0.768110 -2.317120	C -1.870320 -1.206130 3.209180	C 0.269430 1.920620 -2.276220
C -2.888000 2.874000 -1.413000	C -0.200730 0.773740 -2.885420	C -2.283210 -0.431790 -3.111070	C -1.026050 -2.400090 3.181890	C -0.306780 0.663330 -2.855710
C -3.308000 1.891000 -2.417000	C -1.602830 0.756080 -2.352370	C -2.457560 -1.596310 -2.242840	C 0.370680 -1.968290 3.211250	C -1.695030 0.582250 -2.290530
C -4.421000 1.122000 -1.859000	C -1.866770 2.037500 -1.713900	C -2.837450 -1.125200 -0.910270	C 0.401000 -0.506120 3.265660	C -2.012290 1.858890 -1.665530
C -4.696000 1.634000 -0.511000	C -0.621160 2.795310 -1.666840	C -2.895360 0.356840 -0.957090	C -1.003260 -0.027660 3.267000	C -0.806870 2.680700 -1.658370
C -4.139000 -2.418000 -1.227000	C 1.704720 1.984940 -1.692110	C -1.771810 1.928460 -2.537530	C -3.062090 -1.183140 2.452580	C 1.556270 1.991390 -1.726230
C -4.907000 -1.182000 -1.053000	C 1.981790 2.828320 -0.532570	C -1.291240 2.695580 -1.403780	C -3.409340 0.005860 1.698120	C 1.815620 2.866570 -0.586540
C -4.529000 -0.258000 -2.125000	C 0.979740 3.646790 0.014950	C -1.607870 2.273530 -0.103340	C -2.554600 1.118760 1.735400	C 0.784850 3.641290 -0.028100
C -3.527000 -0.922000 -2.964000	C -0.350280 3.634730 -0.563560	C -2.461170 1.123450 0.132610	C -1.362420 1.128990 2.562550	C -0.555610 3.550970 -0.574690
C -3.287000 -2.259000 -2.408000	C -1.304940 3.730690 0.537410	C -2.062660 0.538850 1.453290	C -0.375280 2.044960 1.908810	C -1.488840 3.613470 0.547580
C -0.959000 3.337000 0.094000	C -2.502100 3.002050 0.492430	C -1.999050 -1.090880 1.503570	C 1.171000 1.522560 1.910760	C -2.646120 2.822380 0.542240
C 0.396000 2.786000 0.097000	C -2.794220 2.147180 -0.655290	C -2.349350 -1.787170 0.225120	C 1.390600 0.191000 2.559660	C -2.918190 1.935050 -0.585230
C 0.673000 2.267000 -1.267000	C -3.448310 0.955230 -0.150040	C -1.413450 -2.885020 0.062000	C 2.329980 -0.543210 1.735220	C -3.497880 0.719660 -0.046850
C -0.517000 2.510000 -2.082000	C -3.152240 -0.292470 -0.723480	C -1.063080 -3.362090 -1.210330	C 2.332220 -1.946360 1.701520	C -3.151920 -0.520290 -0.608700
C -1.522000 3.171000 -1.248000	C -2.214600 -0.395960 -1.837460	C -1.596320 -2.705590 -2.389180	C 1.331360 -2.676710 2.455570	C -2.235150 -0.592150 -1.743590
C -1.484000 -3.521000 -1.239000	C -1.457140 -1.647010 -1.638820	C -0.528550 -2.688360 -3.387200	C 0.934030 -3.822050 1.638260	C -1.409620 -1.799630 -1.545010
C -1.986000 -2.800000 -2.414000	C -0.099270 -1.726680 -1.958010	C -0.364180 -1.570900 -4.216630	C -0.406920 -4.229880 1.611790	C -0.057410 -1.814330 -1.897940
C -0.875000 -2.026000 -2.975000	C 0.646290 -0.635100 -2.651490	C -1.260580 -0.424560 -4.084290	C -1.404350 -3.515090 2.404420	C 0.614030 -0.694280 -2.624990
C 0.306000 -2.270000 -2.142000	C 2.456600 0.730790 -1.495970	C -0.702930 1.928160 -3.535660	C -3.444510 -2.333580 1.635120	C 2.376180 0.780460 -1.528830
C -0.066000 -3.191000 -1.077000	C 1.919040 -0.498670 -1.882750	C -0.452040 0.774170 -4.290420	C -2.631490 -3.475700 1.611230	C 1.894400 -0.481080 -1.884080
C -2.306000 -3.673000 -0.105000	C 0.853590 3.771530 1.465040	C -0.597250 2.338610 0.943800	C -2.291730 1.870290 0.515340	C 0.685160 3.782110 1.422830
C -1.740000 -3.501000 1.237000	C 1.794270 3.159600 2.352680	C 0.696660 2.909350 0.699690	C -2.956910 1.551830 -0.715070	C 1.676290 3.233050 2.296540
C -2.750000 -2.846000 2.074000	C 2.859980 2.307190 1.775630	C 1.033640 3.345720 -0.672400	C -3.851360 0.375410 -0.757240	C 2.771840 2.428900 1.707550
C -3.933000 -2.602000 1.249000	C 2.899490 2.125760 0.353980	C 0.051670 3.184980 -1.701480	C -4.019420 -0.398610 0.435360	C 2.787520 2.226280 0.288690
C -3.658000 -3.113000 -0.099000	C -2.995410 2.344390 1.697150	C -0.686060 -1.659940 1.929630	C 1.806360 1.423390 0.560220	C -3.077510 2.159490 1.767910
C -3.216000 2.878000 1.054000	C -2.330900 2.494950 2.958160	C 0.375590 -0.899940 2.511140	C 1.252450 1.970120 -0.638580	C -2.392980 2.364580 3.010570
C -3.603000 1.953000 2.124000	C -1.065220 3.265120 3.006010	C 0.319950 0.590260 2.463220	C -0.162830 2.447730 -0.639860	C -1.168540 3.199930 3.016020
C -2.421000 1.704000 2.953000	C -0.559350 3.826600 1.787900	C -0.794350 1.229310 1.836850	C -0.936400 2.350280 0.558270	C -0.721160 3.768540 1.778530
C -1.309000 2.475000 2.390000	C -2.999710 -1.458990 0.135210	C 0.313290 -3.767170 -1.479590	C 2.571400 -2.638850 0.440050	C -2.919150 -1.663580 0.262850
C -1.796000 3.198000 1.223000	C -3.221830 -1.388280 1.550570	C 1.301610 -3.789620 -0.444430	C 2.912190 -1.923580 -0.752170	C -3.111640 -1.581900 1.682300
C -2.345000 1.256000 -3.224000	C -3.516280 -0.068910 2.155530	C 0.929500 -3.292870 0.898300	C 2.921430 -0.444800 -0.711350	C -3.460730 -0.270090 2.274280
C -0.924000 1.575000 -3.058000	C -3.579250 1.076690 1.300120	C -0.403570 -2.805950 1.109160	C 2.584230 0.213640 0.517790	C -3.602880 0.857010 1.403790
C -0.165000 0.344000 -3.232000	C 0.803350 -2.385080 -1.032180	C 0.978400 -1.080590 -4.515010	C -1.017640 -4.634100 0.349120	C 0.898940 -2.410550 -0.982640
C -1.106000 -0.745000 -3.509000	C 0.337770 -3.116020 0.107920	C 2.147710 -1.765630 -4.049320	C -0.256730 -4.706800 -0.862390	C 0.499040 -3.146120 0.179760
C -2.458000 -0.180000 -3.503000	C -1.100610 -3.069130 0.423130	C 1.974670 -2.947330 -3.172840	C 1.159360 -4.274150 -0.836740	C -0.931850 -3.167360 0.529070
C -5.068000 0.744000 0.517000	C -1.952260 -2.289610 -0.424430	C 0.643740 -3.354590 -2.827970	C 1.709600 -3.802950 0.400810	C -1.842720 -2.447360 -0.309810
C -5.172000 -0.692000 0.241000	C 3.187120 0.833200 -0.235830	C 0.415590 2.714120 -3.021930	C -4.045430 -1.846420 0.396680	C 3.128320 0.940960 -0.288320
C -4.677000 -1.416000 1.415000	C 3.443890 -0.309550 0.590010	C 1.774520 2.386280 -3.343050	C -3.896760 -2.557290 -0.840350	C 3.463800 -0.173760 0.546940
C -4.269000 -0.430000 2.418000	C 2.841760 -1.595940 0.200540	C 2.037470 1.167590 -4.143220	C -3.037960 -3.762790 -0.864510	C 2.920560 -1.495310 0.190490
C -4.510000 0.907000 1.862000	C 2.040540 -1.633670 -0.986770	C 0.924010 0.368290 -4.561050	C -2.391730 -4.168980 0.348660	C 2.094810 -1.593810 -0.976260
C -2.356000 -1.900000 3.041000	C 3.383790 1.236010 2.567650	C 2.402460 3.294070 -1.087280	C -3.997410 -0.327870 -1.995580	C 3.370400 1.398850 2.502010
C -0.938000 -1.569000 3.203000	C 2.946940 1.018900 3.942840	C 3.463690 2.917190 -0.159480	C -3.360770 0.150290 -3.218780	C 2.977490 1.181870 3.890460
C -0.838000 -0.141000 3.476000	C 1.932460 1.819760 4.486550	C 3.139910 2.511620 1.144150	C -2.521200 1.273980 -3.177100	C 1.934540 1.937020 4.445720
C -2.191000 0.423000 3.488000	C 1.322610 2.868680 3.673860	C 1.741300 2.469310 1.562640	C -2.285590 1.953720 -1.905950	C 1.251170 2.938730 3.632340
C -3.131000 -0.667000 3.217000	C -0.090930 2.919900 3.996580	C 1.559080 1.312760 2.421310	C -0.898580 2.379240 -1.869320	C -0.154900 2.921460 3.987740
C 2.131000 0.382000 -0.344000	C -0.355940 1.898170 5.006700	C 2.849950 0.641670 2.535200	C -0.276510 1.964470 -3.121980	C -0.342250 1.904960 5.020150
C 1.820000 -1.073000 -0.556000	C -1.553840 1.170570 4.962400	C 2.902800 -0.757800 2.580730	C 1.049610 1.513380 -3.120080	C -1.500760 1.115020 5.014990
C 1.209000 -1.223000 -1.871000	C -2.527310 1.439890 3.906080	C 1.665570 -1.529050 2.512800	C 1.794240 1.464960 -1.866560	C -2.511450 1.315980 3.978190
C 0.968000 0.110000 -2.425000	C -3.113350 0.173400 3.509350	C 1.936030 -2.720780 1.728560	C 2.633690 0.281630 -1.902240	C -3.040060 0.014630 3.614590
C 1.422000 1.099000 -1.458000	C -2.507670 -0.876980 4.322440	C 3.334140 -2.684970 1.310010	C 2.406810 -0.401210 -3.172650	C -2.361460 -0.989500 4.428770
C 0.230000 0.596000 2.927000	C -2.233790 -2.128310 3.751640	C 3.690760 -3.147450 0.034220	C 2.389030 -1.803350 -3.214780	C -2.036080 -2.234640 3.870810
C 1.265000 -0.051000 2.133000	C -2.552730 -2.372130 2.347990	C 2.663730 -3.662290 -0.865540	C 2.598890 -2.569080 -1.990670	C -2.374340 -2.516940 2.478420
C 1.820000 0.954000 1.168000	C -1.503900 -3.203150 1.790610	C 2.997340 -3.246390 -2.215570	C 1.731750 -3.732050 -2.032230	C -1.295760 -3.299640 1.907820
C 0.875000 2.119000 1.231000	C -0.534000 -3.475710 2.846240	C 4.231300 -2.470380 -2.149890	C 0.981900 -3.683660 -3.282950	C -0.288970 -3.504220 2.943800
C -0.009000 1.929000 2.373000	C 0.836030 -3.527270 2.542020	C 4.397520 -1.354010 -2.982470	C -0.357510 -4.099690 -3.309660	C 1.074050 -3.490560 2.607650
C 0.480000 -3.015000 0.213000	C 1.276690 -3.301300 1.171090	C 3.332210 -0.973300 -3.904410	C -0.993720 -4.570780 -2.083500	C 1.471070 -3.264620 1.223100
C 1.432000 -1.936000 0.479000	C 2.517400 -2.548500 1.217410	C 3.278070 0.476210 -3.951110	C -2.368180 -4.104280 -2.084820	C 2.670210 -2.446630 1.228900
C 1.152000 -1.418000 1.843000	C 2.845750 -2.306520 2.616870	C 4.309580 0.993020 -3.057490	C -2.583190 -3.343590 -3.311550	C 3.017880 -2.165450 2.616100
C 0.035000 -2.188000 2.389000	C 3.413660 -1.078490 2.993090	C 4.057700 2.143900 -2.296820	C -3.392500 -2.197750 -3.286670	C 3.529790 -0.903990 2.960740
C -0.378000 -3.174000 1.389000	C 3.674380 -0.058030 1.981860	C 2.769590 2.819820 -2.408970	C -4.019350 -1.778920 -2.037070	C 3.714280 0.112000 1.928700
C 3.229000 0.959000 0.557000	C 0.912400 -0.164050 5.589810	C 4.839690 0.700190 1.038190	C -0.918420 0.173380 -4.728580	C 1.044880 -0.078970 5.602820
C 3.823000 2.304000 0.185000	C 1.972520 -1.000650 5.022260	C 5.180280 1.123830 -0.321930	C -1.795200 -0.998690 -4.772680	C 2.134150 -0.868080 5.021890
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C 4.290000 2.561000 -1.124000	C -0.337720 -0.923620 5.541890	C 4.894700 -0.762500 1.084520	C 0.468800 -0.297680 -4.728190	C -0.164390 -0.902860 5.595650
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C 4.621000 4.514000 0.874000	C -0.052080 -2.229630 4.944850	C 5.268430 -1.244230 -0.246590	C 0.449650 -1.761730 -4.773410	C 0.175780 -2.201450 5.011440
C 5.082000 4.764000 -0.433000	C -1.546890 -0.264060 5.236280	C 3.945570 -1.473840 1.846920	C -0.949810 -2.195420 -4.799880	C -1.413490 -0.312590 5.309810
H 4.159000 1.806000 -1.905000	C 1.377040 -2.279900 4.625850	C 5.443720 -0.079080 -1.117220	C 1.395000 -2.497470 -4.029730	C 1.597120 -2.182330 4.658230
H 5.270000 3.971000 -2.449000	C -0.987010 -2.820920 4.070960	C 4.677150 -2.417410 -0.758770	C -1.340930 -3.343920 -4.082400	C -0.746810 -2.854770 4.169290
H 3.632000 3.105000 2.197000	C 1.810190 -2.919650 3.447800	C 5.015930 -0.137800 -2.459080	C 0.749240 2.815740 2.618940	C 2.036050 -2.818430 3.480510
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H 5.565000 5.716000 -0.673000	C 1.521130 0.495440 -4.829910	C -4.455940 -0.363670 2.062910	H 0.948570 4.193130 0.929370	C 1.400940 0.470930 -4.812040
C 4.251000 -0.028000 1.159000	C 1.505290 1.815700 -5.332950	H -4.594220 -0.582350 0.990510	H 0.571640 4.953040 2.491260	C 1.272520 1.761790 -5.374770
C 5.313000 -0.512000 0.151000	H 0.666940 2.476020 -5.089850	H -4.872290 -1.222120 2.627300	C 2.682630 4.472940 2.206880	H 0.368650 2.349940 -5.187790
C 6.323000 -1.466000 0.814000	C 2.563110 2.288390 -6.132330	C -5.236820 0.921290 2.417120	H 3.282600 3.736470 1.639810	C 2.301130 2.301870 -6.169320
C 7.334000 -2.025000 -0.168000	H 2.539710 3.314940 -6.511270	H -5.072310 1.181170 3.478980	H 2.946550 4.364070 3.275270	H 2.185270 3.303160 -6.595580
O 7.318000 -1.891000 -1.407000	C 3.648940 1.446650 -6.437820	H -4.852800 1.759510 1.805670	C 3.063610 5.895670 1.752700	C 3.473990 1.561660 -6.410230
O 8.318000 -2.747000 0.504000	H 4.473680 1.815050 -7.055770	C -6.753290 0.778370 2.176120	H 2.447520 6.660410 2.262250	H 4.275390 1.984360 -7.024010
C 9.355000 -3.369000 -0.358000	C 3.673100 0.129310 -5.939660	H -7.290070 1.659800 2.580460	H 4.112590 6.118950 2.033290	C 3.613570 0.277740 -5.850160
H 10.006000 -3.907000 0.341000	H 4.517250 -0.528870 -6.168400	H -7.168410 -0.096950 2.710550	C 0.730420 2.823070 4.136510	H 4.524930 -0.302760 -6.025070
H 8.886000 -4.056000 -1.081000	C 2.616070 -0.343390 -5.141700	C -2.656950 -0.246300 3.882470	C -0.378780 3.379170 4.814710	C 2.585490 -0.262830 -5.056650
H 9.910000 -2.590000 -0.904000	H 2.642300 -1.365770 -4.749500	C -2.510400 0.977840 4.574230	H -1.242190 3.727700 4.238010	H 2.708850 -1.256610 -4.614480
H 4.741000 0.485000 2.010000	C -0.670700 -0.831210 -4.906960	H -2.531850 1.920480 4.018080	C -0.383920 3.476740 6.217360	C -0.755860 -0.977870 -4.851340
H 3.724000 -0.904000 1.579000	H -0.121190 -1.645150 -5.420920	C -2.323330 0.992450 5.969640	H -1.252610 3.902620 6.729220	C -0.096020 -2.216260 -5.498630
H 4.822000 -1.032000 -0.694000	H -1.426800 -1.303060 -4.256870	H -2.205230 1.947780 6.490620	C 0.722420 3.021550 6.961350	H -1.522330 -1.345980 -4.140300
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	C -2.403170 -0.729260 -6.805370	H -2.391420 -2.383200 6.563620	C 1.835850 2.369060 4.889950	C -2.685610 -0.770690 -6.546170
	H -2.753720 -0.103170 -7.649940	C -2.615980 -1.454560 4.616710	H 2.694330 1.925270 4.376270	H -2.374230 -1.617530 -7.183620
	H -1.940180 -1.621600 -7.268210	H -2.724610 -2.409100 4.090890	C 1.432560 0.366550 -3.941300	H -3.360710 -1.200690 -5.777110
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	O -3.952410 -0.810920 -4.878790	O -6.369510 0.899370 -0.264450	O 2.806290 5.210020 -0.610260	O -3.443520 1.430280 -7.377710
	O -4.407650 -2.040010 -6.790940	O -8.439950 0.258200 0.559220	O 3.030230 7.451990 -0.065990	O -4.390280 -0.518680 -8.206370
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				H 0.652890 -1.929750 -6.258750
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				H 0.405560 -2.840420 -4.736980

α2-[70]PCMBM -3322.250069 0	β1-[70]PCMBM -3322.245655 0	β2-[70]PCMBM -3322.245499 0	C_{70} -2667.034247 0	Pr -497.5793347 0

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H -1.384070 1.321970 -5.696360	H -5.196830 -1.561670 3.692040	H -0.092350 6.345900 2.209450		
H -1.741300 -0.046490 -6.777400	H -4.587310 -2.520630 2.307010	H -0.345710 5.541820 3.784510		
TS-[a-b]-Pz-PCPr-1	TS-[a-b]-Pz-PCPr-2	TS-[c-c]-Pz-PCPr-1	TS-[c-c]-Pz-PCPr-2	TS-[a-b]-Pz-PCiPr-1
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1 (-277.43)	1 (-277.14)	1 (-279.91)	1 (-282.33)	1 (-284.25)
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H 1.484460 -5.045410 5.393840	H 1.484460 -5.045410 5.393840	C -2.131700 1.150720 7.321750	C -0.476260 -1.495800 1.636060	H 0.999990 -1.872510 5.085320
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C 0.799950 3.444530 2.703570	C -1.443616 2.730155 2.774090	C 0.920731 3.519327 2.177812	C -0.080282 3.551822 2.700772	C -0.369434 3.418688 2.750347
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C 3.273400 2.659840 -3.895750	C 0.089253 0.001004 -4.638526	C -0.206197 -1.312463 -3.945557	C -1.327298 -0.497114 -4.139798	C -1.067272 -0.474677 -4.257149
C 0.999720 -0.059660 -4.539870	C 2.382308 0.056151 -3.680432	N 3.110538 -3.630482 2.441806	C 1.093130 -0.931445 -3.772270	C 1.362615 -0.752702 -3.807642
C 3.395500 -0.202160 -3.883940	C -0.150422 -1.238379 -4.009485	N 2.317540 -4.467533 2.569194	C -1.655758 -1.524114 -3.231767	C -1.356344 -1.552253 -3.395815
C 0.713080 -1.203170 -3.765130	N 3.114050 -3.747313 2.150087	C 0.362766 -3.846614 2.832196	N 2.632344 -2.829786 3.973031	N 2.871307 -2.906802 3.783883
N 4.389300 -2.586960 2.771100	N 2.291282 -4.563984 2.260827	C 2.741789 0.455103 2.118038	N 1.701340 -3.398194 4.379349	N 2.003720 -3.559603 4.191990
N 3.701800 -3.507940 3.266760	C 0.484283 -3.873455 2.763403	C -0.404754 -4.998101 2.200608	C 0.204572 -3.629376 3.070353	C 0.330326 -3.725765 2.980453
C 2.236480 -3.532450 2.947870	C 2.744325 0.415027 2.115369	H -1.498497 -4.837751 2.330130	C 3.121995 0.130891 1.566622	C 3.107105 0.267204 1.639998
C 1.431840 -3.487160 4.254300	C 0.807843 -3.618792 4.238272	H -0.237293 -4.964511 1.108996	C -1.016035 -3.972102 3.851593	C -0.768050 -3.903238 4.016732
C 2.055810 -3.235870 5.495160	H 1.615773 -2.862093 4.282921	C -0.041584 -6.422608 2.706417	C -1.298302 -3.316214 5.078449	H -0.876660 -2.948618 4.563254
H 3.140770 -3.107200 5.540810	H -0.066098 -3.151496 4.733472	H -0.155366 -6.490864 3.803372	H -0.607123 -2.559350 5.455773	H -1.744847 -4.056172 3.504830
C 1.293420 -3.170640 6.677510	C 1.226797 -4.865161 5.059842	H 1.026352 -6.600372 2.493238	C -2.434468 -3.656536 5.828287	C -0.555388 -5.035448 5.057795

H 1.794480 -2.975490 7.630820 C -0.099920 -3.357600 6.637050 H -0.690950 -3.305620 7.556510 C -0.729820 -3.614990 5.403770 H -1.813080 -3.764920 5.359560 C 0.029190 -3.682020 4.223250 H -0.472770 -3.881710 3.271000 C 1.996090 -4.882620 2.152270 H 1.025700 -4.750420 1.631730 C 3.094750 -5.167600 1.096200 H 3.312100 -4.315200 0.434900 H 4.036310 -5.459110 1.593550 H 2.775190 -6.008200 0.454440 C 1.896920 -6.109170 3.092940 H 2.811100 -6.201160 3.705930 H 1.031760 -6.054480 3.771770 H 1.800880 -7.026200 2.483920	H 0.417412 -5.617517 5.042297 H 2.101229 -5.342433 4.581996 C -0.503005 -4.939479 2.435915 C -1.583679 -5.234115 3.308941 H -1.716642 -4.647685 4.221762 C -2.508189 -6.243614 2.994868 H -3.342319 -6.444289 3.672788 C -2.361777 -6.991987 1.811604 H -3.076967 -7.783619 1.571022 C -1.289557 -6.718377 0.939536 H -1.165491 -7.301969 0.023498 C -0.374783 -5.698377 1.242559 H 0.464920 -5.503437 0.573045 C 1.562110 -4.491050 6.516817 H 1.857617 -5.384311 7.093014 H 2.397311 -3.768624 6.563984 H 0.693141 -4.033742 7.024331	C -0.908068 -7.497184 2.022929 H -0.615888 -8.506937 2.359272 H -1.980707 -7.362186 2.256094 H -0.796261 -7.464222 0.923526 C -0.591972 -0.596378 3.339804 C -1.606634 0.455062 3.314523 C 0.302648 -3.698882 4.318092 C -0.751032 -4.304187 5.061016 H -1.541710 -4.847309 4.538217 C -0.826361 -4.172751 6.455326 H -1.657434 -4.632728 6.997137 C 0.156329 -3.444373 7.152668 H 0.100016 -3.344287 8.240463 C 1.208272 -2.840906 6.438017 H 1.978932 -2.275748 6.969496 C 1.279120 -2.956865 5.041553 H 2.111909 -2.491426 4.513855	H -2.625592 -3.151550 6.778407 C -3.322267 -4.645728 5.362734 H -4.210392 -4.904457 5.945748 C -3.061686 -5.299771 4.144194 H -3.750914 -6.062877 3.771940 C -1.916269 -4.973755 3.400721 H -1.735081 -5.477059 2.447120 C 0.862367 -4.738899 2.249052 H 0.198803 -5.013177 1.403540 H 1.778301 -4.323901 1.787333 C 1.218458 -6.033472 3.025204 H 1.886751 -5.783195 3.868239 H 0.306028 -6.467015 3.471832 C 1.898085 -7.069194 2.108212 H 2.139334 -7.989729 2.666132 H 1.243644 -7.349578 1.262636 H 2.839474 -6.674535 1.687144	H -0.392052 -6.004966 4.557129 H 0.368645 -4.815187 5.619466 C 0.695574 -4.906794 2.141842 C -0.218688 -5.988445 1.986633 H -1.208475 -5.932095 2.444847 C 0.105749 -7.108975 1.208050 H -0.622660 -7.916635 1.092488 C 1.358685 -7.190297 0.571049 H 1.615203 -8.066882 -0.029957 C 2.276053 -6.131166 0.708775 H 3.251191 -6.183164 0.217899 C 1.949411 -5.001112 1.473788 H 2.683282 -4.200408 1.573880 C -1.751568 -5.137668 6.023329 H -1.573296 -5.913725 6.787142 H -1.924817 -4.181682 6.549651 H -2.683164 -5.398400 5.488565
TS-[b-c]-PCiPr -3164.555735 1 (-178.09)	TS-[b-c]*-PCiPr -3164.552193 1 (-165.12)	TS-[c-d]-PCiPr -3164.555344 1 (-174.18)	TS-[c-d]*-PCiPr -3164.553061 1 (-159.52)	[a-a]-open-PCPr -3055.1186 0
C -1.438377 0.590352 3.347579 C -0.413707 -0.454997 3.353705 C 0.895665 0.199987 3.457548 C 0.673448 1.641305 3.515037 C -0.768529 1.884309 3.452160 C -2.581494 0.457299 2.535550 C -3.090886 1.605382 1.787218 C -2.445319 2.846473 1.885328 C -1.267624 2.992690 2.737366 C -0.350776 3.894263 2.048452 C 1.031932 3.662640 2.104347 C 1.554240 2.526072 2.855386 C 2.675620 1.992543 2.093344 C 1.975652 -0.322576 2.708722 C 1.867488 -1.530284 1.915199 C 0.616661 -2.394449 1.937438 C -0.582732 -1.600652 2.559289 C -2.725344 -0.710193 1.681705 C -1.723467 -1.694125 1.676342 C -2.259361 3.663404 0.691424 C -2.797299 3.268899 -0.576371 C -3.477569 1.957838 -0.681969 C -3.565766 1.137693 0.490554 C 1.847272 3.845571 0.907492 C 1.284259 4.338082 -0.313783 C -0.176148 4.577945 -0.373775 C -0.964548 4.309864 0.790996 C 3.268977 0.000753 0.766285 C 3.562276 0.786148 -0.393787 C 3.346843 2.248607 -0.324517 C 2.863578 2.811650 0.900910 C 0.094736 -2.588264 0.485010 C 0.902076 -2.483885 -0.686315 C 2.228731 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^{3}TS2-[c-c]-PCPr-1 -3055.053221 1 (-512.29) (BP86/6-31G* opt)	^{3}TS2-[a-b]-PCiPr -3055.048305 1 (-444.43) (BP86/6-31G* opt)	^{3}TS2-[c-c]-PCiPr-1 -3055.04841 1 (-379.68) (BP86/6-31G* opt)	^{3}[a-b]-PCPr -3055.084867 0	^{3}[c-c]-PCPr-1 -3055.082534 0
C -1.260230 1.552445 2.829607	C -1.296894 -0.092927 2.362110	C -1.242530 1.584450 2.843017	C -1.346667 -0.334215 2.296253	C -1.235082 1.671119 2.859683
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C	1.496056	-2.505698	-0.055464	C	-0.758663	-2.497302	-0.900729	C	-1.115351	-3.049353	0.378335	C	2.100084	-1.742543	-4.065531	C	0.296564	-3.109050	0.064114
C	2.753138	-1.805585	-1.742031	C	0.729798	-2.481554	-0.857180	C	-1.955105	-2.257461	-0.469321	C	1.920544	-2.927763	-3.197073	C	-1.141907	-3.049363	0.373558
C	3.027937	-1.491223	-0.371000	C	1.384805	-2.090492	0.356473	C	3.196494	0.833790	-0.211424	C	0.588490	-3.322851	-2.844742	C	-1.981125	-2.256180	-0.473109
C	-2.967623	-0.827354	-0.883264	C	-3.567516	1.437440	0.000218	C	3.440014	-0.316501	0.606597	C	0.429256	2.748681	-2.988414	C	3.183533	0.813990	-0.242736
C	-2.541008	-1.219125	-2.194694	C	-3.611612	0.617493	-1.173555	C	2.835059	-1.595886	0.200731	C	1.780688	2.407444	-3.323128	C	3.425493	-0.335077	0.577369
C	-1.431568	-2.181613	-2.306726	C	-3.128508	-0.774763	-1.083774	C	2.043480	-1.619140	-0.992760	C	2.023263	1.193625	-4.135041	C	2.813482	-1.612918	0.177328
C	-0.845339	-2.680468	-1.094550	C	-2.627134	-1.248833	0.174100	C	3.374374	1.213565	2.595536	C	0.897827	0.409874	-4.549191	C	2.017251	-1.636199	-1.013188
C	-3.052314	1.130552	-2.943610	C	-3.078838	2.685852	-2.490594	C	2.924151	0.987377	3.964689	C	2.438961	3.292204	-1.067474	C	3.373991	1.200858	2.562071
C	-2.412788	1.958417	-3.956428	C	-2.320999	2.858535	-3.728487	C	1.908826	1.788627	4.505498	C	3.502482	2.893741	-0.152309	C	2.928003	0.980415	3.933470
C	-1.864323	3.200980	-3.602043	C	-1.201581	3.698815	-3.740212	C	1.311759	2.846577	3.696951	C	3.184783	2.480936	1.149756	C	1.918107	1.787501	4.475803
C	-1.928650	3.649278	-2.216061	C	-0.808187	4.405842	-2.513611	C	-0.102980	2.902777	4.008301	C	1.790598	2.451349	1.580381	C	1.322488	2.845709	3.666476
C	-0.691288	4.344259	-1.911969	C	0.634945	4.421208	-2.469283	C	-0.381861	1.874868	5.007908	C	1.603037	1.289613	2.429952	C	-0.090797	2.908817	3.982999
C	0.141436	4.322836	-3.109973	C	1.132310	3.742285	-3.668199	C	-1.582831	1.153942	4.947634	C	2.886002	0.604473	2.527299	C	-0.370261	1.884858	4.986512
C	1.530794	4.169315	-2.991084	C	2.285068	2.932265	-3.576830	C	-2.544855	1.436701	3.885625	C	2.922651	-0.795094	2.560949	C	-1.574443	1.168852	4.932766
C	2.134504	4.029641	-1.670241	C	2.964414	2.786622	-2.310375	C	-3.133599	0.177600	3.473438	C	1.677457	-1.550912	2.498919	C	-2.539228	1.452698	3.873614
C	3.224340	3.076997	-1.775535	C	3.441096	1.392486	-2.218234	C	-2.540617	-0.882150	4.281648	C	1.926627	-2.739338	1.704223	C	-3.134869	0.194954	3.467250
C	3.297177	2.628008	-3.160433	C	3.043441	0.710368	-3.425275	C	-2.270543	-2.130217	3.703516	C	3.321125	-2.716309	1.273323	C	-2.543313	-0.865028	4.276204
C	3.615398	1.290710	-3.441845	C	2.630103	-0.644476	-3.372301	C	-2.579902	-2.360349	2.296424	C	3.661535	-3.173044	-0.008552	C	-2.280795	-2.115943	3.700693
C	3.880156	0.361895	-2.351176	C	2.597643	-1.325542	-2.089191	C	-1.531143	-3.192488	1.740781	C	2.621024	-3.668146	-0.902487	C	-2.596379	-2.348754	2.295386
C	3.310134	-0.928962	-2.727194	C	1.437598	-2.207214	-2.067159	C	-0.571774	-3.477604	2.801776	C	2.947406	-3.245759	-2.251209	C	-1.553285	-3.186869	1.738065
C	2.714277	-0.795270	-4.041343	C	0.753459	-2.043314	-3.348895	C	0.799545	-3.533660	2.508639	C	4.190440	-2.484391	-2.190922	C	-0.591166	-3.472923	2.796211
C	1.505477	-1.473716	-4.331339	C	-0.644344	-2.060768	-3.391792	C	1.253530	-3.301110	1.144217	C	4.363012	-1.363581	-3.017027	C	0.778722	-3.535563	2.497892
C	0.886862	-2.298740	-3.327784	C	-1.400460	-2.235484	-2.152071	C	2.496513	-2.554567	1.206686	C	3.294673	-0.963589	-3.926078	C	1.228496	-3.308567	1.131053
C	-0.587516	-2.136108	-3.454569	C	-2.580420	-1.394451	-2.243102	C	2.812459	-2.324765	2.609924	C	3.256687	0.486328	-3.960228	C	2.474836	-2.567323	1.187102
C	-0.834875	-1.215426	-4.531763	C	-2.551172	-0.708896	-3.530037	C	3.382770	-1.103661	3.000732	C	4.301342	0.984243	-3.072375	C	2.797040	-2.334975	2.588484
C	-1.898929	-0.284469	-4.435242	C	-3.004088	0.621165	-3.619815	C	3.658889	-0.077426	2.001476	C	4.069566	2.132198	-2.300422	C	3.374077	-1.115330	2.973754
C	-2.720788	-0.261318	-3.242742	C	-3.498040	1.298681	-2.425886	C	0.868446	-0.198627	5.582731	C	2.788481	2.823601	-2.394989	C	3.650860	-0.093036	1.970655
C	0.105342	2.783081	-5.063784	C	0.041933	2.069899	-5.158567	C	1.928015	-1.035215	5.017361	C	4.863303	0.652570	1.015250	C	0.873453	-0.192312	5.562572
C	-0.465573	1.489514	-5.432934	C	-1.118336	1.192965	-5.137286	C	2.937564	-0.449313	4.227581	C	5.195473	1.082120	-0.344157	C	1.927342	-1.035009	4.995579
C	-1.705166	1.086662	-4.892822	C	-2.283717	1.583410	-4.438728	C	-0.384318	-0.950697	5.520351	C	4.527330	2.184800	-0.913758	C	2.936401	-0.455623	4.200395
C	1.558173	2.621458	-4.939356	C	1.236220	1.225740	-5.052849	C	0.865384	1.189498	5.331847	C	4.900868	-0.810496	1.049359	C	-0.382719	-0.939233	5.506989
C	-0.584571	3.622747	-4.166020	C	-0.000001	3.308814	-4.467505	C	-0.100990	-2.253275	4.915354	C	3.875392	1.343328	1.746254	C	0.875287	1.195100	5.307726
C	1.887833	1.228020	-5.231862	C	0.807125	-0.178561	-5.000811	C	-1.586512	-0.282023	5.208779	C	5.257037	-1.285777	-0.288138	C	-0.107231	-2.244651	4.904603
C	2.253777	3.307774	-3.923236	C	2.334803	1.654014	-4.286265	C	1.330008	-2.307797	4.607144	C	3.950237	-1.516839	1.813656	C	-1.583254	-0.266319	5.198061
C	0.635878	0.524820	-5.529804	C	-0.646112	-0.197229	-5.044102	C	-1.031081	-2.831261	4.027932	C	5.436453	-0.115985	-1.150340	C	1.322352	-2.306131	4.591168
C	2.902988	0.575866	-4.500128	C	1.499061	-1.090738	-4.166807	C	1.768298	-2.939216	3.427025	C	4.648161	-2.447713	-0.803883	C	-1.043067	-2.821243	4.022330
C	0.452150	-0.796519	-5.089908	C	-1.361440	-1.127794	-4.254837	C	0.388171	-0.007355	-4.050522	C	4.997969	-0.159019	-2.488685	C	1.753407	-2.942715	3.411114
C	-0.458461	-2.888092	2.692568	C	-0.105756	-3.046527	2.391862	C	1.575434	0.538370	-4.819920	C	-2.931498	-0.249219	2.430663	C	0.364604	-0.021690	-4.072923
C	0.723356	-3.631537	3.374517	C	-0.150850	-2.990004	3.943100	C	1.599453	1.870724	-5.287287	C	-4.438287	-0.305562	2.105361	C	1.545987	0.557834	-4.826611
H	1.655227	-3.205874	2.957939	H	-0.161124	-1.921788	4.228591	H	0.782497	2.549606	-5.027235	H	-4.585868	-0.523106	1.032638	C	1.479934	1.861518	-5.369602
C	0.745893	-3.391839	4.900729	C	-1.441076	-3.633489	4.500840	C	2.670740	2.331279	-6.075886	H	-4.864759	-1.161897	2.662597	H	0.596153	2.478003	-5.183923
H	-0.141668	-3.828458	5.389518	H	-1.479065	-4.713849	4.278471	H	2.677286	3.366008	-6.429258	C	-5.205651	0.984693	2.469622	C	2.545039	2.374865	-6.131958
H	0.779607	-2.314256	5.139403	H	-2.343981	-3.159170	4.077706	C	3.729139	1.465343	-6.406477	H	-5.063296	1.210752	3.542877	H	2.480126	3.386373	-6.541639
C	-1.841952	-3.319842	3.133631	C	-0.076689	-4.436278	1.792615	H	4.563023	1.824575	-7.016368	H	-4.771764	1.833241	1.905783	C	3.692495	1.592602	-6.360296
C	-2.460186	-2.716137	4.252847	C	-1.280284	-5.124475	1.515258	C	3.712560	0.135056	-5.945043	C	-2.633971	-0.228925	3.916374	H	4.522872	1.993133	-6.948748
H	-1.962751	-1.884805	4.760007	H	-2.237879	-4.621670	1.676325	H	4.533285	-0.543174	-6.195507	C	-2.448675	0.986510	4.611877	C	3.770290	0.295586	-5.819911
C	-3.712987	-3.165064	4.707833	C	-1.255125	-6.441259	1.021246	C	2.642668	-0.325040	-5.157849	H	-2.441973	1.929708	4.057617	H	4.661171	-0.316573	-5.986849
H	-4.179207	-2.684287	5.572052	H	-2.195205	-6.956101	0.804845	H	2.634533	-1.357400	-4.795615	C	-2.262433	0.990132	6.006756	C	2.705335	-0.217508	-5.057555
C	-4.367031	-4.223647	4.049815	C	-0.026363	-7.089773	0.796848	C	-0.623984	-0.762279	-4.937266	H	-2.115810	1.938638	6.531109	H	2.775143	-1.221618	-4.631085
H	-5.342936	-4.569049	4.400410	H	-0.007054	-8.110706	0.406848	H	-0.068330	-1.557327	-5.471911	C	-2.259416	-0.220686	6.722990	C	-0.674738	-0.775447	-4.954122
C	-3.762892	-4.827477	2.931374	C	1.177236	-6.412666	1.067416	H	-1.373828	-1.270850	-4.305598	H	-2.108205	-0.218056	7.806288	H	-1.457022	-1.162069	-4.274552
H	-4.267952	-5.644337	2.408532	H	2.136841	-6.905133	0.887421	C	-1.352666	0.137317	-5.959713	C	-2.445164	-1.436777	6.037960	C	-1.362578	0.174556	-5.959044
C	-2.510086	-4.378122	2.475781	C	1.152377	-5.095787	1.561412	H	-1.895331	0.936215	-5.417912	H	-2.440221	-2.382455	6.587628	H	-1.859691	1.016219	-5.446471
H	-2.050709	-4.842625	1.598941	H	2.090493	-4.570056	1.759074	H	-0.610867	0.642322	-6.606138	C	-2.632018	-1.440623	4.644724	H	-0.637785	0.587274	-6.681675
H	1.641775	-3.864559	5.339316	H	-1.475187	-3.509121	5.597678	C	-3.142229	-0.252695	-0.760453	H	-2.769609	-2.388358	4.114756	H	-2.132247	-0.376910	-6.527010
C	0.713265	-5.140566	3.041620	C	1.110607	-3.626399	4.570673	C	-2.341274	-0.663019	-6.829854	C	-6.711099	0.871251	2.157536	C	-0.042831	-1.989086	-5.671713
H	-0.176318	-5.637633	3.464426	H	1.170854	-4.704922	4.344334	H	-3.116933	-1.148471	-6.210778	H	-7.174750	0.044913	2.725591	H	-0.823748	-2.548985	-6.215581
H	0.723295	-5.311567	1.950802	H	2.031578	-3.141554	4.202270	H	-2.851577	-0.008529	-7.557433	H	-7.242895	1.801582	2.422405	H	0.719732	-1.670748	-6.403264
H	1.608425	-5.623240	3.470467	H	1.080394	-3.508405	5.668323	H	-1.819900	-1.454990	-7.397766	H	-6.883267	0.679422	1.082832	H	0.433089	-2.680969	-4.954602

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C	-2.563018	0.868522	-2.254605	C	-0.491497	0.847487	-4.249366	C	2.005379	1.191604	-4.124528	C	4.283753	0.965069	-3.065973	C	-2.620995	-0.159470	3.938437
C	-2.329705	-0.330571	-3.056772	C	-0.551775	2.376949	0.996446	C	0.872886	0.416435	-4.535639	C	4.062631	2.115795	-2.294913	C	-2.520778	1.077367	4.616037
C	-2.519788	-1.495830	-2.195705	C	0.749361	2.923708	0.741411	C	2.443683	3.290239	-1.060188	C	2.786966	2.817424	-2.387841	H	-2.611904	2.009428	4.051238
C	-2.877738	-1.028012	-0.856958	C	1.080879	3.363704	-0.630303	C	3.505736	2.884429	-0.146593	C	4.850661	0.633806	1.021023	C	-2.289637	1.118134	6.002820
C	-2.904802	0.454947	-0.893965	C	0.085992	3.228855	-1.649867	C	3.187212	2.475873	1.156588	C	5.183768	1.059040	-0.339512	H	-2.210294	2.083546	6.510841
C	-1.768929	2.014593	-2.474755	C	-0.710141	-1.622575	1.956604	C	1.793666	2.458236	1.590135	C	4.523300	2.166330	-0.909132	C	-2.152124	-0.077328	6.732561
C	-1.261818	2.763358	-1.341027	C	0.373059	-0.888733	2.530532	C	1.598308	1.299143	2.441390	C	4.876623	-0.829487	1.056855	H	-1.965229	-0.045442	7.809706
C	-1.573125	2.339564	-0.040424	C	0.346030	0.601858	2.492693	C	2.875895	0.603637	2.536872	C	3.869792	1.333444	1.753054	C	-2.244451	-1.313804	6.066922
C	-2.444796	1.204560	0.197479	C	-0.762420	1.266775	1.884257	C	2.901390	-0.796111	2.571870	C	5.226303	-1.309224	-0.280764	H	-2.129971	-2.247600	6.624576
C	-2.048051	0.603019	1.510410	C	0.212381	-3.725192	-1.477061	C	1.650025	-1.541711	2.512769	C	3.921683	-1.527154	1.823728	C	-2.475858	-1.354494	4.680120
C	-2.018439	-1.025229	1.551411	C	1.210490	-3.772422	-0.452845	C	1.888012	-2.733316	1.719284	C	5.413548	-0.141948	-1.144696	H	-2.533379	-2.317523	4.165051
C	-2.391917	-1.705371	0.269993	C	0.862052	-3.277555	0.895595	C	3.281873	-2.722180	1.285987	C	4.607209	-2.466868	-0.793935	H	-6.242746	1.017093	2.261768
C	-1.479524	-2.818083	0.087512	C	-0.458527	-2.766867	1.124285	C	3.616196	-3.183246	0.004115	C	4.972193	-0.183086	-2.482162	C	-5.150425	-1.505059	2.679014
C	-1.151737	-3.294200	-1.190700	C	0.899157	-1.032845	-4.499186	C	2.570021	-3.671093	-0.887202	C	-2.947215	-0.203976	2.459375	H	-5.129318	-1.515190	3.782755
C	-1.685230	-2.622448	-2.360040	C	2.058622	-1.745011	-4.051447	C	2.897226	-3.252944	-2.237049	C	-4.465191	-0.239264	2.116115	H	-6.206371	-1.531059	2.358209
C	-0.628193	-2.620336	-3.369973	C	1.871074	-2.927628	-3.181135	C	4.146489	-2.501550	-2.180055	H	-4.546494	-0.281436	1.013952	H	-4.663744	-2.425959	2.312660
C	-0.448797	-1.498466	-4.190651	C	0.536500	-3.311600	-2.825820	C	4.326531	-1.383143	-3.007816	C	-5.187049	1.045182	2.582999				
C	-1.319426	-0.336638	-4.039540	C	0.426197	2.760804	-2.976762	C	3.259744	-0.975651	-3.915307	H	-5.168199	1.139295	3.682767				
C	-0.711791	2.000710	-3.484176	C	1.774161	2.408311	-3.313634	C	3.233392	0.474497	-3.951220	H	-4.724862	1.948638	2.148594				