

Hetero-intermolecular [2+2] Photocycloaddition of 1,4-dihydropyridines: A Combined Experimental and DFT Study

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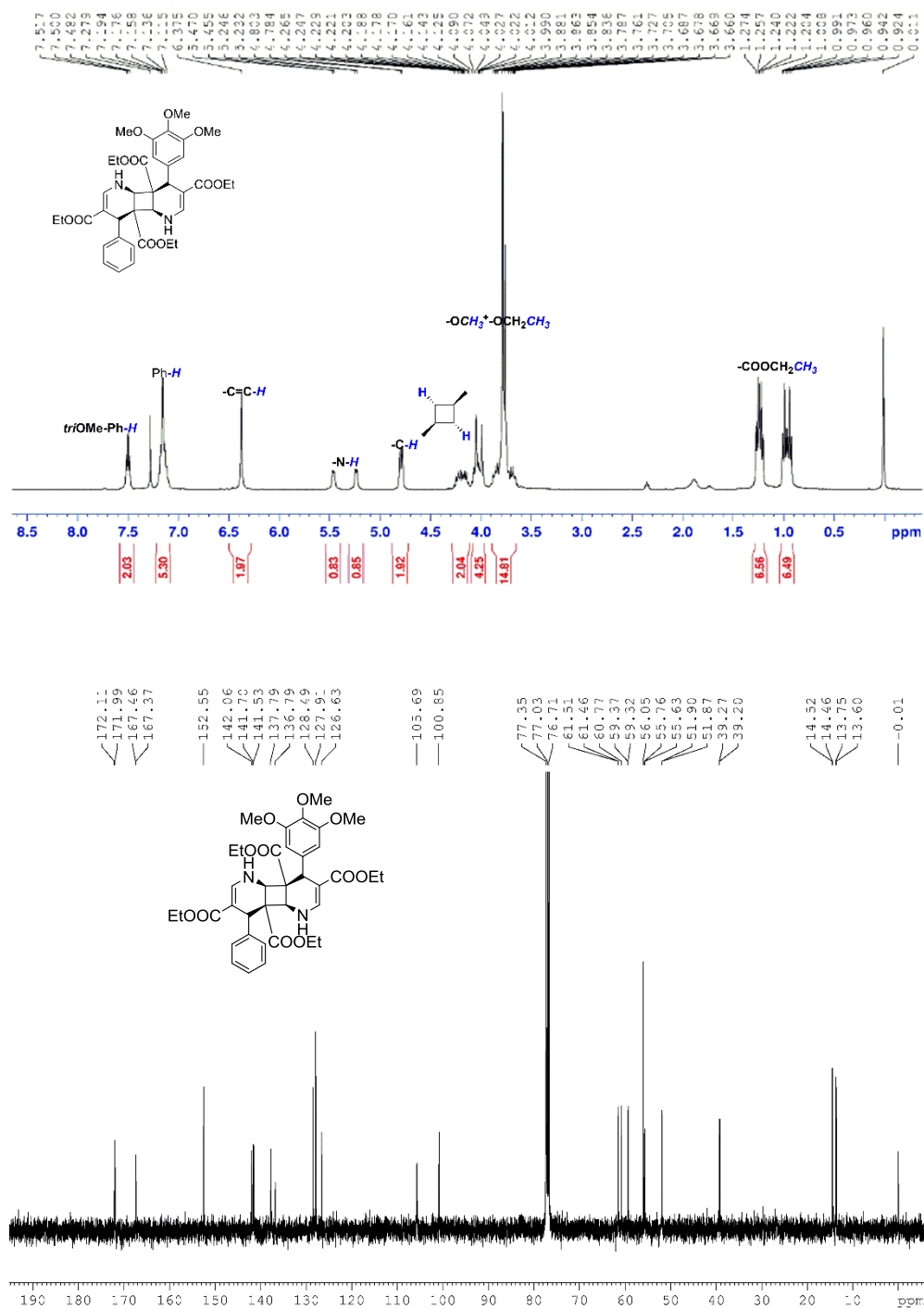
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¹H NMR and ¹³C NMR spectra of new compounds



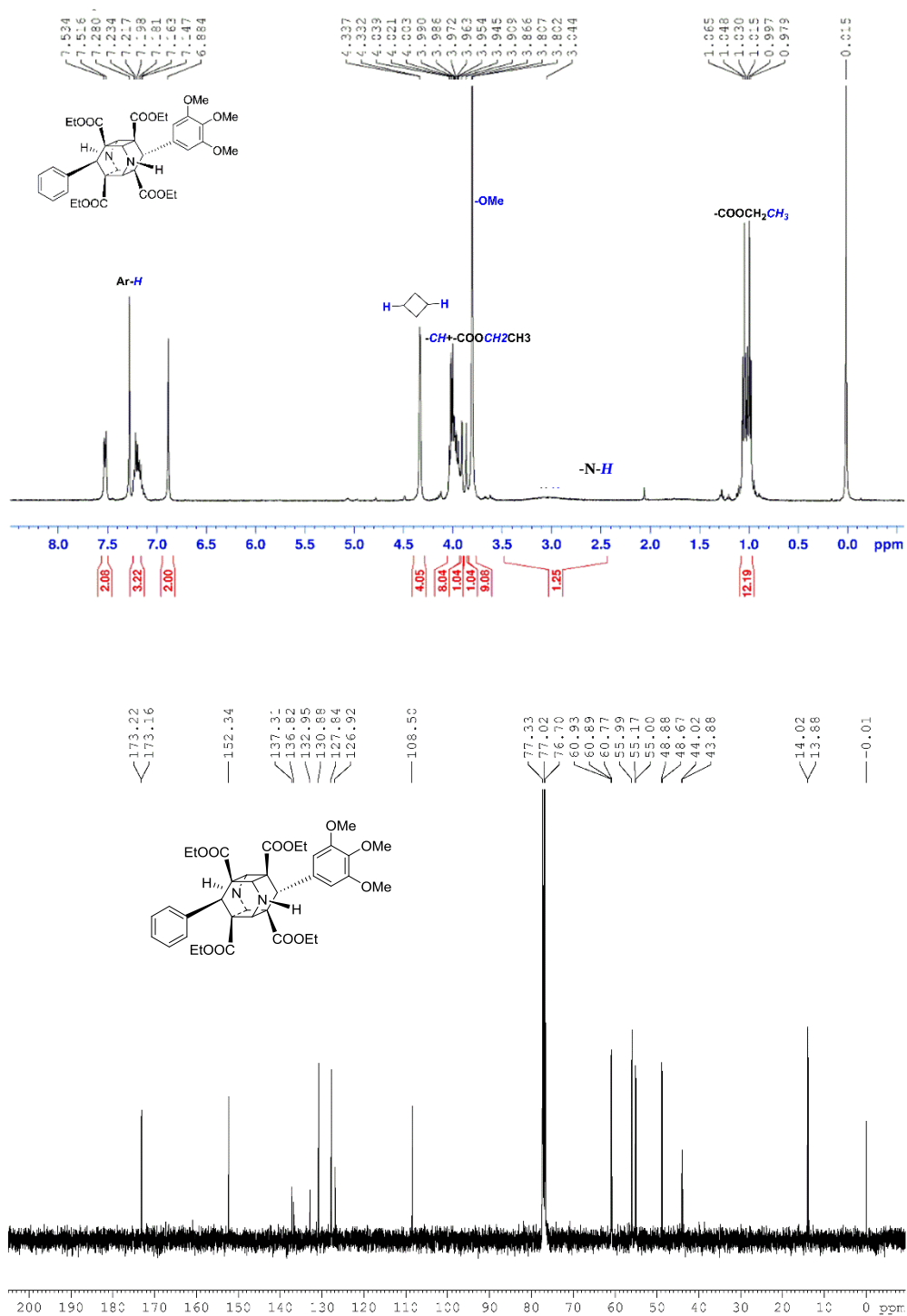


Figure S2 ¹H NMR and ¹³C NMR spectra of **3a**.

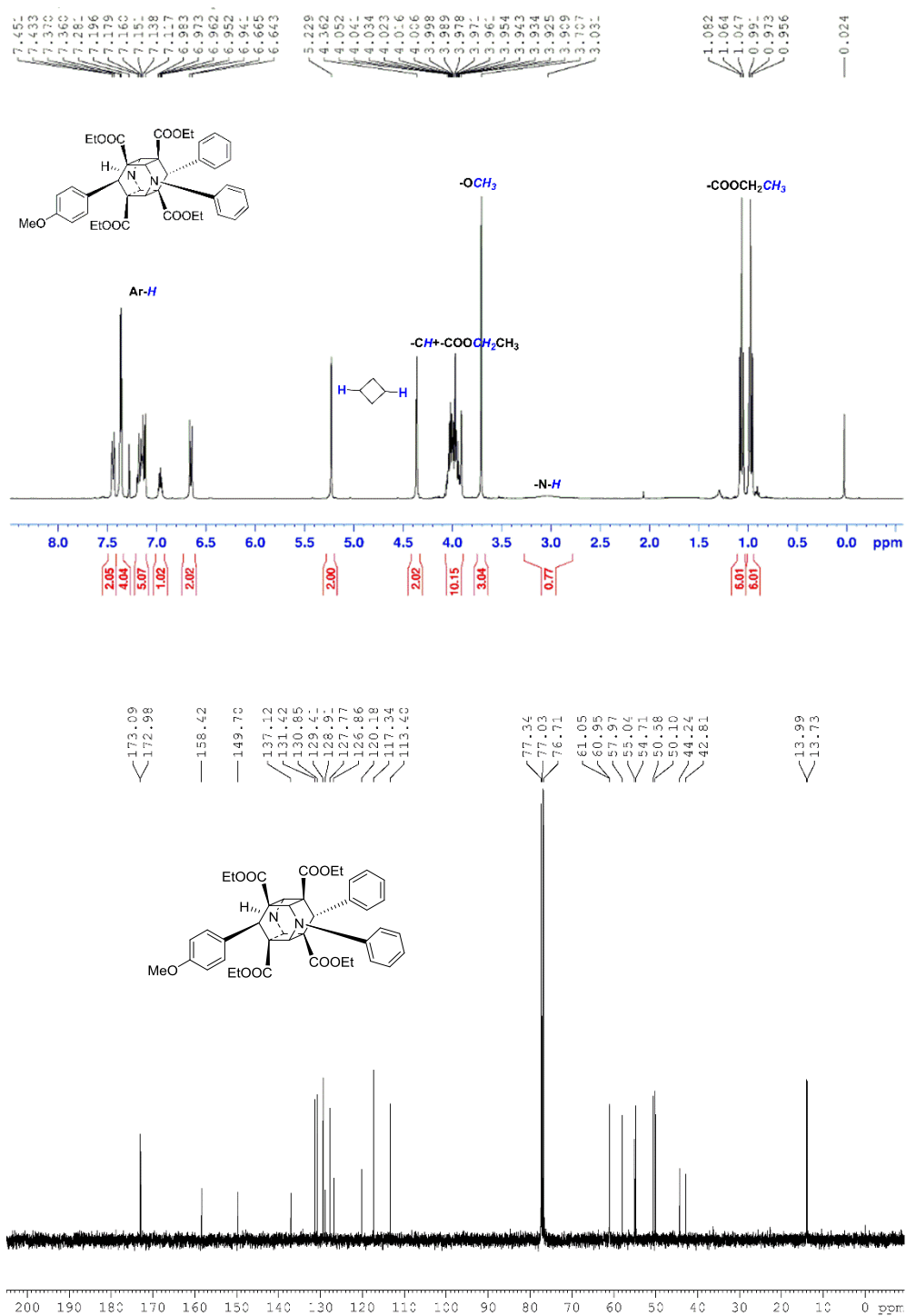


Figure S3 ¹H NMR and ¹³C NMR spectra of **3b**.

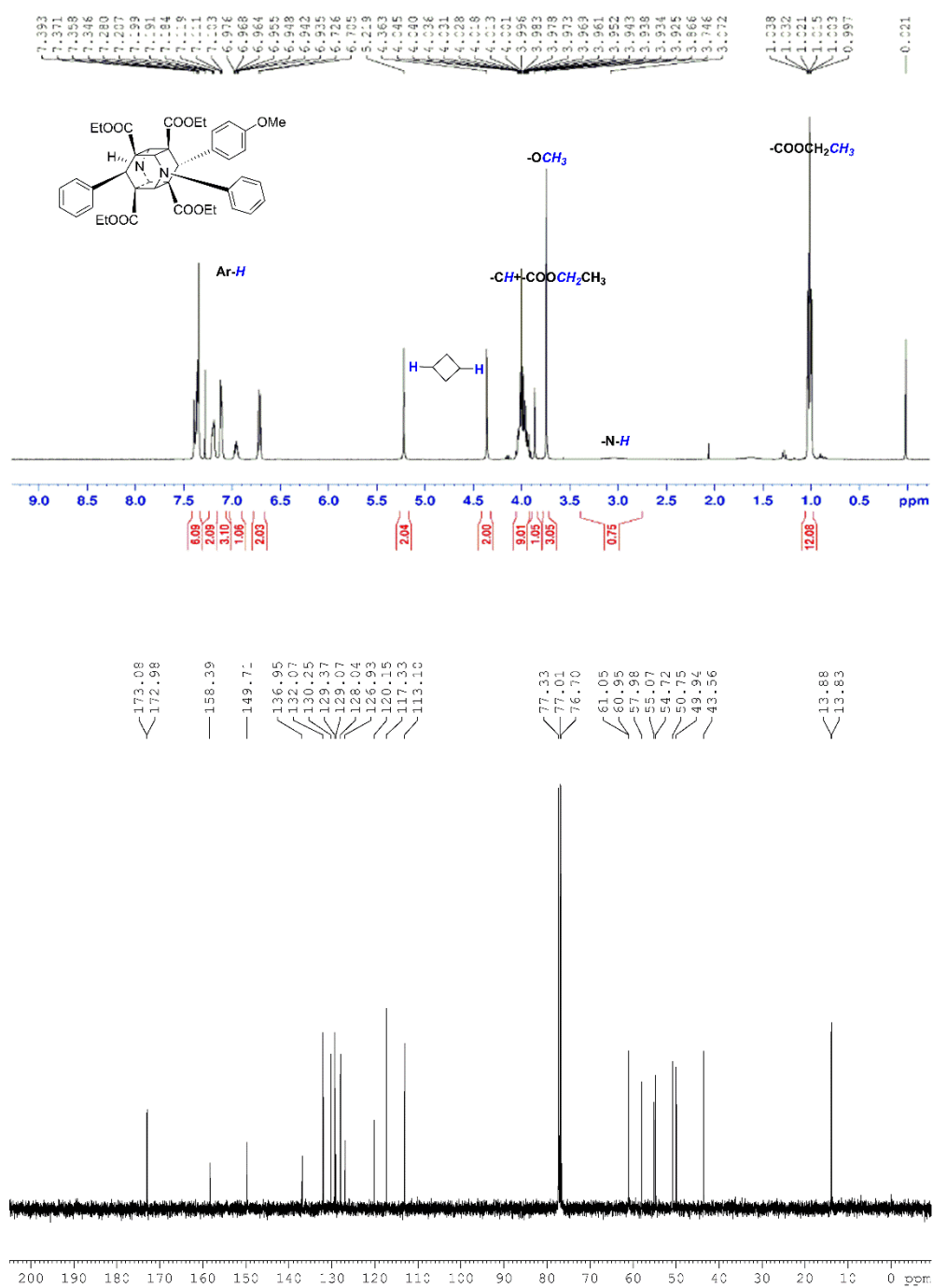


Figure S4 ¹H NMR and ¹³C NMR spectra of 3c.

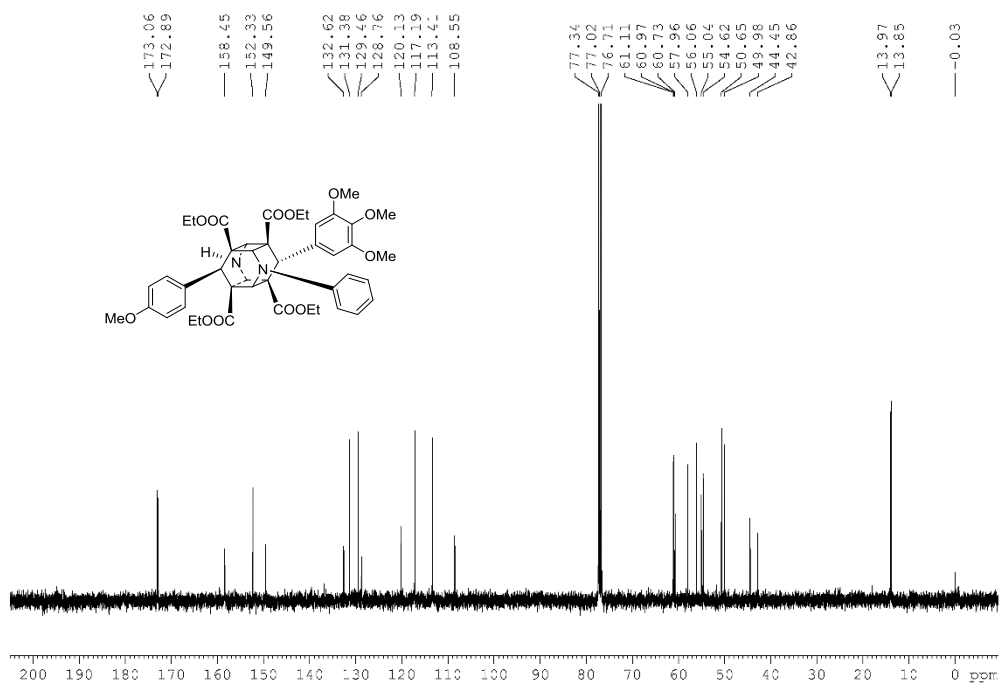
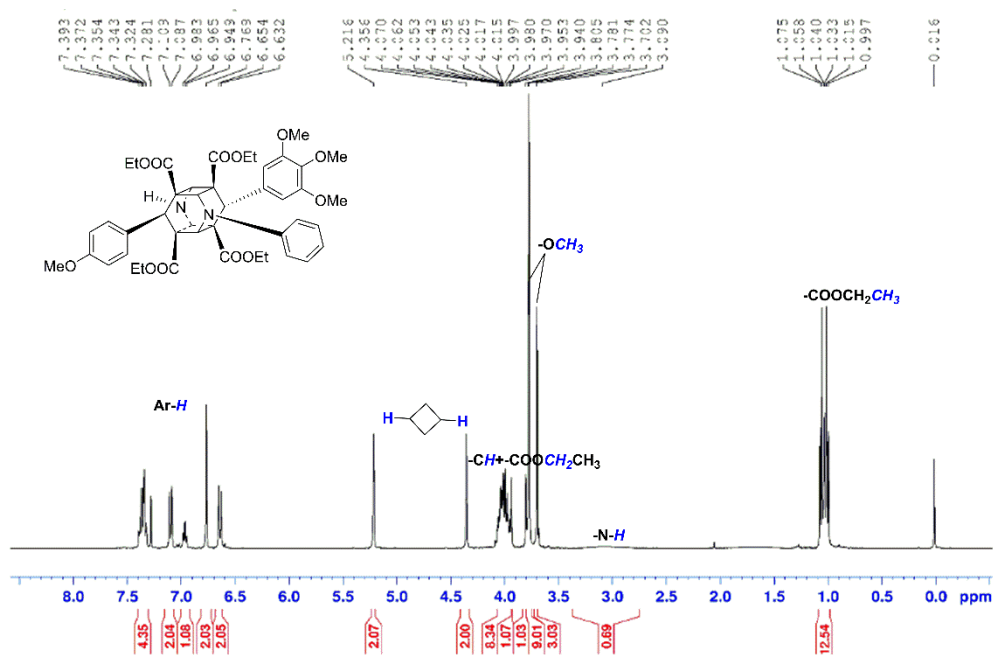


Figure S7 ¹H NMR and ¹³C NMR spectra of 3f.

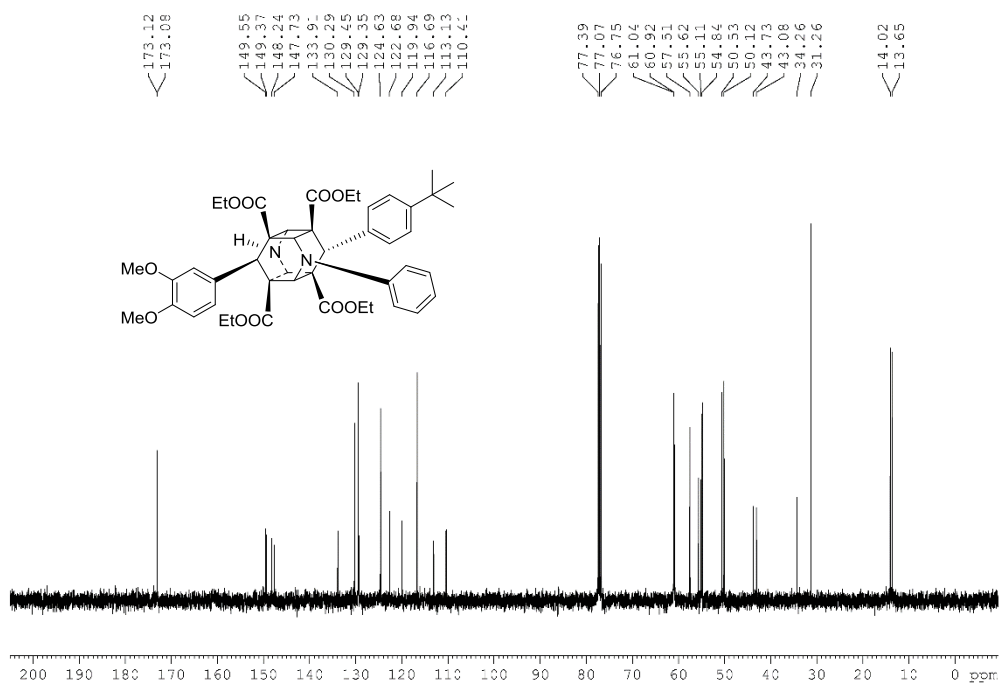
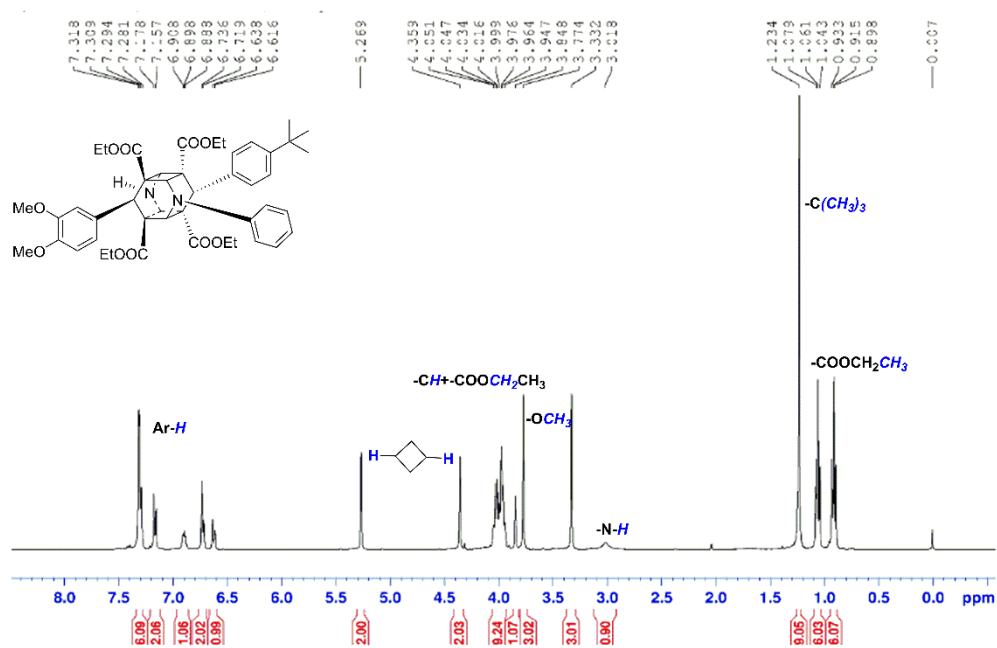


Figure S8 ¹H NMR and ¹³C NMR spectra of **3g**.

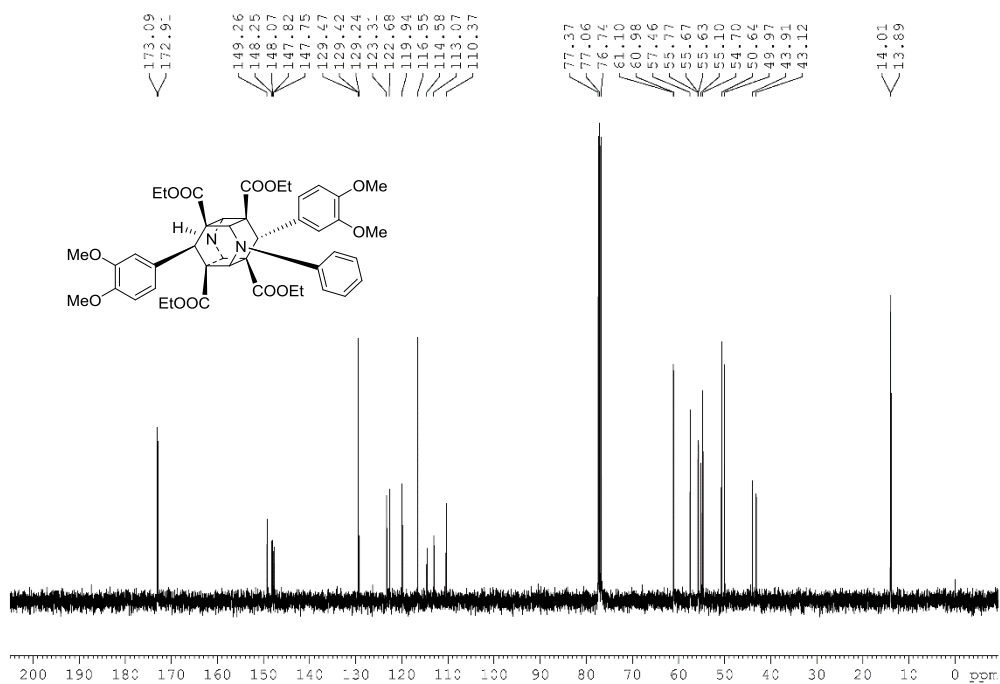
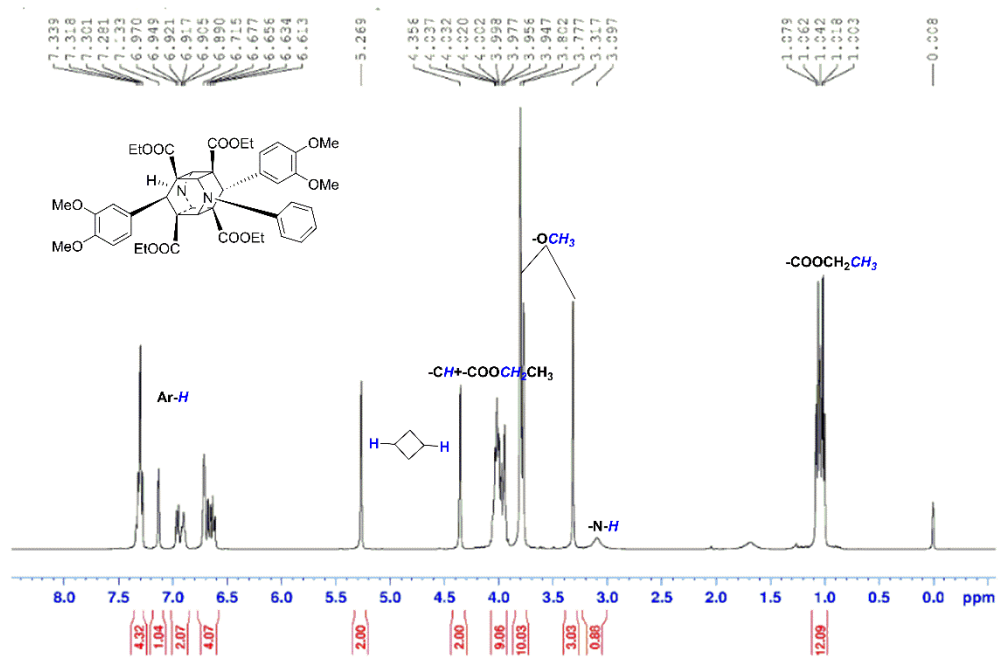


Figure S9 ¹H NMR and ¹³C NMR spectra of 3h.

X-ray single crystal structures of 2a, 3a and 3d

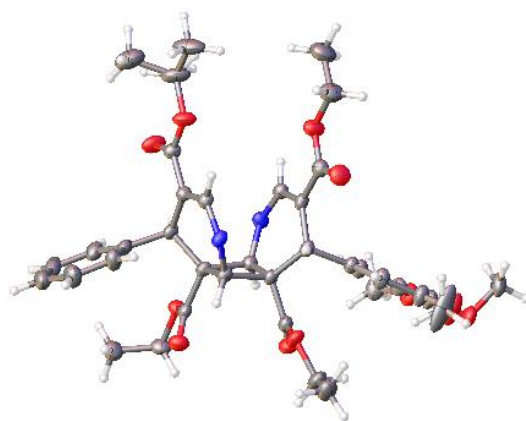


Fig S10 X-ray single crystal structure of **2a** (ellipsoid contours of probability levels are 50%).

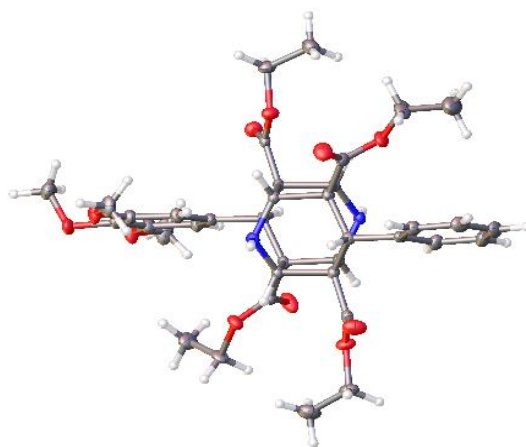


Fig S11 X-ray single crystal structure of **3a** (ellipsoid contours of probability levels are 50%).

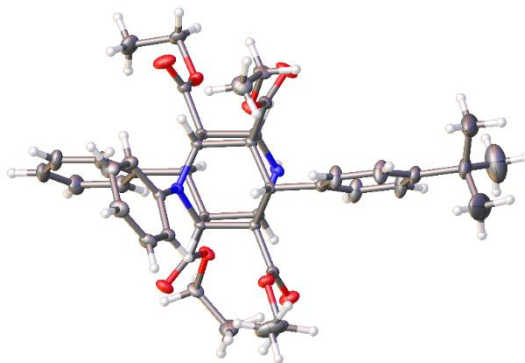


Fig S12 X-ray single crystal structure of **3d** (ellipsoid contours of probability levels are 50%).

A summary of crystallographic data of 2a, 3a and 3d

Table S1 A collection of crystallographic data for **2a**, **3a** and **3d**. The single-crystals suitable for X-ray diffraction were obtained from solution of ethyl acetate and hexane (V:V=1:4). The structures were solved by direct methods and refined by full matrix least squares on F^2 using the SHELX-97 program. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms, located by Fourier difference synthesis, were refined isotropically and were then normalized to the average neutron diffraction values.

Parameters	2a	3a	3d
Empirical Formula	C ₃₇ H ₄₂ N ₂ O ₁₁	C ₃₇ H ₄₄ N ₂ O ₁₁	C ₄₄ H ₅₀ N ₂ O ₈
Formula weight	670.72	692.74	734.86
Temperature (K)	113(2)	113(2)	113(2)
Crystal size (mm ³)	0.23*0.22*0.18	0.20*0.18*0.12	0.20*0.18*0.14
Space group	P-1	P21/n	P21/c
Crystal system	triclinic	Prism	Monoclinic
a (Å)	10.9132(13)	7.0677(17)	11.8540(13)
b (Å)	16.828(2)	38.091(8)	22.738(2)
c (Å)	21.963(3)	12.609(3)	14.8160(18)
α (deg)	88.088(9)	90.00	90.00
β (deg)	75.632(7)	95.486(5)	100.020(3)
γ (deg)	76.611(7)	90.00	90.00
V (Å ³)	3799.9(9)	3379.0(13)	3932.5(7)
ρ_{calc} (g/cm ³)	1.207	1.362	1.241
Z	4	4	4
Crystal F_{000}	1464.0	1472.0	1568
θ range for data collection	3.1-27.5°	3.1-27.4°	3.0-27.5°
Goodness-of-fit on F^2	0.976	0.990	0.995
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0783 wR2 = 0.2147	R1 = 0.0572 wR2 = 0.1372	R1 = 0.0539 wR2 = 0.1515

Conformational Searching of **1a**

Conformers of **1a** produced by rotation of C₁-C₂ (C_{1'}-C_{2'}) and C₃-C₄ (C_{3'}-C_{4'}) were considered in this searching. In this way, 36 initial conformers were generated by the gentor tool, a module of the molclus program,¹ which were subjected to pre-optimize by the semi-empirical PM7 method inserted in the MOPAC2016 program.² After removing duplicated conformers using the default energy (0.25 kcal/mol) and geometry threshold (0.1 Å) for distinguishing different structures set in the isostat tool, a module of the molclus program as well, 23 conformers were remained, which were then optimized at the B3LYP/6-31G(d) level.³⁻⁵ Finally, 21 rotamers were located and their structures associating with relative energies (kcal/mol) were presented in Fig.S13.

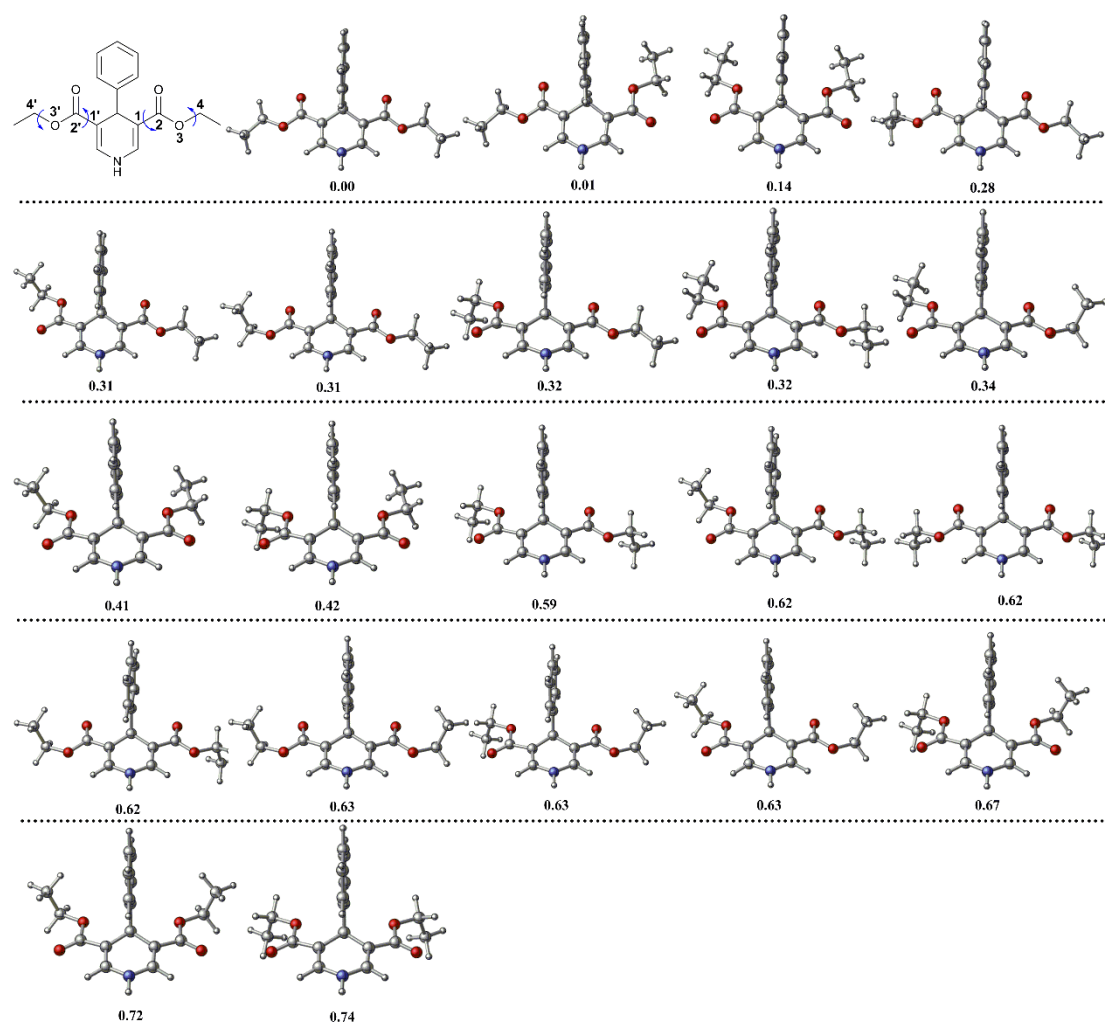


Figure S13 Rotamers of **1a** and their relative energy (kcal/mol).

[1]. Lu, T. Molclus Program 2016, Beijing Keinsci Research Center for Natural Science, China.
<http://www.keinsci.com/research/molclus.html>

- [2]. Stewart, J.J.P. MOPAC2016, Stewart Computational Chemistry, Colorado Springs, CO, USA.
<http://openmopac.net/MOPAC2016.html>
- [3]. Becke A D. Density-functional thermochemistry. III. The role of exact exchange. Journal of chemical physics, 1993, 98(7): 5648-5652.
- [4]. Stephens P J, Devlin F J, Chabalowski C F N, et al. Ab initio calculation of vibrational absorption and circular dichroism spectra using density functional force fields. The Journal of Physical Chemistry, 1994, 98(45): 11623-11627.
- [5]. Hehre W J, Ditchfield R, Pople J A. Self-consistent molecular orbital methods. XII. Further extensions of Gaussian-type basis sets for use in molecular orbital studies of organic molecules. The Journal of Chemical Physics, 1972, 56(5): 2257-2261.

Locating the MECP of 1a*, IM1-4 and IM42-2

Location of MECP was performed via Gaussian 09 together with sobMECP program, which is a modified version of Harvey's MECP program. The location of MECP between singlet excited state (S1) and triplet state (T1) of **1e** was carried out at the B3LYP/6-31G* theoretical level, while location of other MECPs was carried out at the M062X/de2-SV theoretical level. All triplet states were calculated using an unrestricted formalism. The default thresholds were used in these calculations. Initial input Cartesian coordinates used to locate the MECP were presented at the end of this file. The resulting curves of relative energies against optimized steps were presented in **Figure S14**, along with the presence of absolute energy values (E_{abs} , Hartree).

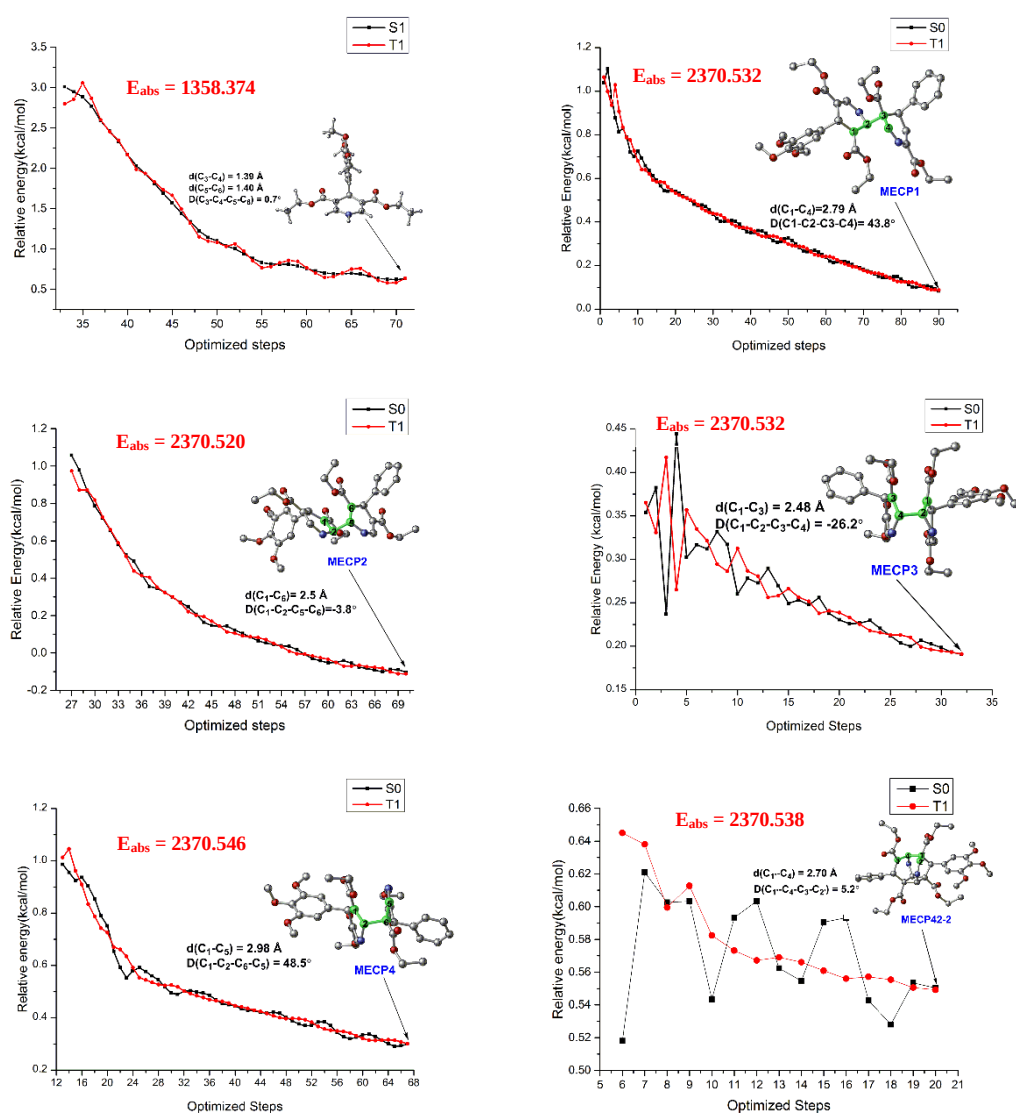


Figure S14 MECP locating curves for **1a***, **IM1-4** and **IM42-2** and the selected absolute energy values used to calculated relative energies.

Relaxed-scanning of ring closure step in every pathways

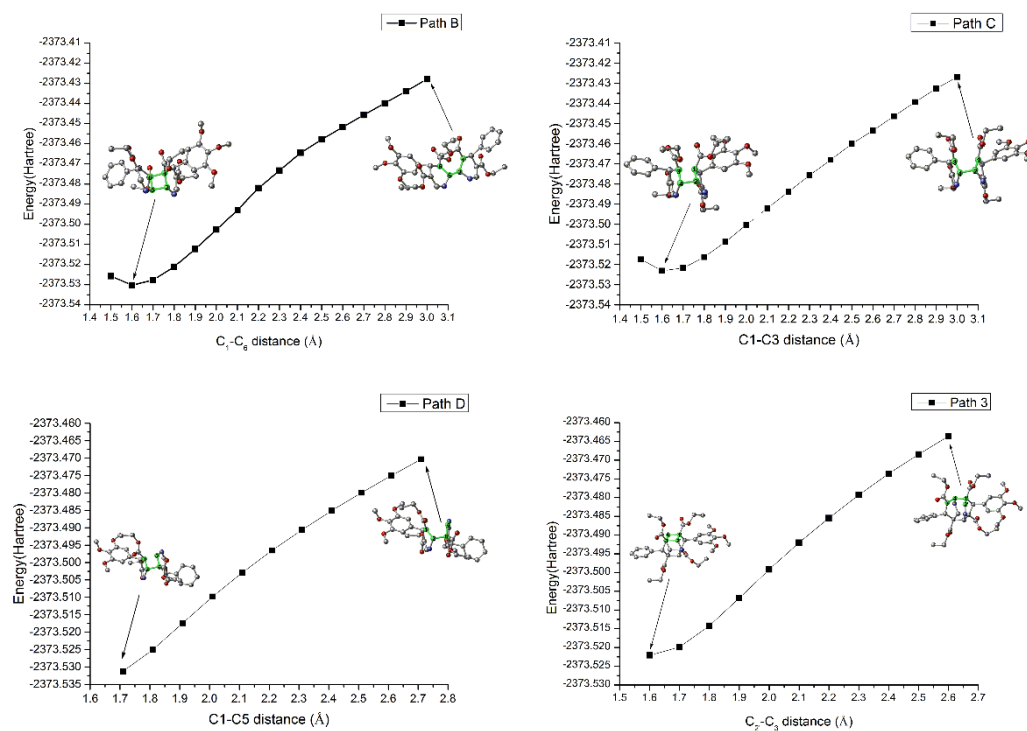
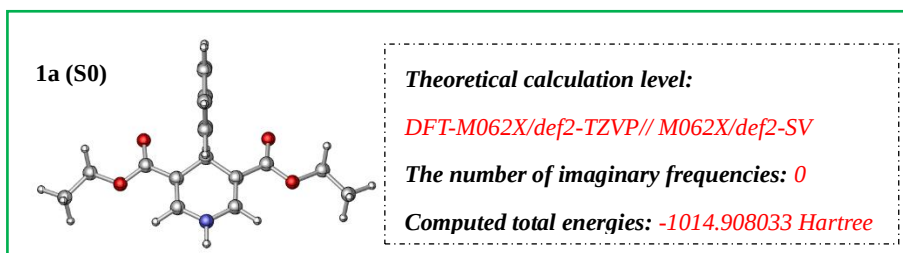


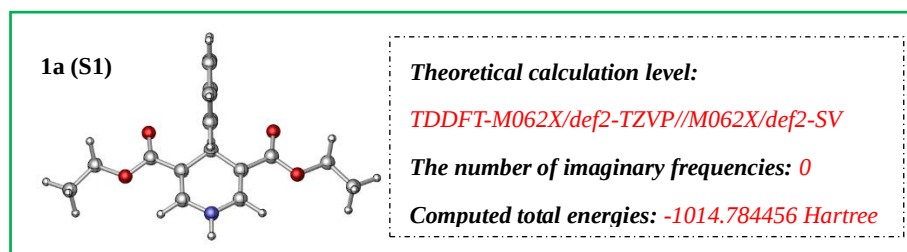
Figure S15 Relaxed scanning curves for the ring closure step of each paths

Cartesian coordinates, the number of imaginary frequencies, computed total energies of every stationary points



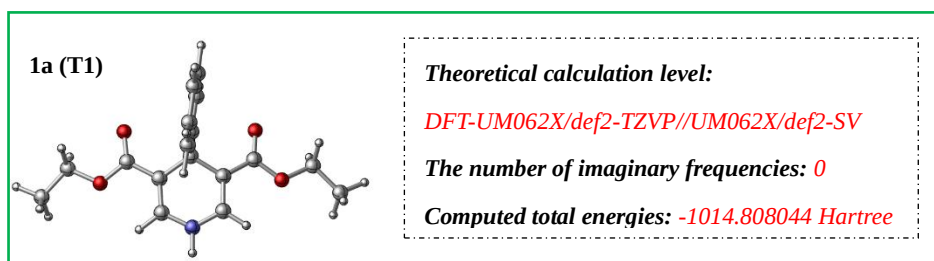
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C	-0.09751400	-0.47505400	0.00000000
C	-0.83776100	0.00208200	-1.23507400
C	-1.79037100	0.96038200	-1.18689700
C	-1.79037100	0.96038200	1.18689700
H	-2.27551700	1.33507300	-2.08912400
H	-2.27551700	1.33507300	2.08912400
C	-0.44489700	-0.60753800	2.51704400
O	0.37422000	-1.49321200	2.61237200
O	-1.08332600	-0.09590000	3.57781500
C	-0.75002800	-0.64771500	4.85256500
C	-1.58874400	0.05680500	5.89457100
H	0.32817700	-0.50637400	5.03076200
H	-0.94557200	-1.73186300	4.83410000
H	-1.35759400	-0.34333500	6.89390800
H	-1.38041900	1.13840100	5.89376200
H	-2.66145300	-0.09601000	5.69642800
C	-0.44489700	-0.60753800	-2.51704400
O	0.37422000	-1.49321200	-2.61237200
O	-1.08332600	-0.09590000	-3.57781500
C	-0.75002800	-0.64771500	-4.85256500
C	-1.58874400	0.05680500	-5.89457100
H	-0.94557200	-1.73186300	-4.83410000
H	0.32817700	-0.50637400	-5.03076200
H	-1.35759400	-0.34333500	-6.89390800
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H	-1.38041900	1.13840100	-5.89376200
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H	-2.95349400	2.19300500	0.00000000



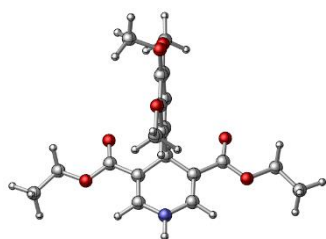
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C	-1.20248200	-1.81888100	0.97550100
C	1.20209200	-1.81889900	0.97554900
H	-2.08881600	-2.26181500	1.42382100
H	2.08838700	-2.26196700	1.42381800
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O	3.57093000	-1.01899100	-0.10522000
C	4.84061000	-0.65835600	-0.64310600
C	5.89448500	-1.48004800	0.06470100
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H	-6.89320800	-1.22441400	-0.32325700
H	-5.72047200	-2.55529300	-0.09803200
H	-5.87855300	-1.28027700	1.14772900
N	-0.00021300	-2.24163600	1.43618900
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C	-0.00001000	1.49681300	1.41108200
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H	-2.95349400	2.19300500	0.00000000



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C	-1.26111100	-0.81346100	0.02440900
C	-1.21289600	-1.72924100	1.05251900
C	1.17403700	-1.55075900	1.29105800
H	-2.09907100	-2.22318500	1.44740400
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C	2.46510400	-0.50727200	-0.65121200
O	2.55825200	0.19230000	-1.64641100
O	3.52216400	-1.11914500	-0.08396400
C	4.78417800	-0.92314100	-0.71941200

C	5.81802000	-1.71353600	0.05062000
H	5.01672200	0.15441600	-0.72810000
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H	6.80985300	-1.58187300	-0.40909000
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O	-2.59737400	0.39557500	-1.50684100
O	-3.58476400	-1.07746200	-0.13126400
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H	-5.04040100	0.32087400	-0.57695100
H	-6.88844500	-1.38695500	-0.47760000
H	-5.68353500	-2.67785400	-0.20000100
H	-5.93250500	-1.40526700	1.03345700
N	-0.03209700	-2.04165000	1.64776100
H	0.00962200	-0.09699500	-1.54447500
C	0.01362000	1.34931300	0.02187600
C	0.24405500	2.37600900	-0.89695600
C	-0.15147400	1.66497900	1.37625800
C	0.29915800	3.70351900	-0.46976900
H	0.38230300	2.13125300	-1.95286900
C	-0.08960400	2.99057600	1.80322100
H	-0.33864500	0.86608100	2.10187600
C	0.13445500	4.01531000	0.88035300
H	0.47038600	4.49928200	-1.19919500
H	-0.22113800	3.22475000	2.86263800
H	0.17788000	5.05487600	1.21426500
H	-0.06389800	-2.68057100	2.44016300



1e (S0)

Theoretical calculation level:

DFT-M062X/def2-TZVP//M062X/def2-SV

The number of imaginary frequencies: 0

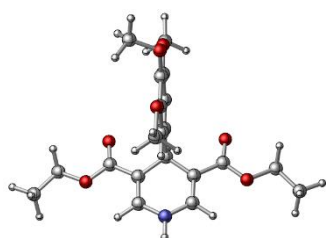
Computed total energies: -1358.479822 Hartree

C	1.85640800	-1.28321200	-0.02530000
C	0.47077100	-1.06178300	-0.60094600

s20

C	-0.46141300	-2.13472700	-0.07155700
C	-0.14906300	-2.90449300	0.99514300
C	2.07908100	-2.08618300	1.03946300
H	-0.85031900	-3.63245000	1.40493400
H	3.06992100	-2.19317300	1.48271400
C	2.96349300	-0.55020100	-0.66317100
O	2.82714600	0.14644500	-1.64306600
O	4.14702200	-0.72955700	-0.06215000
C	5.26558900	-0.04775500	-0.63218600
C	6.48851900	-0.40358000	0.18256800
H	5.06633100	1.03600000	-0.61974100
H	5.37159100	-0.35519100	-1.68501800
H	7.37392600	0.10319800	-0.23159400
H	6.36229200	-0.08764600	1.23027900
H	6.66531400	-1.49062700	0.16070400
C	-1.75687700	-2.28310100	-0.75710800
O	-2.06042100	-1.66536200	-1.75243200
O	-2.57411300	-3.17394100	-0.18067200
C	-3.84054200	-3.38371100	-0.80794700
C	-4.60016200	-4.40098600	0.01302300
H	-3.67420800	-3.73271500	-1.84002200
H	-4.37508700	-2.42179300	-0.86340300
H	-5.58556000	-4.58708300	-0.44168300
H	-4.04897300	-5.35369700	0.05743100
H	-4.75248700	-4.03308000	1.04014200
N	1.07842700	-2.83570600	1.60099200
H	0.51804600	-1.12966800	-1.69955700
C	-0.04966300	0.33414100	-0.26491400
C	-0.35160200	1.23870900	-1.28146400
C	-0.22210100	0.68813500	1.07578500
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C	-0.70281100	1.96046400	1.40423000
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O	-1.42595600	4.13654800	0.70303900
O	-1.16422100	3.45880800	-1.86443700

C	-0.66158000	1.51066100	3.72763300
H	-1.28473000	0.60173600	3.65656700
H	0.40329600	1.21961000	3.75232100
H	-0.91144700	2.05130900	4.65024500
C	-2.83329300	4.22912600	0.82220100
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H	-1.33989600	4.03581400	-3.78888600



1e (S1)

Theoretical calculation level:

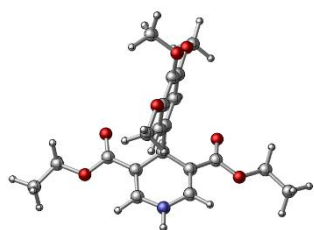
TDDFT-M062X/def2-TZVP//M062X/def2-SV

The number of imaginary frequencies: 0

Computed total energies: -1358.355444 Hartree

C	1.81386100	-1.37025800	-0.06645200
C	0.45706400	-1.17182100	-0.62024100
C	-0.56402600	-2.11181300	-0.10801600
C	-0.30526200	-2.86271700	1.05049200
C	1.99191500	-2.14993100	1.08773100
H	-1.04740000	-3.48652000	1.54346700
H	2.94181300	-2.24949800	1.60790400
C	2.90978300	-0.65910600	-0.70505500
O	2.80340000	0.03621000	-1.70051400
O	4.08787100	-0.85641600	-0.07942300
C	5.22715300	-0.21879100	-0.65181000
C	6.43577300	-0.59779600	0.17449900
H	5.06294300	0.87138300	-0.65853400
H	5.33079700	-0.54347300	-1.70037500
H	7.33834700	-0.12351900	-0.24130300
H	6.31306500	-0.26317700	1.21689800
H	6.58048500	-1.68983800	0.16989800
C	-1.85120700	-2.13828100	-0.78386800
O	-2.12469300	-1.50366100	-1.78805100
O	-2.73418500	-2.96108900	-0.18174400
C	-4.01452200	-3.07841600	-0.79685100

C	-4.84368200	-4.03032400	0.03585200
H	-3.88456800	-3.44606000	-1.82835000
H	-4.47740700	-2.07990600	-0.85866100
H	-5.84007000	-4.15484000	-0.41604600
H	-4.35874000	-5.01790100	0.09271000
H	-4.96919500	-3.64069500	1.05865400
N	0.93929800	-2.84252900	1.58669700
H	0.48297400	-1.18874200	-1.72428600
C	-0.00644300	0.27333600	-0.25619300
C	-0.28330700	1.17834300	-1.27737800
C	-0.14726500	0.63197300	1.08930400
C	-0.71266100	2.47324400	-0.94803900
H	-0.17353000	0.86882900	-2.31557300
C	-0.57618500	1.92029300	1.41308400
H	0.06741500	-0.09844400	1.87194000
C	-0.83853800	2.85500800	0.39358400
H	1.09892100	-3.40035400	2.42484000
O	-0.76708200	2.36838600	2.67276400
O	-1.23114000	4.12109500	0.71227600
O	-1.02382200	3.42188700	-1.85746100
C	-0.51956500	1.48240100	3.73885500
H	-1.17369200	0.59432700	3.68221700
H	0.53549500	1.15637500	3.75077900
H	-0.73901000	2.03640500	4.66121800
C	-2.63248500	4.25938500	0.85527600
H	-3.14796000	4.02268900	-0.09244900
H	-3.01169200	3.59909600	1.65514300
H	-2.83010900	5.30728300	1.12417700
C	-0.89809800	3.10063100	-3.22353500
H	0.14450200	2.84076500	-3.47763800
H	-1.56029400	2.26192600	-3.50125300
H	-1.19480500	3.99812700	-3.78246300



1e

Theoretical calculation level:

DFT-UM062X/def2-TZVP//UM062X/def2-SV

The number of imaginary frequencies: 0

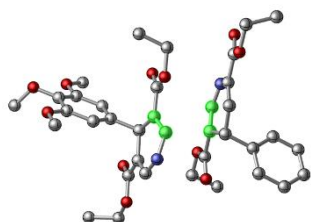
Computed total energies: -1358.380071 Hartree

C	1.00880900	-1.84827800	0.16100500
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s23

C	-0.10896300	-1.15171100	-0.54217100
C	-1.45360900	-1.66976100	-0.12324300
C	-1.59281100	-2.43769400	1.00725600
C	0.75820600	-2.38578500	1.50544600
H	-2.55723200	-2.80744800	1.35240100
H	1.53938200	-2.65526100	2.21023100
C	2.30546600	-1.90489200	-0.47810400
O	2.56074300	-1.41541500	-1.56643200
O	3.22449800	-2.54034900	0.27253600
C	4.53644700	-2.64048900	-0.27919600
C	5.40145400	-3.38048600	0.71602300
H	4.91871400	-1.62625900	-0.47965500
H	4.47967800	-3.17036200	-1.24432700
H	6.42347100	-3.48434800	0.31990900
H	5.44933200	-2.83248500	1.67045200
H	4.99577600	-4.38669500	0.90723100
C	-2.60070200	-1.26777400	-0.93209300
O	-2.52517100	-0.56665000	-1.92032300
O	-3.76871200	-1.75398600	-0.47906300
C	-4.93513400	-1.41638300	-1.22869900
C	-6.12221300	-2.07302400	-0.56045800
H	-4.80698400	-1.76443900	-2.26655200
H	-5.03844500	-0.31951600	-1.25664600
H	-7.04296200	-1.83478300	-1.11536100
H	-5.99890600	-3.16747600	-0.53988700
H	-6.23371600	-1.71135500	0.47410600
N	-0.51633900	-2.74901800	1.77940800
H	0.02105600	-1.27000500	-1.62894600
C	0.06496300	0.34631700	-0.23261600
C	0.69373800	1.16805300	-1.16827700
C	-0.33926800	0.84782100	1.00798500
C	0.91517900	2.51662500	-0.86285300
H	1.01257000	0.74502600	-2.12023700
C	-0.11715300	2.19603800	1.31294800
H	-0.84180800	0.18803100	1.71748600
C	0.53067000	3.02879900	0.38628400
H	-0.68971300	-3.26269300	2.64124400
O	-0.48256300	2.78572400	2.47055200
O	0.77243300	4.33323800	0.69447000

O	1.49801600	3.39991300	-1.69996000
C	-1.12329500	1.99460900	3.44408800
H	-2.07792200	1.58904500	3.06521800
H	-0.47678800	1.16038200	3.76863500
H	-1.32274700	2.65450200	4.29882300
C	-0.26278400	5.21369000	0.29663500
H	-0.40769500	5.17843300	-0.79736200
H	-1.21023100	4.95665400	0.80252200
H	0.04304600	6.22802300	0.59091900
C	1.94218800	2.93326200	-2.95358300
H	2.70068900	2.13944000	-2.83683900
H	1.10227800	2.54817000	-3.55791100
H	2.39244100	3.79510000	-3.46382000



TS23

Theoretical calculation level:

DFT-UM062X/def2-TZVP//UM062X/def2-SV

The number of imaginary frequencies: 1

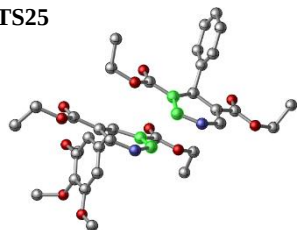
Computed total energies: -2373.285408 Hartree

C	3.29777100	0.68819800	-0.87288500
C	2.17016700	0.85608400	0.13878400
C	3.82949100	-0.72283700	-0.82501600
C	2.13507500	0.03375200	1.27298100
C	3.63957700	-1.51142000	0.25431500
H	4.45323300	-1.08501700	-1.64286000
N	2.86150700	-1.10838000	1.32429000
H	1.52264600	0.27076000	2.14167800
C	1.54858200	2.18763300	0.20685200
O	1.66962300	3.03293300	-0.65312400
O	0.79911000	2.36310700	1.30873800
C	0.14569200	3.62432900	1.46838000
C	1.08043900	4.64667000	2.08662500
H	-0.71581300	3.41471700	2.11888100
H	-0.22372900	3.96189000	0.48843300
H	0.54302100	5.59323800	2.25722200
H	1.46533800	4.28351000	3.05297000
H	1.93114800	4.84405600	1.41524600
H	2.91082100	0.90285900	-1.88389900
C	-1.54488500	0.44346200	0.29429900

C	-0.37552700	-0.35996700	-0.19492500
C	-1.69030900	1.73895800	-0.46744600
C	0.45901800	0.11358800	-1.27792200
C	-0.97900300	1.99752300	-1.59974200
N	-0.00434200	1.15288600	-2.04116100
H	1.13386400	-0.58363100	-1.77397900
H	-1.13836500	2.90196000	-2.18666900
C	-0.10610400	-1.64469000	0.43451800
O	-0.59173800	-2.01927100	1.48637200
O	0.73370200	-2.40097900	-0.29980000
C	1.03459500	-3.70929000	0.18195200
C	-0.10175100	-4.67854100	-0.08773400
H	1.93947400	-4.00490100	-0.37003600
H	1.27056100	-3.65621300	1.25629700
H	0.18934900	-5.69397700	0.22552800
H	-0.33897700	-4.69869400	-1.16362000
H	-1.00147900	-4.38156100	0.47244100
H	-1.40286900	0.66216200	1.36911500
H	0.52293700	1.41641500	-2.86718000
H	2.81098200	-1.72970400	2.12649300
C	-2.63961200	2.71334100	0.06872500
O	-3.23099100	2.57472500	1.11974500
O	-2.76782700	3.81341800	-0.69496500
C	-3.64011500	4.84056400	-0.22017300
C	-5.09347500	4.51752800	-0.51247200
H	-3.32029200	5.74783000	-0.75122100
H	-3.47374000	4.97932000	0.85893600
H	-5.73444700	5.35845200	-0.20224000
H	-5.23952300	4.34725400	-1.59124700
H	-5.40509100	3.61662800	0.03819300
C	4.23289000	-2.86340500	0.44051100
O	4.09835700	-3.48812800	1.46662400
O	4.89291000	-3.29509800	-0.62331200
C	5.50834900	-4.58985700	-0.53864500
C	6.82601500	-4.52632400	0.20770700
H	5.65189900	-4.89372800	-1.58375900
H	4.80311800	-5.28178300	-0.05451500
H	6.66608200	-4.23512600	1.25737800
H	7.30821400	-5.51664800	0.19025300

H	7.50375200	-3.79996300	-0.26811000
C	4.42970100	1.68513900	-0.62839900
C	4.77283900	2.62507900	-1.60340200
C	5.13741500	1.67397300	0.57996100
C	5.80374000	3.53906200	-1.38039900
H	4.21696100	2.64662800	-2.54527600
C	6.16415200	2.58975600	0.80919500
H	4.88222100	0.93814300	1.35027700
C	6.50091100	3.52530000	-0.17175800
H	6.05902500	4.26878700	-2.15303700
H	6.70729800	2.57143400	1.75746900
H	7.30567700	4.24289100	0.00607000
C	-2.82432700	-0.39118200	0.16184900
C	-3.59433800	-0.69458600	1.28134800
C	-3.20035100	-0.83970600	-1.10791100
C	-4.76378500	-1.45204100	1.13266400
H	-3.27940600	-0.32910400	2.25851200
C	-4.36471600	-1.59966500	-1.25970800
H	-2.58561900	-0.57517000	-1.97109700
C	-5.13941400	-1.92521500	-0.13365500
O	-4.82588300	-2.06801800	-2.43921300
O	-5.59247700	-1.78347100	2.14633200
O	-6.26270700	-2.68420400	-0.27625200
C	-4.06696300	-1.81099400	-3.59735800
H	-3.98539800	-0.72697200	-3.79118800
H	-3.05398800	-2.24282200	-3.51409700
H	-4.59841900	-2.28981400	-4.43052000
C	-5.28167000	-1.31598900	3.43834800
H	-4.31347000	-1.71591800	3.78727000
H	-5.25077300	-0.21267100	3.46760400
H	-6.08147100	-1.67519000	4.09962200
C	-7.43862800	-1.92186800	-0.47549500
H	-8.27257400	-2.63182200	-0.57441900
H	-7.62535900	-1.25613900	0.38539200
H	-7.36228600	-1.31816900	-1.39720300

TS25



Theoretical calculation level:

DFT-UM062X/def2-TZVP//UM062X/def2-SV

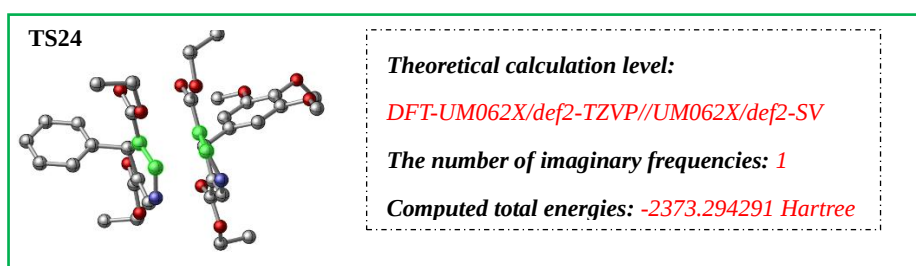
The number of imaginary frequencies: 1

Computed total energies: -2373.286483 Hartree

C	-3.05999700	0.14019800	0.21210000
C	-2.06317900	1.05609500	-0.43884300
C	-3.77373400	-0.72216600	-0.79749800
C	-1.92127300	1.13974900	-1.87984700
C	-3.67169000	-0.49481300	-2.13054900
N	-2.84403500	0.46602600	-2.63960900
H	-1.51653400	2.05322100	-2.31673600
H	-4.24235600	-1.07061600	-2.85977800
C	-1.28665500	1.93667200	0.42596900
O	-1.22068200	1.82743900	1.63491300
O	-0.64835700	2.89669100	-0.26332300
C	0.13032100	3.83662600	0.47955900
C	-0.74503900	4.90640500	1.10495200
H	0.82220900	4.26744100	-0.25872100
H	0.71629700	3.29772000	1.24014800
H	-0.11616500	5.65054700	1.61927100
H	-1.33279400	5.42264000	0.32898400
H	-1.43382500	4.46162400	1.83977400
H	-2.53202300	-0.49933300	0.94666200
C	1.52862500	0.57345600	-0.13211500
C	0.41497900	-0.16318100	-0.84296600
C	2.05451100	1.70357200	-0.99090900
C	0.04875300	0.11502000	-2.17300500
C	1.71001200	1.83838300	-2.29434000
N	0.80113000	1.02072800	-2.89880200
H	-0.48445400	-0.63676300	-2.75480900
H	2.14230400	2.61905900	-2.92165700
C	-0.22575700	-1.25480700	-0.12239600
O	-0.06683600	-1.49047400	1.06043300
O	-1.03521200	-1.99560000	-0.90578200
C	-1.66713700	-3.13043300	-0.31441700

C	-0.70701000	-4.29967200	-0.19422100
H	-2.50011100	-3.36977000	-0.99193000
H	-2.07887500	-2.84785800	0.66714300
H	-1.23578200	-5.17990700	0.20536300
H	-0.29337300	-4.55920700	-1.18208200
H	0.12167800	-4.04906100	0.48606700
H	1.15706600	0.97448200	0.82956700
H	0.57424300	1.17396200	-3.87447100
H	-2.83834900	0.61260400	-3.64410500
C	2.98200500	2.64289400	-0.35350000
O	3.28907300	2.59410100	0.81846100
O	3.43984600	3.59661500	-1.18341200
C	4.34628700	4.55775700	-0.63774100
C	5.75713000	4.00608800	-0.55730500
H	3.98344400	4.86752400	0.35386400
H	4.29243000	5.41523100	-1.32267700
H	6.44571700	4.78602900	-0.19452600
H	5.79721900	3.15309700	0.13769700
H	6.09770600	3.67445900	-1.55132700
C	-4.61018000	-1.80351900	-0.26481800
O	-4.70408100	-2.05692500	0.91651400
O	-5.23756400	-2.51362600	-1.21541200
C	-6.06522500	-3.59670100	-0.78125500
C	-7.42785700	-3.10725400	-0.32884500
H	-5.54836600	-4.13581000	0.02655900
H	-6.14758200	-4.25522800	-1.65677100
H	-8.06298000	-3.96622300	-0.05876800
H	-7.33055100	-2.45428000	0.55234400
H	-7.92404000	-2.54677700	-1.13723200
C	-4.07645900	0.97517100	0.99989500
C	-4.20422500	0.84807000	2.38378000
C	-4.88725900	1.89092100	0.32109200
C	-5.13182000	1.62341800	3.08083300
H	-3.56957200	0.13584300	2.91729200
C	-5.81264600	2.67031400	1.01493900
H	-4.79342300	1.99142100	-0.76602700
C	-5.93737000	2.53722100	2.39929600
H	-5.22491900	1.51369200	4.16432600
H	-6.43870700	3.38295300	0.47219600

H	-6.66239900	3.14453400	2.94674700
C	2.66177100	-0.39860900	0.20515200
C	3.05037500	-0.62302500	1.52052100
C	3.30633500	-1.07431000	-0.83994400
C	4.08378300	-1.52105400	1.79905900
H	2.56169300	-0.10797600	2.34977600
C	4.34440400	-1.96972400	-0.57018900
H	2.99138300	-0.87950600	-1.86779200
C	4.72814500	-2.20662400	0.76479500
O	5.03892800	-2.64670400	-1.50954400
O	5.73367000	-3.08898300	1.03159800
O	4.48135000	-1.71185200	3.09104300
C	4.16537800	-2.98494500	3.63040300
H	4.49879000	-2.97815700	4.67779000
H	3.07466700	-3.15664500	3.59713000
H	4.68369200	-3.78765800	3.08148800
C	6.98774500	-2.46913700	1.25947200
H	7.30567000	-1.89927200	0.36838500
H	6.93695200	-1.79438600	2.13130800
H	7.71381800	-3.27067000	1.45678600
C	4.69012500	-2.44846700	-2.85935600
H	3.64316600	-2.74400200	-3.04943100
H	4.82884500	-1.39410200	-3.15740600
H	5.36041400	-3.08513900	-3.45198700

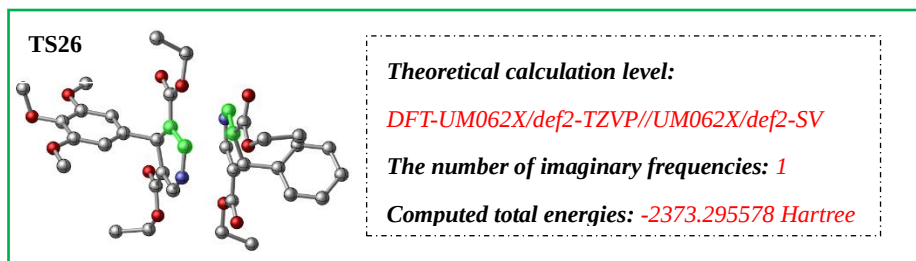


C	-2.45375500	0.35200000	0.25842300
C	-1.94118600	1.58466600	-0.45104100
C	-2.63536500	-0.78708000	-0.70845500
C	-1.97115400	1.70247400	-1.80138100
C	-2.44384500	-0.61798300	-2.10356000
N	-2.30156000	0.64994800	-2.60671600
H	-1.68031300	2.62490400	-2.30632400
H	-2.80779300	-1.37057900	-2.80144200

C	-1.43274400	2.67292400	0.39621600
O	-1.25860800	2.55440100	1.58986200
O	-1.16295900	3.80043700	-0.27616600
C	-0.64776600	4.89819500	0.48248500
C	-1.74477700	5.61080800	1.25186600
H	-0.19852800	5.56624500	-0.26537800
H	0.14332700	4.52337000	1.14818500
H	-1.32431100	6.48630100	1.77245000
H	-2.53316700	5.95953500	0.56555700
H	-2.19177200	4.93931500	2.00049800
H	-1.73432000	0.04731900	1.04302900
C	0.89041400	0.04749400	-0.37259200
C	1.07278700	1.02617000	-1.50798600
C	0.09706300	-1.15734800	-0.80503700
C	0.81754100	0.67544700	-2.79555100
C	-0.27189800	-1.36646500	-2.16912900
N	0.25224000	-0.52599400	-3.11747800
H	1.02997600	1.34459700	-3.62991900
H	-0.56864300	-2.35930100	-2.50659600
C	1.54671300	2.37092600	-1.16985500
O	1.72567500	2.75926600	-0.03445200
O	1.74559000	3.15078100	-2.24597300
C	2.27587200	4.45777100	-2.01946000
C	3.78314300	4.41558800	-1.85154800
H	1.98880700	5.03840000	-2.90709700
H	1.79191400	4.89279100	-1.13328200
H	4.17840700	5.43764200	-1.73700500
H	4.25625800	3.95449100	-2.73329900
H	4.05438500	3.83415900	-0.95614500
H	0.37283900	0.55012100	0.46539400
H	0.09903800	-0.74386800	-4.09693100
H	-2.29062700	0.78024700	-3.61226800
C	-3.08954000	-2.06495700	-0.18052200
O	-3.21289300	-2.31177500	1.00369700
O	-3.36864300	-2.96086300	-1.14824900
C	-3.91541500	-4.21329600	-0.73806900
C	-5.41520500	-4.10883800	-0.53079500
H	-3.41396200	-4.54025300	0.18390300
H	-3.67005500	-4.91357300	-1.54914500

H	-5.82979900	-5.09419100	-0.26362100
H	-5.63972200	-3.40296100	0.28462400
H	-5.90857400	-3.75843500	-1.45152500
C	-0.14710800	-2.16030300	0.22364000
O	-0.01526300	-1.94679000	1.41361300
O	-0.50050200	-3.36140500	-0.27188900
C	-0.64914700	-4.42436400	0.67250700
C	0.70044600	-4.95050900	1.12769900
H	-1.21095000	-5.20033900	0.13420700
H	-1.25371000	-4.06211300	1.51797500
H	0.55945800	-5.80822800	1.80489500
H	1.29456600	-5.28300000	0.26087500
H	1.25843200	-4.16794000	1.66453000
C	-3.76680600	0.68248900	0.97117800
C	-3.85995500	0.65537900	2.36363800
C	-4.89638700	1.02883200	0.22120200
C	-5.06344600	0.96613900	2.99906900
H	-2.97809000	0.38820700	2.95215000
C	-6.10146400	1.33711200	0.85144800
H	-4.82711100	1.05703900	-0.87199500
C	-6.18800300	1.30588000	2.24525500
H	-5.12361600	0.94065500	4.09017200
H	-6.97644000	1.60387500	0.25311700
H	-7.13069600	1.54613700	2.74323000
C	2.25794800	-0.39295400	0.16271300
C	2.72753500	0.11041000	1.37399000
C	3.02930800	-1.28774200	-0.58481300
C	3.98635500	-0.28230900	1.84630700
H	2.11023800	0.81804500	1.92684100
C	4.28477000	-1.68673100	-0.11276800
H	2.64539500	-1.66240600	-1.53597000
C	4.75773100	-1.19994400	1.11697100
O	4.54182900	0.16128200	2.99466100
O	5.96943700	-1.60793900	1.58943700
O	5.11012800	-2.53737200	-0.75973400
C	4.66700800	-3.09515500	-1.97423300
H	5.46564000	-3.76550000	-2.31886500
H	3.73847100	-3.67592500	-1.83052600
H	4.49303800	-2.31428000	-2.73544200

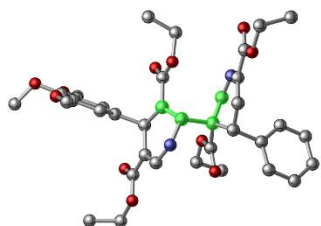
C	7.03126800	-0.73360900	1.25471900
H	7.14143300	-0.65357100	0.15855300
H	6.86177000	0.27008500	1.68220300
H	7.95035300	-1.16037400	1.68188200
C	3.82165000	1.09969700	3.76054200
H	3.61654300	2.01626500	3.17998500
H	2.86692800	0.67576100	4.11807900
H	4.45437200	1.34857100	4.62289900



C	-3.05999700	0.14019800	0.21210000
C	-2.06317900	1.05609500	-0.43884300
C	-3.77373400	-0.72216600	-0.79749800
C	-1.92127300	1.13974900	-1.87984700
C	-3.67169000	-0.49481300	-2.13054900
N	-2.84403500	0.46602600	-2.63960900
H	-1.51653400	2.05322100	-2.31673600
H	-4.24235600	-1.07061600	-2.85977800
C	-1.28665500	1.93667200	0.42596900
O	-1.22068200	1.82743900	1.63491300
O	-0.64835700	2.89669100	-0.26332300
C	0.13032100	3.83662600	0.47955900
C	-0.74503900	4.90640500	1.10495200
H	0.82220900	4.26744100	-0.25872100
H	0.71629700	3.29772000	1.24014800
H	-0.11616500	5.65054700	1.61927100
H	-1.33279400	5.42264000	0.32898400
H	-1.43382500	4.46162400	1.83977400
H	-2.53202300	-0.49933300	0.94666200
C	1.52862500	0.57345600	-0.13211500
C	0.41497900	-0.16318100	-0.84296600
C	2.05451100	1.70357200	-0.99090900
C	0.04875300	0.11502000	-2.17300500
C	1.71001200	1.83838300	-2.29434000

N	0.80113000	1.02072800	-2.89880200
H	-0.48445400	-0.63676300	-2.75480900
H	2.14230400	2.61905900	-2.92165700
C	-0.22575700	-1.25480700	-0.12239600
O	-0.06683600	-1.49047400	1.06043300
O	-1.03521200	-1.99560000	-0.90578200
C	-1.66713700	-3.13043300	-0.31441700
C	-0.70701000	-4.29967200	-0.19422100
H	-2.50011100	-3.36977000	-0.99193000
H	-2.07887500	-2.84785800	0.66714300
H	-1.23578200	-5.17990700	0.20536300
H	-0.29337300	-4.55920700	-1.18208200
H	0.12167800	-4.04906100	0.48606700
H	1.15706600	0.97448200	0.82956700
H	0.57424300	1.17396200	-3.87447100
H	-2.83834900	0.61260400	-3.64410500
C	2.98200500	2.64289400	-0.35350000
O	3.28907300	2.59410100	0.81846100
O	3.43984600	3.59661500	-1.18341200
C	4.34628700	4.55775700	-0.63774100
C	5.75713000	4.00608800	-0.55730500
H	3.98344400	4.86752400	0.35386400
H	4.29243000	5.41523100	-1.32267700
H	6.44571700	4.78602900	-0.19452600
H	5.79721900	3.15309700	0.13769700
H	6.09770600	3.67445900	-1.55132700
C	-4.61018000	-1.80351900	-0.26481800
O	-4.70408100	-2.05692500	0.91651400
O	-5.23756400	-2.51362600	-1.21541200
C	-6.06522500	-3.59670100	-0.78125500
C	-7.42785700	-3.10725400	-0.32884500
H	-5.54836600	-4.13581000	0.02655900
H	-6.14758200	-4.25522800	-1.65677100
H	-8.06298000	-3.96622300	-0.05876800
H	-7.33055100	-2.45428000	0.55234400
H	-7.92404000	-2.54677700	-1.13723200
C	-4.07645900	0.97517100	0.99989500
C	-4.20422500	0.84807000	2.38378000
C	-4.88725900	1.89092100	0.32109200

C	-5.13182000	1.62341800	3.08083300
H	-3.56957200	0.13584300	2.91729200
C	-5.81264600	2.67031400	1.01493900
H	-4.79342300	1.99142100	-0.76602700
C	-5.93737000	2.53722100	2.39929600
H	-5.22491900	1.51369200	4.16432600
H	-6.43870700	3.38295300	0.47219600
H	-6.66239900	3.14453400	2.94674700
C	2.66177100	-0.39860900	0.20515200
C	3.05037500	-0.62302500	1.52052100
C	3.30633500	-1.07431000	-0.83994400
C	4.08378300	-1.52105400	1.79905900
H	2.56169300	-0.10797600	2.34977600
C	4.34440400	-1.96972400	-0.57018900
H	2.99138300	-0.87950600	-1.86779200
C	4.72814500	-2.20662400	0.76479500
O	5.03892800	-2.64670400	-1.50954400
O	5.73367000	-3.08898300	1.03159800
O	4.48135000	-1.71185200	3.09104300
C	4.16537800	-2.98494500	3.63040300
H	4.49879000	-2.97815700	4.67779000
H	3.07466700	-3.15664500	3.59713000
H	4.68369200	-3.78765800	3.08148800
C	6.98774500	-2.46913700	1.25947200
H	7.30567000	-1.89927200	0.36838500
H	6.93695200	-1.79438600	2.13130800
H	7.71381800	-3.27067000	1.45678600
C	4.69012500	-2.44846700	-2.85935600
H	3.64316600	-2.74400200	-3.04943100
H	4.82884500	-1.39410200	-3.15740600
H	5.36041400	-3.08513900	-3.45198700



IM1 (T1)

Theoretical calculation level:

DFT-UM062X/def2-TZVP//UM062X/def2-SV

The number of imaginary frequencies: 0

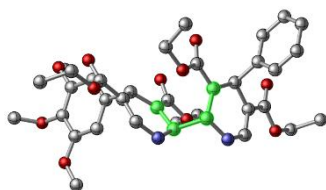
Computed total energies: -2373.300147 Hartree

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C	-1.95577300	0.72049500	-0.00463800

C	-3.79440900	-0.57105600	1.09515700
C	-2.30939300	-0.03459600	-1.24163300
C	-3.75543700	-1.44183100	0.05602200
H	-4.33422600	-0.83913500	2.00284800
N	-3.08892900	-1.14213600	-1.11074900
H	-1.81913300	0.13262300	-2.19771900
C	-1.42886900	2.11453700	-0.31312900
O	-1.58921800	3.06330000	0.40960100
O	-0.69929600	2.14930400	-1.42766300
C	-0.02671500	3.38147300	-1.72882000
C	-0.93692700	4.32558200	-2.48817300
H	0.84866500	3.08729900	-2.32479400
H	0.31645000	3.82670700	-0.78239400
H	-0.38394400	5.24043400	-2.75449200
H	-1.29775500	3.85266900	-3.41534100
H	-1.80350500	4.60829000	-1.86966900
H	-2.83853600	1.16153900	1.92805500
C	1.55924100	0.46893800	-0.30690200
C	0.36379000	-0.41392800	-0.09830400
C	1.56786100	1.61495000	0.67766800
C	-0.76415600	-0.03739200	0.80825600
C	0.72583500	1.64349500	1.74493800
N	-0.27899300	0.75082800	1.91774300
H	-1.23452100	-0.95387800	1.19339700
H	0.82696500	2.41323700	2.51333400
C	0.25100500	-1.60489500	-0.94602800
O	0.86656300	-1.75707200	-1.97900300
O	-0.60538700	-2.51215200	-0.45702000
C	-0.86262000	-3.66844100	-1.25954800
C	0.19607100	-4.73252200	-1.04165600
H	-1.85862000	-4.01372100	-0.94812900
H	-0.90502500	-3.36193400	-2.31633900
H	-0.05433800	-5.63467800	-1.62240800
H	0.25071600	-5.00656300	0.02410400
H	1.18202000	-4.36710100	-1.36869000
H	1.51653100	0.86255400	-1.34013700
H	-0.86083100	0.82840700	2.74265400
H	-3.18408600	-1.80412300	-1.87712800
C	2.54676200	2.67487700	0.44723200

O	3.26340000	2.73090700	-0.53076900
O	2.56075200	3.61685500	1.40823100
C	3.49593600	4.68634900	1.25980900
C	4.88742700	4.27070400	1.70007300
H	3.10318900	5.49391400	1.89307500
H	3.49458200	5.01938800	0.21116900
H	5.57387800	5.13078300	1.64260400
H	4.86862900	3.90833600	2.74051300
H	5.27298700	3.47044700	1.04950500
C	-4.42171900	-2.77024000	0.03930200
O	-4.34719100	-3.52175800	-0.90653400
O	-5.09115400	-3.03173700	1.15213100
C	-5.78770900	-4.28493700	1.22227600
C	-7.12125600	-4.21068800	0.50528400
H	-5.91855400	-4.46810500	2.29681600
H	-5.14458200	-5.06896700	0.79661200
H	-6.97469800	-4.03064500	-0.57099700
H	-7.66090400	-5.16303200	0.62896800
H	-7.73971700	-3.40136400	0.92450200
C	-4.25351500	1.79700500	0.48504400
C	-4.51163700	2.95608900	1.22590200
C	-5.00191300	1.56767800	-0.67770400
C	-5.48324200	3.86861200	0.81473500
H	-3.93106800	3.15173500	2.13156100
C	-5.96789500	2.48315200	-1.09695600
H	-4.84257500	0.65637000	-1.25856700
C	-6.21221800	3.63775800	-0.35321000
H	-5.66948100	4.76746000	1.40811700
H	-6.53816200	2.28601600	-2.00827700
H	-6.97145900	4.35273700	-0.67987300
C	2.84856600	-0.34853100	-0.19269700
C	3.77577200	-0.34263400	-1.23122100
C	3.07902500	-1.09589800	0.96565800
C	4.95284100	-1.09189100	-1.11520200
H	3.57497700	0.25864400	-2.11758600
C	4.25274600	-1.85022000	1.08384300
H	2.34254500	-1.07138100	1.77193200
C	5.18291100	-1.86656600	0.03185900
O	4.57737500	-2.59820800	2.16060400

O	5.92215600	-1.14077400	-2.05457400
O	6.31302200	-2.62216600	0.13153900
C	3.66456400	-2.65123500	3.23169200
H	3.51139400	-1.65314000	3.67859100
H	2.69055300	-3.05712800	2.90591600
H	4.10412600	-3.32150100	3.98227600
C	5.75299000	-0.37170300	-3.22238300
H	4.85506600	-0.68614200	-3.78259300
H	5.67527000	0.70403900	-2.98555900
H	6.64430100	-0.54521400	-3.84011500
C	7.41504800	-1.92284900	0.67907100
H	8.26257000	-2.62289300	0.70790200
H	7.67997800	-1.05440500	0.05085600
H	7.18977500	-1.58014400	1.70462400



IM2 (T1)

Theoretical calculation level:

DFT-UM062X/def2-TZVP//UM062X/def2-SV

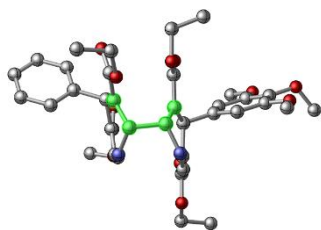
The number of imaginary frequencies: 0

Computed total energies: -2373.301070 Hartree

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C	-2.14071700	0.91668300	-0.33209300
C	-3.77525800	-0.91582700	-0.74340800
C	-1.65355100	0.82122500	-1.74094000
C	-3.43377000	-0.84959700	-2.05542600
N	-2.54643600	0.03670200	-2.55995700
H	-1.58952000	1.84352300	-2.14765700
H	-3.88392500	-1.53202000	-2.77985800
C	-1.47350200	1.85532100	0.57360800
O	-1.57219000	1.82286700	1.78099400
O	-0.72893300	2.75321800	-0.08693500
C	-0.03852600	3.74188100	0.68583900
C	-0.98229600	4.81979600	1.18500000
H	0.70771700	4.15635600	-0.00570100
H	0.48373400	3.24299800	1.51811300
H	-0.40696800	5.60052500	1.70761000
H	-1.51202400	5.28585100	0.33870500
H	-1.72059600	4.40126400	1.88552200
H	-2.83961900	-0.44498700	1.13978500

C	1.66506200	0.65954500	0.05902700
C	0.49155900	-0.05916600	-0.54072500
C	2.09563100	1.82722400	-0.78898100
C	-0.12515800	0.26904700	-1.86127600
C	1.62514800	1.98866600	-2.05159600
N	0.69247400	1.18925000	-2.61613500
H	-0.23280800	-0.67003800	-2.42832400
H	2.00378600	2.79292900	-2.68636800
C	-0.10092900	-1.13853800	0.25341500
O	0.10703600	-1.30911700	1.43504700
O	-0.91100100	-1.91733500	-0.47726300
C	-1.52739900	-3.03269600	0.17666700
C	-0.54264000	-4.16772200	0.38632500
H	-2.34098600	-3.32976200	-0.49928900
H	-1.96197100	-2.69069200	1.12981000
H	-1.06415800	-5.03241200	0.82677500
H	-0.10585000	-4.47757400	-0.57661600
H	0.26689900	-3.86312400	1.06705800
H	1.37944000	1.00572600	1.07049800
H	0.41149100	1.38247100	-3.57037600
H	-2.36371800	0.01617800	-3.55632400
C	3.03953200	2.76421300	-0.19218900
O	3.46683500	2.66432100	0.93955100
O	3.37193300	3.78748400	-1.00337300
C	4.30851200	4.74196200	-0.50155400
C	5.73492700	4.24398400	-0.63949400
H	4.06634300	4.96271500	0.54863100
H	4.14150500	5.64532000	-1.10463400
H	6.43955600	5.02034300	-0.30039900
H	5.88766700	3.34210000	-0.02625200
H	5.95909300	4.00389900	-1.69126000
C	-4.65485200	-1.95556200	-0.22417100
O	-4.94169700	-2.07228000	0.94977200
O	-5.09319300	-2.81500000	-1.16438500
C	-5.95005200	-3.87320900	-0.73265200
C	-7.38504500	-3.40386400	-0.58538400
H	-5.56676800	-4.27746300	0.21604300
H	-5.86122500	-4.64334500	-1.51152500
H	-8.03181500	-4.25364500	-0.31353300

H	-7.46145300	-2.64005800	0.20395600
H	-7.75026000	-2.97683000	-1.53322300
C	-4.36018400	0.99780400	0.75505700
C	-4.76948900	0.98227700	2.08923400
C	-4.98824700	1.87089400	-0.13994100
C	-5.79223600	1.82679400	2.52442700
H	-4.28408900	0.29776200	2.78985100
C	-6.00803500	2.71879000	0.29162000
H	-4.67561200	1.88199000	-1.19025100
C	-6.41296300	2.69814800	1.62803500
H	-6.10567600	1.80433200	3.57137900
H	-6.48784300	3.39781400	-0.41776700
H	-7.21183100	3.36071900	1.97018600
C	2.81395000	-0.33673700	0.24542100
C	3.29481700	-0.65266100	1.50990500
C	3.36469800	-0.94602300	-0.89046600
C	4.33355300	-1.57848100	1.64703000
H	2.87885400	-0.19004400	2.40671000
C	4.40452600	-1.86965100	-0.76057200
H	2.97974600	-0.67428300	-1.87632800
C	4.88367900	-2.20076200	0.52315400
O	5.01471100	-2.49016500	-1.79101100
O	5.89220100	-3.10903500	0.65318800
O	4.82953200	-1.85648000	2.88702200
C	4.53342100	-3.15749400	3.36904600
H	4.96943900	-3.23102300	4.37530400
H	3.44036700	-3.30356700	3.43403800
H	4.97294700	-3.92974700	2.71748000
C	7.17325500	-2.51766200	0.79174500
H	7.42481300	-1.92236000	-0.10362400
H	7.20941600	-1.87376600	1.68745200
H	7.89779400	-3.33729900	0.89912700
C	4.58865500	-2.18090500	-3.09759500
H	3.52489400	-2.43869700	-3.24317200
H	4.73742900	-1.10999600	-3.32240400
H	5.20525800	-2.78477000	-3.77638600



IM3 (T1)

Theoretical calculation level:

DFT-UM062X/def2-TZVP//UM062X/def2-SV

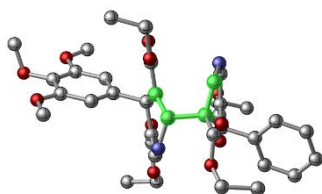
The number of imaginary frequencies: 0

Computed total energies: -2373.307906 Hartree

C	-2.60294400	0.38007700	0.33199100
C	-1.88934700	1.57885600	-0.25710100
C	-2.75272200	-0.72345200	-0.67999500
C	-1.74349400	1.72390600	-1.59682100
C	-2.06076500	-0.63577100	-2.00085200
N	-2.05310000	0.73061800	-2.46932900
H	-1.34130500	2.64629600	-2.02232200
H	-2.58635200	-1.25468000	-2.73909400
C	-1.34757700	2.57214400	0.67113500
O	-1.28373400	2.40168200	1.87152600
O	-0.88196500	3.67558400	0.06720500
C	-0.20792700	4.63184900	0.88722900
C	-1.19082700	5.53750700	1.60473700
H	0.42702600	5.19977300	0.19321100
H	0.44005400	4.09462800	1.59482800
H	-0.64617800	6.30968600	2.17178100
H	-1.85133400	6.03955200	0.87937500
H	-1.80845300	4.95626100	2.30670100
H	-2.02348300	-0.00058900	1.19557200
C	1.04183300	0.11225500	-0.32858100
C	1.24990900	0.92867000	-1.58174200
C	0.08035800	-1.01319300	-0.56946300
C	0.93513900	0.42434900	-2.80286200
C	-0.56589200	-1.25731700	-1.89547300
N	0.26324100	-0.74753400	-2.96567800
H	1.20736300	0.95927700	-3.71634000
H	-0.70468900	-2.34036400	-2.02104000
C	1.80940300	2.26890000	-1.41456100
O	2.05693800	2.76809300	-0.33624500
O	1.99439500	2.92225900	-2.57553000
C	2.55217600	4.23529600	-2.50634300
C	4.05864000	4.19215000	-2.33180200

H	2.27553700	4.70954200	-3.45829400
H	2.07232800	4.78322600	-1.68155400
H	4.46794400	5.21515700	-2.34350500
H	4.52491800	3.62084800	-3.15053600
H	4.32132800	3.72077600	-1.37193200
H	0.63430600	0.75496500	0.47334400
H	0.04872800	-1.05254900	-3.90873700
H	-1.83822500	0.87849900	-3.44825900
C	-3.42698700	-1.95596600	-0.27207900
O	-3.82056400	-2.17222600	0.85400900
O	-3.55775500	-2.82807300	-1.28298900
C	-4.28444800	-4.03198200	-1.01869400
C	-5.77879600	-3.79808900	-1.13268200
H	-4.01751700	-4.39792100	-0.01672600
H	-3.92966700	-4.74847300	-1.77196700
H	-6.31913200	-4.74599300	-0.98016200
H	-6.11613100	-3.07803300	-0.37026200
H	-6.03222900	-3.40682900	-2.13082600
C	-0.23063200	-1.86931000	0.57636700
O	0.04353200	-1.58425900	1.72301200
O	-0.85638700	-3.00464400	0.22931800
C	-1.16083500	-3.92642900	1.28314500
C	0.06654200	-4.72445100	1.68074600
H	-1.94155600	-4.57673800	0.86582300
H	-1.57749700	-3.36600700	2.13270100
H	-0.20659100	-5.47282800	2.44163700
H	0.48243300	-5.25042300	0.80639800
H	0.83911200	-4.06277700	2.10222200
C	-3.96272900	0.81938400	0.87668700
C	-4.18857300	0.90900300	2.25133500
C	-4.98833500	1.17106600	-0.00786400
C	-5.42446100	1.33900300	2.73774600
H	-3.38542600	0.64207100	2.94324900
C	-6.22548800	1.59626500	0.47489600
H	-4.81134700	1.11187200	-1.08745900
C	-6.44652400	1.68129300	1.85155700
H	-5.59011900	1.40455400	3.81613500
H	-7.02020000	1.86458900	-0.22580800
H	-7.41464900	2.01641900	2.23206300

C	2.38274200	-0.42607000	0.17897800
C	3.01238700	0.18994000	1.25821600
C	2.97260700	-1.51927500	-0.46332500
C	4.25182300	-0.28774200	1.70420400
H	2.53524300	1.04963800	1.72750600
C	4.20382000	-2.00735000	-0.01069800
H	2.46943400	-1.97511600	-1.31873800
C	4.83665100	-1.40455600	1.08900800
O	4.95476000	0.25268200	2.72198800
O	6.02308200	-1.89345900	1.54774100
O	4.86056700	-3.05302700	-0.55702500
C	4.27185800	-3.70571500	-1.65771800
H	4.95668800	-4.51553000	-1.94236200
H	3.29040000	-4.13491900	-1.38857400
H	4.14545200	-3.01652300	-2.51111000
C	7.15199200	-1.36387400	0.87763300
H	7.11677400	-1.60431500	-0.19945700
H	7.20654600	-0.26861700	1.00913300
H	8.04255900	-1.82835600	1.32529100
C	4.43323200	1.40069700	3.35102900
H	4.30776300	2.22781700	2.63020500
H	3.46274000	1.18851700	3.83258500
H	5.16258700	1.69273900	4.11837900



IM4 (T1)

Theoretical calculation level:

DFT-UM062X/def2-TZVP//UM062X/def2-SV

The number of imaginary frequencies: 0

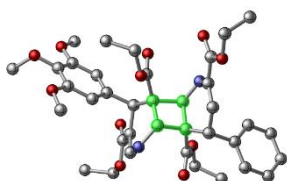
Computed total energies: -2373.311855 Hartree

C	-2.63550900	0.00428200	-0.12196000
C	-2.15675100	-1.47537900	-0.07600600
C	-1.93135600	0.73018900	-1.24667000
C	-2.12398100	-2.06792500	-1.44690900
C	-1.59039800	0.06844800	-2.39176600
N	-1.75235700	-1.27778200	-2.49690800
H	-2.23155600	-3.13462500	-1.62258400
H	-1.16025200	0.57400100	-3.25639900
C	-3.10124100	-2.32460700	0.77801200
O	-3.53883300	-3.39670000	0.45270000

O	-3.35987500	-1.74727800	1.95083900
C	-4.34657400	-2.37246700	2.78978400
C	-5.74469300	-2.10223600	2.26897600
H	-4.13259400	-3.45000100	2.84226300
H	-4.18930900	-1.92353300	3.77923600
H	-5.91295800	-1.01780900	2.16187000
H	-6.48677000	-2.51082100	2.97377600
H	-5.89303000	-2.57791300	1.28680600
H	-2.34948100	0.48883300	0.81988600
C	1.08159300	0.22778700	-0.10842000
C	0.40141600	-1.10114900	-0.27587900
C	0.50929800	0.99721500	1.05700900
C	-0.70003700	-1.58630100	0.62095300
C	-0.24015800	0.37602200	2.00037100
N	-0.64318200	-0.91817900	1.90468400
H	-0.54796900	-2.66637400	0.77616500
H	-0.56666500	0.91464400	2.89324600
C	0.90342200	-1.95346400	-1.35846400
O	1.54075300	-1.53251000	-2.29935900
O	0.59231400	-3.24753000	-1.19832700
C	1.03049200	-4.15558400	-2.21370800
C	2.48078000	-4.54797100	-2.00486100
H	0.36201000	-5.02270100	-2.12307800
H	0.88094800	-3.68658000	-3.19802900
H	2.78258500	-5.28845500	-2.76274100
H	2.61776900	-4.99384100	-1.00647900
H	3.13534700	-3.66685600	-2.09554600
H	0.94669500	0.81284600	-1.03591600
H	-1.57284800	-1.71836100	-3.39407900
H	-1.30218600	-1.24865800	2.60106800
C	-1.67734200	2.16071900	-1.08394200
O	-2.00388600	2.80684700	-0.10756500
O	-1.02100000	2.70083500	-2.12550100
C	-0.73808100	4.10068800	-2.06933600
C	-1.95643000	4.92879200	-2.43372600
H	0.07296100	4.24911700	-2.79620900
H	-0.36164900	4.34376100	-1.06553200
H	-1.69116800	5.99829800	-2.45376400
H	-2.33217100	4.64446800	-3.42993700

H	-2.75827200	4.78128800	-1.69373000
C	0.77828800	2.43194300	1.11674400
O	1.33107200	3.05155300	0.22980900
O	0.33321600	3.01780900	2.23985300
C	0.47170900	4.43471300	2.33904600
C	1.87272200	4.83226300	2.76561200
H	-0.27106600	4.73811400	3.09028400
H	0.20462900	4.88893100	1.37246000
H	2.13531500	4.34460800	3.71821700
H	2.60619300	4.53779500	1.99930400
H	1.92836600	5.92389600	2.90548800
C	-4.14954600	0.16091200	-0.22135700
C	-4.77656700	1.14354100	0.55625200
C	-4.94036900	-0.62068400	-1.07448200
C	-6.15599400	1.33655100	0.49331700
H	-4.16357400	1.76652300	1.21289700
C	-6.32337100	-0.43633900	-1.13069100
H	-4.48018000	-1.39283500	-1.69754800
C	-6.93691000	0.54147100	-0.34823400
H	-6.62490300	2.10776200	1.10993000
H	-6.92476600	-1.06349000	-1.79395600
H	-8.01914900	0.68559000	-0.39484000
C	2.58788200	0.03285600	0.08490300
C	3.48841900	0.85098400	-0.59398800
C	3.04398200	-0.95161300	0.96723800
C	4.86496200	0.68652400	-0.39029900
H	3.10312100	1.61402900	-1.26940900
C	4.41871000	-1.12446500	1.16546700
H	2.32021400	-1.57744400	1.49345100
C	5.33289500	-0.28923000	0.50319000
O	5.81843500	1.41850400	-1.00493300
O	6.67078800	-0.43641700	0.71805200
O	4.96293200	-2.05906900	1.97368400
C	5.40941100	2.40893800	-1.91974000
H	4.78686000	3.17592100	-1.42640000
H	6.32689100	2.87557100	-2.30242500
H	4.84548200	1.96837900	-2.76054900
C	4.09329700	-2.93547600	2.65147700
H	3.41927900	-2.38356200	3.32984200

H	3.48909500	-3.52791300	1.94146900
H	4.72823500	-3.60972200	3.24150000
C	7.29467300	-1.33071700	-0.18444100
H	8.36137600	-1.36793000	0.08010500
H	6.86021600	-2.34225700	-0.09503700
H	7.18853600	-0.97469500	-1.22436200



P1 (S0)

Theoretical calculation level:

DFT-M062X/def2-TZVP//M062X/def2-SV

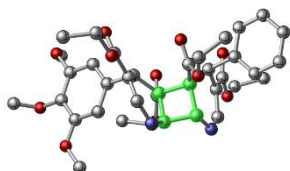
The number of imaginary frequencies: 0

Computed total energies: -2373.388003 Hartree

C	2.54104000	-0.38954000	-0.31766400
C	1.57492900	0.47174900	0.53510800
C	2.72174100	-1.75230100	0.29757900
C	1.65250700	0.31377500	2.07649800
C	2.58069400	-1.93299200	1.63581900
N	2.20761900	-0.95398500	2.49048600
H	2.13062600	1.14420700	2.61319000
H	2.77151000	-2.90844200	2.08919600
C	1.71397100	1.90365100	0.02679100
O	1.53407500	2.18654900	-1.13018100
O	2.08616100	2.77251700	0.95743800
C	2.28647400	4.12922800	0.53253100
C	3.63948900	4.28635100	-0.13417200
H	2.21645000	4.72238500	1.45427900
H	1.45974800	4.40750400	-0.13881700
H	3.77990500	5.33155700	-0.45385000
H	4.44764800	4.02087700	0.56609600
H	3.71201000	3.63127200	-1.01769300
H	2.08326900	-0.50595700	-1.31050000
C	-0.98180100	0.85316800	-0.23096800
C	0.04669300	0.05248500	0.60985400
C	-1.13139600	2.25481200	0.30038100
C	0.09091400	0.32859500	2.13745200
C	-0.89066400	2.53275000	1.60745600
N	-0.44117500	1.62137200	2.49942700
H	-0.33594100	-0.45995000	2.77234000
H	-1.05552400	3.53773900	2.00272500

C	-0.13699300	-1.41410500	0.22804800
O	-0.05694100	-1.78883000	-0.91376900
O	-0.43547400	-2.20306800	1.25246800
C	-0.70872000	-3.57996500	0.95456600
C	-2.13612100	-3.74981700	0.46903800
H	-0.53738700	-4.10929000	1.90165400
H	0.02358400	-3.92742100	0.21025300
H	-2.32528000	-4.80941400	0.23240900
H	-2.85388400	-3.43107200	1.24314400
H	-2.31141000	-3.14786900	-0.43907900
H	-0.59547200	0.90401500	-1.25881600
H	-0.23251800	1.94215700	3.43886700
H	2.07523000	-1.20219500	3.46506800
C	-1.57332500	3.27967100	-0.63959500
O	-1.86197100	3.05925500	-1.79708600
O	-1.61787300	4.51658800	-0.10566600
C	-2.09161100	5.57190400	-0.94269000
C	-3.60727400	5.59217300	-1.00893900
H	-1.65355900	5.45723100	-1.94526300
H	-1.70106100	6.49197400	-0.48584400
H	-3.94568200	6.44930400	-1.61326900
H	-3.98404200	4.66721300	-1.47264800
H	-4.03670300	5.68631400	0.00149600
C	3.09243500	-2.84322300	-0.59710300
O	3.30392600	-2.70444100	-1.78359900
O	3.16775700	-4.04192700	0.01481400
C	3.59171000	-5.15105700	-0.77835300
C	5.09959200	-5.17129300	-0.94664800
H	3.08571900	-5.10707100	-1.75432300
H	3.24099100	-6.03840700	-0.23297600
H	5.40353500	-6.06951400	-1.50812000
H	5.43562300	-4.28200900	-1.50230700
H	5.59710000	-5.18878500	0.03640800
C	3.88246300	0.31081600	-0.50007000
C	4.31263600	0.69971900	-1.77202400
C	4.69903900	0.59383200	0.60275700
C	5.53022800	1.36048700	-1.94246800
H	3.68038400	0.48268300	-2.63748900
C	5.91408100	1.25843700	0.43713700

H	4.38469200	0.28186600	1.60431700
C	6.33341500	1.64462400	-0.83751600
H	5.85218700	1.65544900	-2.94453700
H	6.53780900	1.47511800	1.30822500
H	7.28658700	2.16286400	-0.96906600
C	-2.32569700	0.13745700	-0.27037100
C	-2.89410500	-0.23086000	-1.48568700
C	-2.97316400	-0.19145700	0.92946500
C	-4.10298400	-0.93274900	-1.50757300
H	-2.40831400	0.01064300	-2.43305100
C	-4.17090100	-0.90835400	0.91385300
H	-2.53047000	0.11613700	1.87853100
C	-4.73862800	-1.29107000	-0.31650400
O	-4.84141100	-1.30070200	2.01731200
O	-5.89436900	-2.01352900	-0.33448700
O	-4.66916800	-1.27049800	-2.70231600
C	-4.58517200	-2.65019400	-3.02162900
H	-5.06395700	-2.78142500	-4.00233100
H	-3.52827000	-2.96587900	-3.08706200
H	-5.10855700	-3.26152300	-2.26836600
C	-7.05611900	-1.22300100	-0.51897700
H	-7.16716700	-0.49641200	0.30515100
H	-7.01183300	-0.68558400	-1.48192900
H	-7.91625900	-1.90745200	-0.51990600
C	-4.28645200	-0.98487600	3.27342800
H	-3.28432300	-1.43577500	3.38881800
H	-4.21248400	0.10759000	3.41559100
H	-4.96488100	-1.40465400	4.02780300



P2 (S0)

Theoretical calculation level:

DFT-M062X/def2-TZVP//M062X/def2-SV

The number of imaginary frequencies: 0

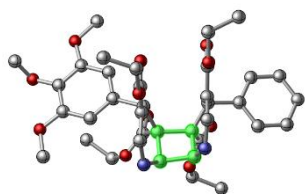
Computed total energies: -2373.385029 Hartree

C	3.26757300	0.08264000	1.07092500
C	1.95506100	-0.54419800	0.52913100
C	3.27564700	1.56270800	0.79966900
C	1.37424500	0.04354300	-0.77858900
C	2.68579000	2.04518000	-0.30840800

H	3.78203400	2.24163100	1.48512000
N	2.04836100	1.23575700	-1.24109300
H	1.29328700	-0.67943300	-1.60039500
C	2.12629200	-2.04965200	0.56331000
O	2.30207300	-2.64591000	1.59739300
O	2.11304800	-2.62108200	-0.63372700
C	2.33222500	-4.03821800	-0.68335200
C	3.81179900	-4.35585400	-0.58687400
H	1.91191600	-4.35080000	-1.64899000
H	1.75783800	-4.50862800	0.12901500
H	3.96769800	-5.44307000	-0.67687600
H	4.36601600	-3.85128200	-1.39508500
H	4.21841100	-4.01769200	0.37987700
H	3.26157100	-0.08896600	2.15946300
C	-1.10815700	-0.71491000	-0.48676500
C	-0.00420200	0.28754800	-0.04661200
C	-1.00520100	-2.02974100	0.25792500
C	0.67345100	-0.04566400	1.30165900
C	-0.58161000	-2.06881900	1.54631400
N	-0.01374200	-0.98536800	2.14860800
H	0.91186600	0.86130400	1.87282300
H	-0.66938000	-2.97863700	2.14428500
C	-0.47938800	1.70525900	-0.29096000
O	-0.77606400	2.08824900	-1.39543000
O	-0.48560000	2.47698400	0.78910900
C	-0.92228600	3.83555500	0.61172200
C	-2.43359800	3.92498300	0.52134800
H	-0.53639200	4.36550800	1.49297700
H	-0.44003400	4.23441400	-0.29344600
H	-2.73248500	4.98106700	0.42161700
H	-2.91163300	3.51165300	1.42422300
H	-2.80268900	3.37059900	-0.35625600
H	-0.97942800	-0.90593200	-1.56202500
H	0.41276600	-1.14853700	3.05495000
H	1.51709600	1.76522300	-1.93101900
C	-1.53748600	-3.21795500	-0.41334100
O	-2.02119700	-3.20778300	-1.52519100
O	-1.41205300	-4.34236400	0.31287800
C	-1.92126400	-5.54841700	-0.26009900

C	-3.42314400	-5.65814000	-0.07716100
H	-1.39519400	-6.35541900	0.26845600
H	-1.64773500	-5.57950900	-1.32524800
H	-3.78168500	-6.62189500	-0.47327400
H	-3.68568800	-5.60087100	0.99143300
H	-3.93656300	-4.84626500	-0.61550000
C	2.63827600	3.50525600	-0.62862200
O	1.96660500	3.94444500	-1.53203200
O	3.37513800	4.24673400	0.18554400
C	3.34399000	5.66865900	-0.00726300
C	4.26315200	6.09305200	-1.13565700
H	3.67174800	6.08377600	0.95493300
H	2.30445300	5.97501000	-0.19770100
H	3.91724800	5.67903800	-2.09536500
H	4.27147600	7.19195500	-1.21215600
H	5.29175200	5.74849300	-0.94425100
C	4.51078800	-0.60431700	0.51449000
C	5.33394000	-1.35530600	1.35902800
C	4.83319900	-0.52403600	-0.84768700
C	6.46035100	-2.01218100	0.85930000
H	5.08552800	-1.43207500	2.42155100
C	5.95492200	-1.18266000	-1.34891500
H	4.19617700	0.06111900	-1.51815300
C	6.77301100	-1.92847000	-0.49681600
H	7.09378700	-2.59372400	1.53397800
H	6.19288400	-1.11273700	-2.41341500
H	7.65300500	-2.44258000	-0.89143500
C	-2.50868600	-0.14060900	-0.29300000
C	-3.39591800	-0.10202500	-1.36737600
C	-2.88392100	0.36510900	0.95568000
C	-4.66748300	0.46438400	-1.20042300
H	-3.08700300	-0.51784300	-2.32648800
C	-4.14416200	0.94766700	1.11932800
H	-2.17984500	0.31758300	1.78767800
C	-5.03373900	1.01775800	0.03592200
O	-4.58171400	1.49445900	2.27516000
O	-5.60395700	0.53460900	-2.17010800
O	-6.25025200	1.61286600	0.18665200
C	-3.75228500	1.38651600	3.40967600

H	-3.55489100	0.32909000	3.65911700
H	-2.79079600	1.90736700	3.25345600
H	-4.29306500	1.86400600	4.23748600
C	-5.29466500	-0.00788600	-3.43304600
H	-4.43247000	0.50832500	-3.89025000
H	-5.07668400	-1.08793300	-3.36176000
H	-6.18244800	0.14339200	-4.06149800
C	-7.27555300	0.71650400	0.57278800
H	-8.20306800	1.30116700	0.65690300
H	-7.41067700	-0.07416100	-0.18592900
H	-7.04504200	0.25433200	1.54908700



P3 (S0)

Theoretical calculation level:

DFT-M062X/def2-TZVP//M062X/def2-SV

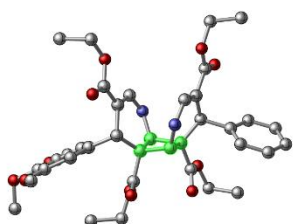
The number of imaginary frequencies: 0

Computed total energies: -2373.379324 Hartree

C	-2.36624400	-0.11038200	0.46011000
C	-2.36082000	1.23387700	-0.22965500
C	-1.69419100	-1.17921800	-0.41452300
C	-2.46788100	1.29674800	-1.58017300
C	-1.90957700	-1.07475100	-1.95318900
N	-2.41795400	0.20498400	-2.38117500
H	-2.57889900	2.25725900	-2.08909800
H	-2.51810800	-1.87971200	-2.38766800
C	-2.31119100	2.43212100	0.60072800
O	-2.19117900	2.41296700	1.80916500
O	-2.39452300	3.57803600	-0.09999200
C	-2.31403700	4.79533300	0.64088400
C	-3.62719600	5.12816400	1.32587300
H	-2.05912800	5.56131500	-0.10504200
H	-1.48995400	4.71355800	1.36559800
H	-3.54946000	6.10543600	1.82929200
H	-4.44282100	5.18191600	0.58679500
H	-3.87474200	4.36416600	2.07830100
H	-1.79809100	-0.04458600	1.40143200
C	0.55262600	0.28963400	-0.27024000
C	0.52810700	1.29398200	-1.39827100
C	-0.11297500	-1.07536400	-0.66193100

C	0.49745500	0.90955300	-2.69729400
C	-0.36375200	-1.28414400	-2.17526700
N	0.30927700	-0.38634600	-3.06667000
H	0.62784500	1.63651200	-3.50213800
H	-0.16246900	-2.31953500	-2.46796400
C	0.60684700	2.70104700	-1.01473000
O	0.68168200	3.08693100	0.13403000
O	0.55936700	3.54643100	-2.06048100
C	0.67905500	4.94060800	-1.77844000
C	2.13091800	5.34786900	-1.61138700
H	0.22017600	5.44509100	-2.64050300
H	0.09721300	5.17313700	-0.87466300
H	2.20193000	6.43658700	-1.45689100
H	2.71165900	5.08397700	-2.50989800
H	2.57412700	4.84197600	-0.73923200
H	0.00308700	0.71310000	0.58188700
H	0.27950300	-0.60309800	-4.05641500
H	-2.44758800	0.35680900	-3.38346700
C	-2.01087100	-2.57764100	0.11116900
O	-2.49277000	-2.82938600	1.17995100
O	-1.61545200	-3.51345500	-0.75973300
C	-1.73122600	-4.88482200	-0.35389800
C	-3.14170000	-5.39995500	-0.56019200
H	-1.42372600	-4.95977300	0.70025900
H	-1.00770400	-5.42230400	-0.98210900
H	-3.19164800	-6.46642200	-0.28866000
H	-3.85153600	-4.84345900	0.07129600
H	-3.43940600	-5.29406300	-1.61556100
C	0.63825600	-2.19590100	0.04440100
O	0.52652800	-2.39589200	1.22795900
O	1.39352500	-2.92329100	-0.76831200
C	2.11040000	-4.02262100	-0.18556600
C	3.39268600	-3.56912900	0.48337600
H	2.31076700	-4.70037300	-1.02633200
H	1.44465800	-4.52524200	0.53211300
H	3.89225300	-4.43886000	0.94049100
H	4.08460700	-3.11195600	-0.24197900
H	3.17712800	-2.83150100	1.27372400
C	-3.81415100	-0.41929900	0.82804700

C	-4.26307800	-0.15094100	2.12465300
C	-4.73408400	-0.89445200	-0.11585200
C	-5.59622000	-0.36383800	2.47822400
H	-3.55369200	0.23530900	2.86122600
C	-6.06589600	-1.11429100	0.23670300
H	-4.41483700	-1.09718400	-1.14284900
C	-6.50293000	-0.85091100	1.53628100
H	-5.92669000	-0.15124200	3.49833800
H	-6.76734300	-1.49401200	-0.51073600
H	-7.54620300	-1.02407400	1.81159500
C	1.99813200	0.12116400	0.19844300
C	2.32453000	0.35481600	1.53395400
C	2.98113900	-0.27155900	-0.71259800
C	3.64670900	0.18956900	1.96657100
H	1.54354000	0.67161100	2.22579100
C	4.29739900	-0.45380600	-0.28106500
H	2.70131800	-0.45552800	-1.75124300
C	4.63404700	-0.23365300	1.06372000
O	4.06777000	0.40444100	3.23197600
O	5.90995500	-0.45108700	1.48907000
O	5.30443900	-0.88169700	-1.07497700
C	5.01474900	-1.12656400	-2.43188800
H	5.95212200	-1.46377200	-2.89411700
H	4.24884500	-1.91525900	-2.54074200
H	4.66525400	-0.20927500	-2.93764300
C	6.69455400	0.72432600	1.57504200
H	6.79195500	1.20245300	0.58395400
H	6.25162800	1.44079800	2.28812000
H	7.68999800	0.42312900	1.93200400
C	3.11288100	0.78566200	4.19522900
H	2.64284800	1.75015800	3.93480100
H	2.32854100	0.01648300	4.30528500
H	3.65423300	0.89060300	5.14483500



P4 (S0)

Theoretical calculation level:

DFT-M062X/def2-TZVP//M062X/def2-SV

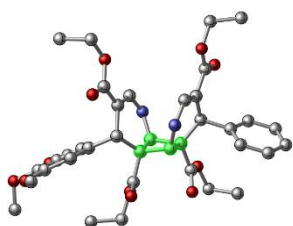
The number of imaginary frequencies: 0

Computed total energies: -2373.390072 Hartree

C	-3.00623000	-0.25501600	0.36842700
C	-1.70146200	-0.95742500	-0.05228500
C	-3.00233500	1.19199900	-0.06733100
C	-0.97894500	-0.48024300	-1.33460400
C	-2.26617100	1.60356400	-1.13209500
N	-1.41063700	0.80634500	-1.81004800
H	-0.99392700	-1.20741000	-2.15812600
H	-2.34208300	2.63153600	-1.49381100
C	-1.86036900	-2.46880000	-0.07068600
O	-1.52591900	-3.18870100	-0.97776100
O	-2.37513200	-2.89995400	1.07303800
C	-2.65180600	-4.30552400	1.18047100
C	-3.90667400	-4.67492200	0.41277300
H	-1.77541800	-4.86286600	0.81676400
H	-2.76945700	-4.48136700	2.25775600
H	-4.76477800	-4.07778300	0.76176100
H	-4.13169100	-5.74284500	0.56535300
H	-3.76936500	-4.49612200	-0.66539800
H	-3.07162900	-0.29404200	1.46733200
C	1.31389100	0.71415900	-0.71683400
C	0.37687600	-0.50229300	-0.53503100
C	0.79579900	1.91618700	0.03344100
C	-0.40809200	-0.63073300	0.79457300
C	0.00102900	1.77350700	1.12447000
N	-0.46608900	0.58236400	1.56531300
H	-0.08997700	-1.45904700	1.44201600
H	-0.29362400	2.64474700	1.71390100
C	1.13818900	-1.75728700	-0.93902100
O	1.53959200	-1.91750600	-2.06270000
O	1.31622800	-2.62302500	0.05130400
C	2.10629800	-3.78679600	-0.23212500
C	3.58217400	-3.47290500	-0.07751600
H	1.77154800	-4.53968100	0.49405300
H	1.86874100	-4.13144200	-1.24857600
H	4.18304800	-4.36310400	-0.32545300
H	3.81030500	-3.17446200	0.95889000
H	3.87691600	-2.64934100	-0.75119800
H	1.34484600	0.94863400	-1.79263000

H	-0.89382200	1.20883000	-2.58384300
H	-1.06754000	0.57853300	2.38132800
C	-3.87142000	2.10791000	0.66359300
O	-4.53025900	1.78705000	1.63263900
O	-3.87159300	3.36208200	0.17514900
C	-4.70726100	4.31767600	0.82879100
C	-6.15390100	4.18605500	0.39010600
H	-4.29366700	5.29507800	0.54342800
H	-4.61120000	4.19271100	1.91776600
H	-6.76158100	4.97887100	0.85538700
H	-6.23394200	4.28197000	-0.70469500
H	-6.55991400	3.20906400	0.69464300
C	1.25350300	3.22575000	-0.41964100
O	1.97647000	3.39332700	-1.38061800
O	0.78998800	4.24860400	0.32258200
C	1.22023200	5.56212700	-0.03558100
C	2.60412700	5.86186900	0.50940100
H	0.46788200	6.23490800	0.39925900
H	1.19726800	5.66003000	-1.13107700
H	2.62213400	5.73822300	1.60412700
H	3.34849300	5.18542500	0.06125900
H	2.88566600	6.90029200	0.27088200
C	-4.24478300	-0.95428700	-0.17730500
C	-5.33714900	-1.20601100	0.65858900
C	-4.32380300	-1.33465200	-1.52326700
C	-6.48194600	-1.83257400	0.16483000
H	-5.28502000	-0.90109100	1.70694800
C	-5.46301200	-1.97072600	-2.01714000
H	-3.48631300	-1.13180800	-2.19940300
C	-6.54642000	-2.22262500	-1.17346000
H	-7.32630400	-2.02369900	0.83225500
H	-5.50511600	-2.26729300	-3.06825400
H	-7.44009000	-2.71863000	-1.56015200
C	2.73854400	0.38805300	-0.28471700
C	3.79275300	0.53350200	-1.18573200
C	2.97215400	-0.08387300	1.01050500
C	5.09671500	0.20318900	-0.79121500
H	3.58638800	0.90506400	-2.18955200
C	4.26758300	-0.43880500	1.39771000

H	2.13613200	-0.19183400	1.70394200
C	5.33923000	-0.26811600	0.50768600
O	6.18265400	0.30251100	-1.58618900
O	6.60746800	-0.58513200	0.89218400
O	4.58350300	-0.97301600	2.59747200
C	6.00056500	0.74485800	-2.91160900
H	5.59056200	1.76961600	-2.93876500
H	6.99411000	0.73914100	-3.37932500
H	5.32976200	0.06918500	-3.47079700
C	3.53430500	-1.23401600	3.50171300
H	3.02763500	-0.30198200	3.80763500
H	2.79208200	-1.92348000	3.06071000
H	3.99209900	-1.70446400	4.38199500
C	6.95441700	-1.93425000	0.63814400
H	8.00252100	-2.06328400	0.94489700
H	6.31514800	-2.61958900	1.22221300
H	6.85661100	-2.16723800	-0.43727800



2a (S1)

Theoretical calculation level:

TDDFT-M062X/def2-TZVP//M062X/def2-SV

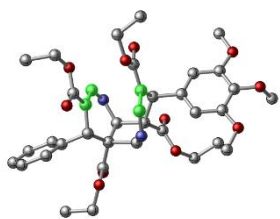
The number of imaginary frequencies: 0

Computed total energies: -2373.238334 Hartree

C	-3.00304800	-0.38408900	0.35819200
C	-1.67573400	-0.94603000	-0.14151400
C	-2.96259400	1.10909500	0.25321400
C	-0.99856100	-0.31436800	-1.38518900
C	-2.29891400	1.73052600	-0.81304700
N	-1.40432600	1.05672900	-1.58807000
H	-1.06367000	-0.87895500	-2.32695200
H	-2.44518600	2.78173900	-1.06044900
C	-1.76062400	-2.45487800	-0.29266800
O	-1.52687000	-3.05638400	-1.31051000
O	-2.12957700	-3.01998400	0.84782100
C	-2.32172500	-4.44454400	0.84197500
C	-3.67638100	-4.80407300	0.26451800
H	-1.50137500	-4.90331700	0.27051100
H	-2.23852200	-4.74019400	1.89596300
H	-4.48442400	-4.34437300	0.85512900

H	-3.80641800	-5.89814400	0.27797600
H	-3.75938800	-4.45439300	-0.77758200
H	-3.09199400	-0.65204100	1.42252100
C	1.37353900	0.67168100	-0.85716500
C	0.37770900	-0.46676000	-0.63645800
C	0.77915200	1.94208100	-0.33895200
C	-0.41016600	-0.52643700	0.69951900
C	-0.01154100	1.93283700	0.81877500
N	-0.53487600	0.77579700	1.31361400
H	-0.09145900	-1.26530700	1.44785500
H	-0.26437400	2.84072400	1.36581900
C	1.07076700	-1.76647600	-1.01411900
O	1.50215000	-1.95974600	-2.11983200
O	1.18969600	-2.61044700	0.00482500
C	1.99552900	-3.78046800	-0.20169800
C	3.45589700	-3.44606900	0.03557700
H	1.62076000	-4.51450400	0.52395800
H	1.81987600	-4.15347000	-1.22070300
H	4.07980100	-4.33921400	-0.13047400
H	3.60739500	-3.09690100	1.07017200
H	3.78838500	-2.64985500	-0.65350700
H	1.51241200	0.76918900	-1.94507600
H	-1.08375300	1.50317500	-2.44263300
H	-0.95818200	0.80148600	2.23694800
C	-3.70248700	1.86059500	1.24481600
O	-4.36652400	1.36786400	2.14528300
O	-3.56478900	3.19873700	1.09277500
C	-4.26453200	4.03123800	2.01441800
C	-5.72823600	4.17347800	1.63816800
H	-3.74817600	5.00069100	1.96971100
H	-4.15793500	3.61449700	3.02745100
H	-6.22800500	4.87494600	2.32574000
H	-5.82550300	4.56206700	0.61154600
H	-6.23521900	3.19826700	1.70194900
C	1.12868000	3.16577000	-1.02791700
O	1.89538200	3.24259600	-1.97713300
O	0.48981900	4.24690700	-0.52113800
C	0.79393600	5.51132500	-1.10463500
C	2.09453000	6.07532100	-0.56178000

H	-0.05734700	6.15643800	-0.84478500
H	0.84000100	5.40148100	-2.19852200
H	2.05065100	6.15492000	0.53641600
H	2.93826500	5.42507900	-0.84046900
H	2.27322600	7.07990500	-0.97826400
C	-4.20785200	-0.97881700	-0.35635500
C	-5.25946100	-1.52386100	0.38794200
C	-4.29990100	-0.97689400	-1.75573700
C	-6.37829500	-2.06204900	-0.24898600
H	-5.19584700	-1.52429700	1.47960100
C	-5.41358500	-1.52123500	-2.39381900
H	-3.49481100	-0.54434600	-2.35849000
C	-6.45729700	-2.06681100	-1.64212900
H	-7.19014400	-2.48629100	0.34746900
H	-5.46719000	-1.51849100	-3.48532200
H	-7.33006500	-2.49369300	-2.14214900
C	2.74028900	0.36832400	-0.25526800
C	3.87368000	0.43168300	-1.06832200
C	2.85369800	0.00913200	1.09184600
C	5.13207100	0.12282500	-0.53469300
H	3.76085100	0.71298600	-2.11522700
C	4.10517500	-0.32303100	1.61921500
H	1.96342100	-0.03131100	1.72023200
C	5.25314900	-0.24096000	0.81525700
O	6.28326600	0.13894900	-1.23818100
O	6.47587700	-0.54578900	1.33373900
O	4.30712500	-0.75124100	2.88378400
C	6.22574700	0.49828700	-2.59941800
H	5.83055400	1.52138400	-2.72554500
H	7.25677700	0.45763100	-2.97512900
H	5.59930000	-0.20674400	-3.17357700
C	3.18084100	-0.90933600	3.71562100
H	2.67010300	0.05484000	3.88461100
H	2.46441700	-1.63059200	3.28279600
H	3.55329100	-1.29558500	4.67362200
C	6.81101600	-1.91634300	1.21306300
H	7.82037200	-2.04243200	1.63102600
H	6.10049000	-2.54431700	1.77936200
H	6.81179600	-2.22608200	0.15272300



2a (T1)

Theoretical calculation level:

DFT-UM062X/def2-TZVP//UM062X/def2-SV

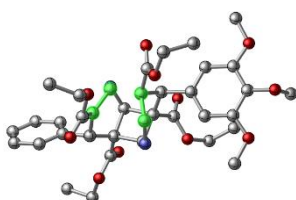
The number of imaginary frequencies: 0

Computed total energies: -2373.285602 Hartree

C	-2.71437300	-0.28969900	0.32441500
C	-1.67582500	-1.33020600	-0.15422200
C	-2.44932300	1.07925900	-0.26259600
C	-0.88424100	-1.01168800	-1.44387000
C	-1.84233400	1.22310200	-1.47103700
N	-1.26344800	0.19029300	-2.13127000
H	-0.90136200	-1.85118900	-2.15037500
H	-1.79535100	2.19784800	-1.96133500
C	-2.24364400	-2.73516200	-0.16016100
O	-2.18253500	-3.50571300	-1.08468200
O	-2.75601300	-3.03633500	1.02841600
C	-3.37253000	-4.32435300	1.17353300
C	-4.74382500	-4.34932600	0.52721900
H	-2.70589000	-5.08347000	0.73754000
H	-3.43403000	-4.48022100	2.25871700
H	-5.38241900	-3.55382900	0.94472400
H	-5.22316300	-5.32458300	0.71129300
H	-4.66208900	-4.19788100	-0.56059000
H	-2.64086000	-0.22448500	1.42073000
C	1.17969300	0.39288500	-0.59363700
C	0.46486200	-0.98150300	-0.61983200
C	0.48604400	1.34897500	0.32629500
C	-0.31371400	-1.36229500	0.66282600
C	0.01930000	0.87883100	1.65144600
N	-0.14662600	-0.48567400	1.77515200
H	-0.08509100	-2.38054100	1.00198200
H	0.35002600	1.39693000	2.55716900
C	1.43819400	-2.00318500	-1.17445000
O	1.83378900	-1.94444200	-2.31117600
O	1.80147500	-2.93738600	-0.30310800
C	2.80405700	-3.87385100	-0.72983000
C	4.19468600	-3.28486000	-0.58422800
H	2.66522700	-4.74844000	-0.08071100

H	2.59572500	-4.15728200	-1.77138300
H	4.94250900	-4.01239100	-0.93960800
H	4.41344600	-3.04541300	0.46891900
H	4.29156400	-2.36244900	-1.18188300
H	1.13771200	0.80741000	-1.61054800
H	-0.81838400	0.37541000	-3.02315800
H	-0.38291200	-0.85343100	2.69065200
C	-3.03011400	2.22381400	0.43830200
O	-3.59656000	2.14561400	1.50830600
O	-2.89655000	3.38884800	-0.22494200
C	-3.54222000	4.53016100	0.34046700
C	-5.03240100	4.52565300	0.05292900
H	-3.05222500	5.39424400	-0.12927900
H	-3.34761200	4.55215800	1.42347100
H	-5.49147500	5.44828200	0.44322300
H	-5.21390600	4.47735100	-1.03275900
H	-5.51609800	3.66251200	0.53584100
C	0.41267000	2.73972400	-0.06947900
O	0.76860900	3.17065500	-1.15591300
O	-0.08198500	3.52035500	0.90714000
C	-0.20068600	4.91308600	0.61978300
C	1.13114600	5.62671100	0.76342800
H	-0.93144200	5.29059600	1.34853900
H	-0.61230500	5.03348500	-0.39397400
H	1.54029300	5.47747300	1.77562700
H	1.85369900	5.24583600	0.02534400
H	0.99653600	6.70767900	0.59744900
C	-4.14786200	-0.68192800	-0.01905700
C	-5.14953700	-0.62123100	0.95427100
C	-4.49292100	-1.07213800	-1.31961800
C	-6.46943900	-0.94692900	0.63830600
H	-4.88725700	-0.30722700	1.96779000
C	-5.80927200	-1.40814500	-1.63572100
H	-3.72125000	-1.11587700	-2.09602000
C	-6.80265400	-1.34650700	-0.65652700
H	-7.24123300	-0.89180000	1.41049800
H	-6.06081600	-1.71647500	-2.65375200
H	-7.83505000	-1.60632000	-0.90370500
C	2.64912800	0.31065900	-0.19269600

C	3.60757500	0.92635300	-1.00157000
C	3.02396100	-0.36123800	0.97320700
C	4.96155600	0.84858400	-0.65220400
H	3.28826100	1.45285100	-1.90131100
C	4.37779500	-0.45551400	1.31113800
H	2.26242000	-0.84545700	1.58491800
C	5.34855300	0.16780800	0.51445700
O	5.96733100	1.38756900	-1.37050300
O	6.66545600	0.08953300	0.85192000
O	4.84434900	-1.14623000	2.37339800
C	5.64313200	2.08464500	-2.55193300
H	4.98927000	2.94811400	-2.33795700
H	6.59253700	2.44308500	-2.97132700
H	5.14640500	1.42265700	-3.28267900
C	3.90478300	-1.78452100	3.20907300
H	3.20940400	-1.05314800	3.65701100
H	3.32482000	-2.54150900	2.65139000
H	4.47911500	-2.27766800	4.00432700
C	7.31853500	-1.04431200	0.30927600
H	8.37248200	-0.99073600	0.61797700
H	6.87057400	-1.97664800	0.69663700
H	7.25924400	-1.03748200	-0.79363000



TS24-2

Theoretical calculation level:

DFT-UM062X/def2-TZVP//UM062X/def2-SV

The number of imaginary frequencies: 1

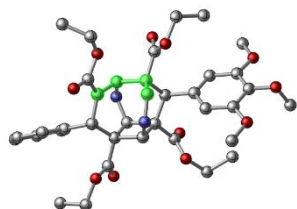
Computed total energies: -2373.278002 Hartree

C	-3.01812700	0.01725300	0.36852900
C	-2.07710000	-1.13978600	0.01572200
C	-2.36428700	1.33276500	0.05092900
C	-1.28646400	-0.99770200	-1.30693800
C	-1.27772900	1.37617400	-0.97074500
N	-1.49483100	0.29358500	-1.90520400
H	-1.46764800	-1.79566400	-2.03903600
H	-1.29919700	2.32715000	-1.51811400
C	-2.73959800	-2.48949100	0.15217300
O	-2.52569900	-3.42973900	-0.57270900
O	-3.53720600	-2.53438700	1.21507900

C	-4.33344300	-3.71213200	1.40020000
C	-5.54829600	-3.67471800	0.49108500
H	-3.70859000	-4.59667800	1.20890100
H	-4.61994600	-3.69458700	2.46000600
H	-6.04959700	-2.69496000	0.57255200
H	-6.26184000	-4.46193400	0.78275900
H	-5.25645100	-3.83363500	-0.55891500
H	-3.20249200	-0.01872700	1.45425200
C	0.93886000	0.09710200	-0.79425000
C	0.06890600	-1.14563000	-0.52977000
C	0.17585500	1.31953400	-0.19010500
C	-0.69706700	-1.17667900	0.82006300
C	0.05831000	1.12999000	1.27942200
N	-0.38595200	-0.10712800	1.71388800
H	-0.57805100	-2.12892000	1.35413300
H	0.24517500	1.90130100	2.02018400
C	0.84504000	-2.38294900	-0.91238900
O	1.17029200	-2.61007900	-2.05063200
O	1.14844100	-3.16370700	0.12073300
C	2.02619000	-4.27090100	-0.12719200
C	3.47450400	-3.81713100	-0.12890300
H	1.82518700	-4.97690300	0.68961400
H	1.74792700	-4.73572000	-1.08390300
H	4.12902700	-4.66531700	-0.38793300
H	3.77065600	-3.43325700	0.86104000
H	3.62815500	-3.01872500	-0.87459700
H	0.95928500	0.23350800	-1.88534700
H	-0.98945200	0.41482900	-2.77936100
H	-0.73807000	-0.18249200	2.66192200
C	-2.61724300	2.48267200	0.90564500
O	-3.37712000	2.48867100	1.85416700
O	-1.91055300	3.55671100	0.51614400
C	-2.01227000	4.74020600	1.31140800
C	-3.13302900	5.63116900	0.81146600
H	-1.03440200	5.23165800	1.21841800
H	-2.17295000	4.45086400	2.35998000
H	-3.12010900	6.59209400	1.35017100
H	-3.01076500	5.83253500	-0.26475700
H	-4.11150100	5.15209200	0.97532600

C	0.96289900	2.55556200	-0.58774900
O	1.18202700	2.82626900	-1.74442700
O	1.40377100	3.28075800	0.43153700
C	2.25049100	4.39748700	0.12222500
C	3.66994000	3.94124800	-0.15801100
H	2.20359900	5.03525400	1.01389700
H	1.82559400	4.94107600	-0.73411800
H	4.12057600	3.48903400	0.74039000
H	3.67819900	3.19688200	-0.96971400
H	4.28525700	4.80173700	-0.46615300
C	-4.38866200	-0.07557800	-0.30854800
C	-5.47960800	0.55597400	0.30366900
C	-4.59754700	-0.76346400	-1.50909100
C	-6.75199600	0.48962700	-0.26196600
H	-5.31862500	1.10096400	1.23770800
C	-5.87221400	-0.83155300	-2.07557800
H	-3.76454700	-1.25322000	-2.01814100
C	-6.95394400	-0.20853600	-1.45452500
H	-7.59201800	0.98261400	0.23412400
H	-6.01736600	-1.37816300	-3.01083700
H	-7.95103700	-0.26588200	-1.89800600
C	2.37893300	-0.02077500	-0.34339200
C	3.38721200	0.36519500	-1.23201400
C	2.70733800	-0.53562800	0.91309100
C	4.73239700	0.23969300	-0.86391000
H	3.11044700	0.75666100	-2.21190600
C	4.05011500	-0.68571700	1.27263900
H	1.91285900	-0.86332000	1.58239200
C	5.06738300	-0.27080500	0.40005400
O	5.77405000	0.57033400	-1.65589500
O	6.37486900	-0.40609100	0.75728700
O	4.46242900	-1.24456900	2.43124500
C	5.49926000	1.16425700	-2.90388500
H	4.88883200	2.07659100	-2.78719100
H	6.47045500	1.43123900	-3.34142100
H	4.97686500	0.46079900	-3.57596300
C	3.48659300	-1.55766700	3.39949900
H	2.86768400	-0.67601500	3.64161300
H	2.83135500	-2.37822200	3.05629800

H	4.03159600	-1.87804100	4.29738400
C	6.92675900	-1.66243700	0.40639000
H	7.97747800	-1.65818200	0.73051600
H	6.38940700	-2.48200900	0.91572700
H	6.88192200	-1.81667200	-0.68641900



IM24-2 (T1)

Theoretical calculation level:

DFT-UM062X/def2-TZVP//UM062X/def2-SV

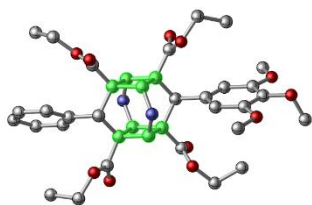
The number of imaginary frequencies: 0

Computed total energies: -2373.296053 Hartree

C	-3.00641600	0.05180800	0.33929800
C	-2.08392800	-1.11942200	-0.03360400
C	-2.35244700	1.35880200	-0.00890800
C	-1.27501300	-0.98068000	-1.34476500
C	-1.24713800	1.38982600	-1.00967700
N	-1.46295500	0.30950800	-1.95054500
H	-1.45719700	-1.78028200	-2.07457300
H	-1.25899300	2.33759500	-1.56150900
C	-2.78177500	-2.45295000	0.07807700
O	-2.63925200	-3.36792800	-0.69472600
O	-3.53059000	-2.51604900	1.17554100
C	-4.36004400	-3.67316500	1.34521600
C	-5.60022000	-3.56684900	0.47801500
H	-3.77246200	-4.57130900	1.10447600
H	-4.61233600	-3.68192700	2.41388100
H	-6.13826800	-2.62761600	0.69098200
H	-6.27271200	-4.41623400	0.67949000
H	-5.32845700	-3.58010500	-0.58962700
H	-3.13390300	0.03356600	1.43357600
C	0.94957300	0.10623300	-0.79931200
C	0.07115100	-1.13646000	-0.54914400
C	0.17879300	1.32623000	-0.20815600
C	-0.71455500	-1.17266600	0.78981600
C	0.04071800	1.13068700	1.26080200
N	-0.44440700	-0.09369900	1.68367800
H	-0.60320700	-2.12236900	1.32908700
H	0.05595800	1.94813200	1.97753000
C	0.85966700	-2.36377500	-0.93719700

O	1.22577300	-2.55412900	-2.06989600
O	1.13359100	-3.17313900	0.08201200
C	2.03011500	-4.26477600	-0.17264200
C	3.47249300	-3.79882000	-0.09715000
H	1.80328200	-5.00546200	0.60563300
H	1.79586600	-4.69081100	-1.15852700
H	4.14803600	-4.64175100	-0.31569100
H	3.70831900	-3.41240500	0.90783100
H	3.66055800	-2.99749500	-0.83213700
H	0.98772800	0.23468300	-1.89116500
H	-0.92452000	0.42185200	-2.80632300
H	-0.64713200	-0.22791100	2.66637000
C	-2.61188600	2.52432200	0.82172200
O	-3.40733000	2.56214000	1.73919800
O	-1.83693900	3.56688200	0.47010300
C	-1.94306900	4.76028800	1.24984200
C	-3.12352200	5.60546200	0.81112400
H	-0.99086000	5.28485000	1.08788700
H	-2.02376700	4.48280600	2.31179400
H	-3.14325800	6.54620100	1.38424100
H	-3.04449700	5.85002100	-0.26015900
H	-4.06890200	5.06919300	0.98745600
C	0.96654900	2.57327500	-0.57413400
O	1.07261500	2.96197800	-1.71197800
O	1.55153400	3.15836300	0.46269000
C	2.40018300	4.28362400	0.19799400
C	3.76955800	3.82821000	-0.26761700
H	2.45795600	4.81828800	1.15555600
H	1.91298900	4.92857000	-0.54801700
H	4.20946700	3.12874300	0.46245600
H	3.69585000	3.31970800	-1.24162800
H	4.43818300	4.69782400	-0.37118800
C	-4.40552000	-0.05458600	-0.26513100
C	-5.50846700	0.34602800	0.49865500
C	-4.62074600	-0.54907400	-1.55671100
C	-6.80216400	0.24298200	-0.01146800
H	-5.34121500	0.74489900	1.50249400
C	-5.91643000	-0.65957400	-2.06529400
H	-3.76952800	-0.84690100	-2.17367900

C	-7.01083700	-0.26561300	-1.29510100
H	-7.65323000	0.55454400	0.59959000
H	-6.06872000	-1.05708600	-3.07198000
H	-8.02430300	-0.35385600	-1.69432200
C	2.38241000	-0.01379900	-0.32742100
C	3.40311700	0.35341200	-1.20884200
C	2.69033000	-0.51360200	0.94032500
C	4.74306700	0.21786100	-0.82413100
H	3.14076000	0.73418500	-2.19711200
C	4.02719000	-0.66992600	1.31825400
H	1.88400000	-0.81971100	1.60524800
C	5.05788800	-0.28163200	0.44891900
O	5.79798900	0.53453600	-1.60379300
O	6.35975600	-0.42587200	0.82296500
O	4.42266100	-1.20968600	2.49172300
C	5.54594900	0.98544400	-2.91482400
H	4.96905900	1.92663600	-2.91115800
H	6.52651800	1.16339200	-3.37588600
H	4.99905300	0.22537500	-3.49989300
C	3.42654200	-1.58175100	3.41723100
H	2.81336100	-0.71199700	3.71209200
H	2.76786700	-2.36632600	3.00390300
H	3.95181400	-1.97450200	4.29784600
C	6.90385500	-1.68785600	0.48004300
H	7.95262100	-1.69029400	0.81048200
H	6.35732100	-2.50117700	0.98970400
H	6.86414300	-1.84609800	-0.61229500



3a (S0)

Theoretical calculation level:

DFT-M062X/def2-TZVP//M062X/def2-SV

The number of imaginary frequencies: 0

Computed total energies: -2373.382528 Hartree

C	-2.72936200	-0.20010900	0.55026400
C	-1.83362000	-1.30043900	-0.02698700
C	-1.94995600	1.13386500	0.44275400
C	-1.12118500	-0.96956400	-1.36040600
C	-1.24716400	1.38866600	-0.91584100
N	-1.47546800	0.33197400	-1.87081500

H	-1.27352500	-1.73269300	-2.13478000
H	-1.48090600	2.35756000	-1.37497000
C	-2.51153300	-2.64725100	-0.02240900
O	-2.45284300	-3.45290000	-0.91744400
O	-3.16153700	-2.85084600	1.12115800
C	-3.99494100	-4.01325100	1.21622000
C	-5.30720200	-3.78050600	0.49058900
H	-3.45204500	-4.87828700	0.80781400
H	-4.14876300	-4.15926300	2.29360700
H	-5.78602000	-2.85656600	0.85702300
H	-5.98914900	-4.62854900	0.66340700
H	-5.13940300	-3.68070600	-0.59371900
H	-2.81071500	-0.40088400	1.63208600
C	1.03877800	0.25531000	-0.77259500
C	0.27611100	-1.07805200	-0.64214400
C	0.14363000	1.36226100	-0.17903200
C	-0.43112100	-1.33172700	0.71382600
C	-0.56015700	1.02660800	1.16258100
N	-0.21540800	-0.27966400	1.67389800
H	-0.18944000	-2.30050800	1.16884600
H	-0.41884300	1.77889900	1.94823400
C	1.16499700	-2.17009400	-1.18464300
O	1.49073800	-2.22022400	-2.34454500
O	1.58174200	-3.02382700	-0.25364000
C	2.60842900	-3.95357200	-0.62656200
C	3.97201300	-3.30287000	-0.48497900
H	2.49052300	-4.80119900	0.06165200
H	2.42430800	-4.29198800	-1.65585700
H	4.76091600	-4.00670700	-0.79638400
H	4.15386300	-3.01014700	0.56209300
H	4.03583000	-2.39861500	-1.11562200
H	1.07198700	0.46215100	-1.85562200
H	-1.04741400	0.52474200	-2.77451700
H	-0.66114600	-0.47416400	2.56901100
C	-2.83206200	2.24045000	0.96373100
O	-2.94037300	2.51570800	2.13282200
O	-3.53636100	2.81775000	-0.00216300
C	-4.58747000	3.70647800	0.39502600
C	-5.43645200	3.98047900	-0.82451300

H	-4.13843000	4.62417200	0.80785900
H	-5.16688000	3.21943300	1.19576400
H	-6.26421900	4.65686000	-0.56050900
H	-4.83768700	4.45223500	-1.61973400
H	-5.85987000	3.03846500	-1.21050000
C	0.90535100	2.66193600	-0.25626200
O	1.03544600	3.28680100	-1.27980700
O	1.45497900	3.00408200	0.90330300
C	2.33125300	4.13997300	0.91412500
C	3.70289100	3.76964600	0.38483600
H	2.37440300	4.44643200	1.96774400
H	1.87252500	4.94561700	0.32187100
H	4.10910900	2.90717500	0.94007500
H	3.64822400	3.50182000	-0.68215200
H	4.39124800	4.62234800	0.50065000
C	-4.15050200	-0.17783600	0.01660000
C	-5.17985700	0.22980700	0.87665800
C	-4.48383200	-0.57313600	-1.28298200
C	-6.50616200	0.25785000	0.44897200
H	-4.93466000	0.52576900	1.90205200
C	-5.81345600	-0.55863200	-1.71118100
H	-3.69803900	-0.89105800	-1.97097100
C	-6.82805000	-0.14070100	-0.85026000
H	-7.29233800	0.58096600	1.13616100
H	-6.05577400	-0.87655400	-2.72842000
H	-7.86724400	-0.12918500	-1.18821700
C	2.48337800	0.22479200	-0.30584300
C	3.47088600	0.60738900	-1.21872400
C	2.83767900	-0.21308300	0.97243900
C	4.82238400	0.55537800	-0.85453100
H	3.17635000	0.93722900	-2.21575500
C	4.18762200	-0.28910300	1.32837200
H	2.04780200	-0.50671600	1.66320600
C	5.18405600	0.11764900	0.42774300
O	5.84554700	0.90263100	-1.66346500
O	6.49742400	0.05707500	0.78469900
O	4.63031800	-0.76399700	2.51255300
C	5.54335900	1.36059400	-2.96110100
H	4.92439400	2.27461000	-2.92871600

H	6.50421200	1.58938300	-3.44093900
H	5.01886900	0.58575700	-3.54733500
C	3.66945700	-1.17154800	3.45966900
H	3.00740200	-0.33415600	3.74156000
H	3.05517400	-2.00434200	3.07339000
H	4.22793700	-1.50870700	4.34298500
C	7.10582200	-1.18182300	0.46682200
H	8.15643900	-1.11982100	0.78549500
H	6.60879900	-2.01016100	1.00222100
H	7.06363200	-1.36986500	-0.62084000

Initial input Cartesian coordinates for locating MECP

Initial input Cartesian coordinates for locating MECP between S1 and T1 of 1e

C	-2.09246200	0.82397800	0.07169100
C	-0.71366800	0.87587700	-0.48533000
C	0.08315800	2.08769900	0.04910300
C	-0.40741200	2.76555900	1.09583100
C	-2.33594900	1.35850000	1.32170900
H	-0.01342600	3.75474000	1.33057700
H	-3.33060600	1.38855400	1.72194800
C	-3.02405500	0.06997400	-0.70282500
O	-2.77669200	-0.56523200	-1.76281800
O	-4.30884300	0.02837200	-0.14417800
C	-5.30850800	-0.69859800	-0.85158200
C	-6.58684800	-0.58934900	-0.03709800
H	-5.00474100	-1.74389600	-0.98532500
H	-5.44253900	-0.28299600	-1.85900200
H	-7.41547600	-1.12347800	-0.52100400
H	-6.42581100	-1.01226000	0.96188700
H	-6.86437500	0.46554200	0.08045400
C	1.26640700	2.44464700	-0.64455000
O	1.74701400	1.83101000	-1.59290700
O	1.88012000	3.55590600	-0.11583000
C	3.10212400	3.95675400	-0.74083300
C	3.56943500	5.22195100	-0.04171500
H	2.93280800	4.12693000	-1.80971400
H	3.83855600	3.15063900	-0.64589500
H	4.51828400	5.55728100	-0.47676800
H	2.83460400	6.02688600	-0.15441200
H	3.72439200	5.04299100	1.02826500
N	-1.43319400	2.35655500	1.89239100
H	-0.75238700	0.97710500	-1.58418700
H	-1.88999600	3.08720600	2.42680100
C	0.09649300	-0.35723100	-0.23218300
C	0.34246800	-0.77976800	1.11767700
C	1.04287100	-1.91885500	1.42506500
C	1.63348900	-2.66796600	0.36197600
C	1.41830600	-2.19911100	-1.03569300

C	0.66091400	-1.04539700	-1.27922900
H	-0.06252400	-0.14355200	1.89785800
H	0.44510900	-0.70992000	-2.26506000
O	1.93002700	-2.94610500	-1.96405500
O	2.36668900	-3.74259500	0.56959100
O	1.25804100	-2.35784900	2.68005300
C	3.79797300	-3.50667000	0.78237500
H	3.95792100	-3.24954400	1.82784600
H	4.30595900	-4.42618100	0.51581300
H	4.11570300	-2.69484700	0.12897100
C	0.61609800	-1.55695300	3.69316700
H	0.79710400	-2.04535200	4.64150900
H	1.03991600	-0.54764900	3.70308300
H	-0.46154000	-1.50555800	3.50132500
C	1.73093500	-2.55658500	-3.36582800
H	2.70544100	-2.55498800	-3.83840000
H	1.04401400	-3.27054700	-3.81283700
H	1.31450300	-1.56179000	-3.42968300

Initial input Cartesian coordinates for locating MECP between S0 and T1 of IM1

C	-3.19168400	0.80348300	0.94930600
C	-1.95577300	0.72049500	-0.00463800
C	-3.79440900	-0.57105600	1.09515700
C	-2.30939300	-0.03459600	-1.24163300
C	-3.75543700	-1.44183100	0.05602200
H	-4.33422600	-0.83913500	2.00284800
N	-3.08892900	-1.14213600	-1.11074900
H	-1.81913300	0.13262300	-2.19771900
C	-1.42886900	2.11453700	-0.31312900
O	-1.58921800	3.06330000	0.40960100
O	-0.69929600	2.14930400	-1.42766300
C	-0.02671500	3.38147300	-1.72882000
C	-0.93692700	4.32558200	-2.48817300
H	0.84866500	3.08729900	-2.32479400
H	0.31645000	3.82670700	-0.78239400
H	-0.38394400	5.24043400	-2.75449200
H	-1.29775500	3.85266900	-3.41534100
H	-1.80350500	4.60829000	-1.86966900
H	-2.83853600	1.16153900	1.92805500
C	1.55924100	0.46893800	-0.30690200

C	0.36379000	-0.41392800	-0.09830400
C	1.56786100	1.61495000	0.67766800
C	-0.76415600	-0.03739200	0.80825600
C	0.72583500	1.64349500	1.74493800
N	-0.27899300	0.75082800	1.91774300
H	-1.23452100	-0.95387800	1.19339700
H	0.82696500	2.41323700	2.51333400
C	0.25100500	-1.60489500	-0.94602800
O	0.86656300	-1.75707200	-1.97900300
O	-0.60538700	-2.51215200	-0.45702000
C	-0.86262000	-3.66844100	-1.25954800
C	0.19607100	-4.73252200	-1.04165600
H	-1.85862000	-4.01372100	-0.94812900
H	-0.90502500	-3.36193400	-2.31633900
H	-0.05433800	-5.63467800	-1.62240800
H	0.25071600	-5.00656300	0.02410400
H	1.18202000	-4.36710100	-1.36869000
H	1.51653100	0.86255400	-1.34013700
H	-0.86083100	0.82840700	2.74265400
H	-3.18408600	-1.80412300	-1.87712800
C	2.54676200	2.67487700	0.44723200
O	3.26340000	2.73090700	-0.53076900
O	2.56075200	3.61685500	1.40823100
C	3.49593600	4.68634900	1.25980900
C	4.88742700	4.27070400	1.70007300
H	3.10318900	5.49391400	1.89307500
H	3.49458200	5.01938800	0.21116900
H	5.57387800	5.13078300	1.64260400
H	4.86862900	3.90833600	2.74051300
H	5.27298700	3.47044700	1.04950500
C	-4.42171900	-2.77024000	0.03930200
O	-4.34719100	-3.52175800	-0.90653400
O	-5.09115400	-3.03173700	1.15213100
C	-5.78770900	-4.28493700	1.22227600
C	-7.12125600	-4.21068800	0.50528400
H	-5.91855400	-4.46810500	2.29681600
H	-5.14458200	-5.06896700	0.79661200
H	-6.97469800	-4.03064500	-0.57099700
H	-7.66090400	-5.16303200	0.62896800

H	-7.73971700	-3.40136400	0.92450200
C	-4.25351500	1.79700500	0.48504400
C	-4.51163700	2.95608900	1.22590200
C	-5.00191300	1.56767800	-0.67770400
C	-5.48324200	3.86861200	0.81473500
H	-3.93106800	3.15173500	2.13156100
C	-5.96789500	2.48315200	-1.09695600
H	-4.84257500	0.65637000	-1.25856700
C	-6.21221800	3.63775800	-0.35321000
H	-5.66948100	4.76746000	1.40811700
H	-6.53816200	2.28601600	-2.00827700
H	-6.97145900	4.35273700	-0.67987300
C	2.84856600	-0.34853100	-0.19269700
C	3.77577200	-0.34263400	-1.23122100
C	3.07902500	-1.09589800	0.96565800
C	4.95284100	-1.09189100	-1.11520200
H	3.57497700	0.25864400	-2.11758600
C	4.25274600	-1.85022000	1.08384300
H	2.34254500	-1.07138100	1.77193200
C	5.18291100	-1.86656600	0.03185900
O	4.57737500	-2.59820800	2.16060400
O	5.92215600	-1.14077400	-2.05457400
O	6.31302200	-2.62216600	0.13153900
C	3.66456400	-2.65123500	3.23169200
H	3.51139400	-1.65314000	3.67859100
H	2.69055300	-3.05712800	2.90591600
H	4.10412600	-3.32150100	3.98227600
C	5.75299000	-0.37170300	-3.22238300
H	4.85506600	-0.68614200	-3.78259300
H	5.67527000	0.70403900	-2.98555900
H	6.64430100	-0.54521400	-3.84011500
C	7.41504800	-1.92284900	0.67907100
H	8.26257000	-2.62289300	0.70790200
H	7.67997800	-1.05440500	0.05085600
H	7.18977500	-1.58014400	1.70462400

Initial input Cartesian coordinates for locating MECP between S0 and T1 of IM2

C	-3.24168100	0.08117400	0.25207900
C	-2.14071700	0.91668300	-0.33209300
C	-3.77525800	-0.91582700	-0.74340800

C	-1.65355100	0.82122500	-1.74094000
C	-3.43377000	-0.84959700	-2.05542600
N	-2.54643600	0.03670200	-2.55995700
H	-1.58952000	1.84352300	-2.14765700
H	-3.88392500	-1.53202000	-2.77985800
C	-1.47350200	1.85532100	0.57360800
O	-1.57219000	1.82286700	1.78099400
O	-0.72893300	2.75321800	-0.08693500
C	-0.03852600	3.74188100	0.68583900
C	-0.98229600	4.81979600	1.18500000
H	0.70771700	4.15635600	-0.00570100
H	0.48373400	3.24299800	1.51811300
H	-0.40696800	5.60052500	1.70761000
H	-1.51202400	5.28585100	0.33870500
H	-1.72059600	4.40126400	1.88552200
H	-2.83961900	-0.44498700	1.13978500
C	1.66506200	0.65954500	0.05902700
C	0.49155900	-0.05916600	-0.54072500
C	2.09563100	1.82722400	-0.78898100
C	-0.12515800	0.26904700	-1.86127600
C	1.62514800	1.98866600	-2.05159600
N	0.69247400	1.18925000	-2.61613500
H	-0.23280800	-0.67003800	-2.42832400
H	2.00378600	2.79292900	-2.68636800
C	-0.10092900	-1.13853800	0.25341500
O	0.10703600	-1.30911700	1.43504700
O	-0.91100100	-1.91733500	-0.47726300
C	-1.52739900	-3.03269600	0.17666700
C	-0.54264000	-4.16772200	0.38632500
H	-2.34098600	-3.32976200	-0.49928900
H	-1.96197100	-2.69069200	1.12981000
H	-1.06415800	-5.03241200	0.82677500
H	-0.10585000	-4.47757400	-0.57661600
H	0.26689900	-3.86312400	1.06705800
H	1.37944000	1.00572600	1.07049800
H	0.41149100	1.38247100	-3.57037600
H	-2.36371800	0.01617800	-3.55632400
C	3.03953200	2.76421300	-0.19218900
O	3.46683500	2.66432100	0.93955100

O	3.37193300	3.78748400	-1.00337300
C	4.30851200	4.74196200	-0.50155400
C	5.73492700	4.24398400	-0.63949400
H	4.06634300	4.96271500	0.54863100
H	4.14150500	5.64532000	-1.10463400
H	6.43955600	5.02034300	-0.30039900
H	5.88766700	3.34210000	-0.02625200
H	5.95909300	4.00389900	-1.69126000
C	-4.65485200	-1.95556200	-0.22417100
O	-4.94169700	-2.07228000	0.94977200
O	-5.09319300	-2.81500000	-1.16438500
C	-5.95005200	-3.87320900	-0.73265200
C	-7.38504500	-3.40386400	-0.58538400
H	-5.56676800	-4.27746300	0.21604300
H	-5.86122500	-4.64334500	-1.51152500
H	-8.03181500	-4.25364500	-0.31353300
H	-7.46145300	-2.64005800	0.20395600
H	-7.75026000	-2.97683000	-1.53322300
C	-4.36018400	0.99780400	0.75505700
C	-4.76948900	0.98227700	2.08923400
C	-4.98824700	1.87089400	-0.13994100
C	-5.79223600	1.82679400	2.52442700
H	-4.28408900	0.29776200	2.78985100
C	-6.00803500	2.71879000	0.29162000
H	-4.67561200	1.88199000	-1.19025100
C	-6.41296300	2.69814800	1.62803500
H	-6.10567600	1.80433200	3.57137900
H	-6.48784300	3.39781400	-0.41776700
H	-7.21183100	3.36071900	1.97018600
C	2.81395000	-0.33673700	0.24542100
C	3.29481700	-0.65266100	1.50990500
C	3.36469800	-0.94602300	-0.89046600
C	4.33355300	-1.57848100	1.64703000
H	2.87885400	-0.19004400	2.40671000
C	4.40452600	-1.86965100	-0.76057200
H	2.97974600	-0.67428300	-1.87632800
C	4.88367900	-2.20076200	0.52315400
O	5.01471100	-2.49016500	-1.79101100
O	5.89220100	-3.10903500	0.65318800

O	4.82953200	-1.85648000	2.88702200
C	4.53342100	-3.15749400	3.36904600
H	4.96943900	-3.23102300	4.37530400
H	3.44036700	-3.30356700	3.43403800
H	4.97294700	-3.92974700	2.71748000
C	7.17325500	-2.51766200	0.79174500
H	7.42481300	-1.92236000	-0.10362400
H	7.20941600	-1.87376600	1.68745200
H	7.89779400	-3.33729900	0.89912700
C	4.58865500	-2.18090500	-3.09759500
H	3.52489400	-2.43869700	-3.24317200
H	4.73742900	-1.10999600	-3.32240400
H	5.20525800	-2.78477000	-3.77638600

Initial input Cartesian coordinates for locating MECP between S0 and T1 of IM3

C	-2.60294400	0.38007700	0.33199100
C	-1.88934700	1.57885600	-0.25710100
C	-2.75272200	-0.72345200	-0.67999500
C	-1.74349400	1.72390600	-1.59682100
C	-2.06076500	-0.63577100	-2.00085200
N	-2.05310000	0.73061800	-2.46932900
H	-1.34130500	2.64629600	-2.02232200
H	-2.58635200	-1.25468000	-2.73909400
C	-1.34757700	2.57214400	0.67113500
O	-1.28373400	2.40168200	1.87152600
O	-0.88196500	3.67558400	0.06720500
C	-0.20792700	4.63184900	0.88722900
C	-1.19082700	5.53750700	1.60473700
H	0.42702600	5.19977300	0.19321100
H	0.44005400	4.09462800	1.59482800
H	-0.64617800	6.30968600	2.17178100
H	-1.85133400	6.03955200	0.87937500
H	-1.80845300	4.95626100	2.30670100
H	-2.02348300	-0.00058900	1.19557200
C	1.04183300	0.11225500	-0.32858100
C	1.24990900	0.92867000	-1.58174200
C	0.08035800	-1.01319300	-0.56946300
C	0.93513900	0.42434900	-2.80286200
C	-0.56589200	-1.25731700	-1.89547300
N	0.26324100	-0.74753400	-2.96567800

H	1.20736300	0.95927700	-3.71634000
H	-0.70468900	-2.34036400	-2.02104000
C	1.80940300	2.26890000	-1.41456100
O	2.05693800	2.76809300	-0.33624500
O	1.99439500	2.92225900	-2.57553000
C	2.55217600	4.23529600	-2.50634300
C	4.05864000	4.19215000	-2.33180200
H	2.27553700	4.70954200	-3.45829400
H	2.07232800	4.78322600	-1.68155400
H	4.46794400	5.21515700	-2.34350500
H	4.52491800	3.62084800	-3.15053600
H	4.32132800	3.72077600	-1.37193200
H	0.63430600	0.75496500	0.47334400
H	0.04872800	-1.05254900	-3.90873700
H	-1.83822500	0.87849900	-3.44825900
C	-3.42698700	-1.95596600	-0.27207900
O	-3.82056400	-2.17222600	0.85400900
O	-3.55775500	-2.82807300	-1.28298900
C	-4.28444800	-4.03198200	-1.01869400
C	-5.77879600	-3.79808900	-1.13268200
H	-4.01751700	-4.39792100	-0.01672600
H	-3.92966700	-4.74847300	-1.77196700
H	-6.31913200	-4.74599300	-0.98016200
H	-6.11613100	-3.07803300	-0.37026200
H	-6.03222900	-3.40682900	-2.13082600
C	-0.23063200	-1.86931000	0.57636700
O	0.04353200	-1.58425900	1.72301200
O	-0.85638700	-3.00464400	0.22931800
C	-1.16083500	-3.92642900	1.28314500
C	0.06654200	-4.72445100	1.68074600
H	-1.94155600	-4.57673800	0.86582300
H	-1.57749700	-3.36600700	2.13270100
H	-0.20659100	-5.47282800	2.44163700
H	0.48243300	-5.25042300	0.80639800
H	0.83911200	-4.06277700	2.10222200
C	-3.96272900	0.81938400	0.87668700
C	-4.18857300	0.90900300	2.25133500
C	-4.98833500	1.17106600	-0.00786400
C	-5.42446100	1.33900300	2.73774600

H	-3.38542600	0.64207100	2.94324900
C	-6.22548800	1.59626500	0.47489600
H	-4.81134700	1.11187200	-1.08745900
C	-6.44652400	1.68129300	1.85155700
H	-5.59011900	1.40455400	3.81613500
H	-7.02020000	1.86458900	-0.22580800
H	-7.41464900	2.01641900	2.23206300
C	2.38274200	-0.42607000	0.17897800
C	3.01238700	0.18994000	1.25821600
C	2.97260700	-1.51927500	-0.46332500
C	4.25182300	-0.28774200	1.70420400
H	2.53524300	1.04963800	1.72750600
C	4.20382000	-2.00735000	-0.01069800
H	2.46943400	-1.97511600	-1.31873800
C	4.83665100	-1.40455600	1.08900800
O	4.95476000	0.25268200	2.72198800
O	6.02308200	-1.89345900	1.54774100
O	4.86056700	-3.05302700	-0.55702500
C	4.27185800	-3.70571500	-1.65771800
H	4.95668800	-4.51553000	-1.94236200
H	3.29040000	-4.13491900	-1.38857400
H	4.14545200	-3.01652300	-2.51111000
C	7.15199200	-1.36387400	0.87763300
H	7.11677400	-1.60431500	-0.19945700
H	7.20654600	-0.26861700	1.00913300
H	8.04255900	-1.82835600	1.32529100
C	4.43323200	1.40069700	3.35102900
H	4.30776300	2.22781700	2.63020500
H	3.46274000	1.18851700	3.83258500
H	5.16258700	1.69273900	4.11837900

Initial input Cartesian coordinates for locating MECF between S0 and T1 of IM4

C	-2.63550900	0.00428200	-0.12196000
C	-2.15675100	-1.47537900	-0.07600600
C	-1.93135600	0.73018900	-1.24667000
C	-2.12398100	-2.06792500	-1.44690900
C	-1.59039800	0.06844800	-2.39176600
N	-1.75235700	-1.27778200	-2.49690800
H	-2.23155600	-3.13462500	-1.62258400
H	-1.16025200	0.57400100	-3.25639900

C	-3.10124100	-2.32460700	0.77801200
O	-3.53883300	-3.39670000	0.45270000
O	-3.35987500	-1.74727800	1.95083900
C	-4.34657400	-2.37246700	2.78978400
C	-5.74469300	-2.10223600	2.26897600
H	-4.13259400	-3.45000100	2.84226300
H	-4.18930900	-1.92353300	3.77923600
H	-5.91295800	-1.01780900	2.16187000
H	-6.48677000	-2.51082100	2.97377600
H	-5.89303000	-2.57791300	1.28680600
H	-2.34948100	0.48883300	0.81988600
C	1.08159300	0.22778700	-0.10842000
C	0.40141600	-1.10114900	-0.27587900
C	0.50929800	0.99721500	1.05700900
C	-0.70003700	-1.58630100	0.62095300
C	-0.24015800	0.37602200	2.00037100
N	-0.64318200	-0.91817900	1.90468400
H	-0.54796900	-2.66637400	0.77616500
H	-0.56666500	0.91464400	2.89324600
C	0.90342200	-1.95346400	-1.35846400
O	1.54075300	-1.53251000	-2.29935900
O	0.59231400	-3.24753000	-1.19832700
C	1.03049200	-4.15558400	-2.21370800
C	2.48078000	-4.54797100	-2.00486100
H	0.36201000	-5.02270100	-2.12307800
H	0.88094800	-3.68658000	-3.19802900
H	2.78258500	-5.28845500	-2.76274100
H	2.61776900	-4.99384100	-1.00647900
H	3.13534700	-3.66685600	-2.09554600
H	0.94669500	0.81284600	-1.03591600
H	-1.57284800	-1.71836100	-3.39407900
H	-1.30218600	-1.24865800	2.60106800
C	-1.67734200	2.16071900	-1.08394200
O	-2.00388600	2.80684700	-0.10756500
O	-1.02100000	2.70083500	-2.12550100
C	-0.73808100	4.10068800	-2.06933600
C	-1.95643000	4.92879200	-2.43372600
H	0.07296100	4.24911700	-2.79620900
H	-0.36164900	4.34376100	-1.06553200

H	-1.69116800	5.99829800	-2.45376400
H	-2.33217100	4.64446800	-3.42993700
H	-2.75827200	4.78128800	-1.69373000
C	0.77828800	2.43194300	1.11674400
O	1.33107200	3.05155300	0.22980900
O	0.33321600	3.01780900	2.23985300
C	0.47170900	4.43471300	2.33904600
C	1.87272200	4.83226300	2.76561200
H	-0.27106600	4.73811400	3.09028400
H	0.20462900	4.88893100	1.37246000
H	2.13531500	4.34460800	3.71821700
H	2.60619300	4.53779500	1.99930400
H	1.92836600	5.92389600	2.90548800
C	-4.14954600	0.16091200	-0.22135700
C	-4.77656700	1.14354100	0.55625200
C	-4.94036900	-0.62068400	-1.07448200
C	-6.15599400	1.33655100	0.49331700
H	-4.16357400	1.76652300	1.21289700
C	-6.32337100	-0.43633900	-1.13069100
H	-4.48018000	-1.39283500	-1.69754800
C	-6.93691000	0.54147100	-0.34823400
H	-6.62490300	2.10776200	1.10993000
H	-6.92476600	-1.06349000	-1.79395600
H	-8.01914900	0.68559000	-0.39484000
C	2.58788200	0.03285600	0.08490300
C	3.48841900	0.85098400	-0.59398800
C	3.04398200	-0.95161300	0.96723800
C	4.86496200	0.68652400	-0.39029900
H	3.10312100	1.61402900	-1.26940900
C	4.41871000	-1.12446500	1.16546700
H	2.32021400	-1.57744400	1.49345100
C	5.33289500	-0.28923000	0.50319000
O	5.81843500	1.41850400	-1.00493300
O	6.67078800	-0.43641700	0.71805200
O	4.96293200	-2.05906900	1.97368400
C	5.40941100	2.40893800	-1.91974000
H	4.78686000	3.17592100	-1.42640000
H	6.32689100	2.87557100	-2.30242500
H	4.84548200	1.96837900	-2.76054900

C	4.09329700	-2.93547600	2.65147700
H	3.41927900	-2.38356200	3.32984200
H	3.48909500	-3.52791300	1.94146900
H	4.72823500	-3.60972200	3.24150000
C	7.29467300	-1.33071700	-0.18444100
H	8.36137600	-1.36793000	0.08010500
H	6.86021600	-2.34225700	-0.09503700
H	7.18853600	-0.97469500	-1.22436200

Initial input Cartesian coordinates for locating MECP between S0 and T1 of IM42-2

C	-3.00641600	0.05180800	0.33929800
C	-2.08392800	-1.11942200	-0.03360400
C	-2.30019509	1.35382138	0.01881461
C	-1.27501300	-0.98068000	-1.34476500
C	-1.24713800	1.38982600	-1.00967700
N	-1.46295500	0.30950800	-1.95054500
H	-1.45719700	-1.78028200	-2.07457300
H	-1.25899300	2.33759500	-1.56150900
C	-2.78177500	-2.45295000	0.07807700
O	-2.63925200	-3.36792800	-0.69472600
O	-3.53059000	-2.51604900	1.17554100
C	-4.36004400	-3.67316500	1.34521600
C	-5.60022000	-3.56684900	0.47801500
H	-3.77246200	-4.57130900	1.10447600
H	-4.61233600	-3.68192700	2.41388100
H	-6.13826800	-2.62761600	0.69098200
H	-6.27271200	-4.41623400	0.67949000
H	-5.32845700	-3.58010500	-0.58962700
H	-3.13390300	0.03356600	1.43357600
C	0.94957300	0.10623300	-0.79931200
C	0.07115100	-1.13646000	-0.54914400
C	0.17879300	1.32623000	-0.20815600
C	-0.71455500	-1.17266600	0.78981600
C	-0.01153391	1.13566762	1.23307939
N	-0.44440700	-0.09369900	1.68367800
H	-0.60320700	-2.12236900	1.32908700
H	0.05595800	1.94813200	1.97753000
C	0.85966700	-2.36377500	-0.93719700
O	1.22577300	-2.55412900	-2.06989600
O	1.13359100	-3.17313900	0.08201200

C	2.03011500	-4.26477600	-0.17264200
C	3.47249300	-3.79882000	-0.09715000
H	1.80328200	-5.00546200	0.60563300
H	1.79586600	-4.69081100	-1.15852700
H	4.14803600	-4.64175100	-0.31569100
H	3.70831900	-3.41240500	0.90783100
H	3.66055800	-2.99749500	-0.83213700
H	0.98772800	0.23468300	-1.89116500
H	-0.92452000	0.42185200	-2.80632300
H	-0.64713200	-0.22791100	2.66637000
C	-2.61188600	2.52432200	0.82172200
O	-3.40733000	2.56214000	1.73919800
O	-1.83693900	3.56688200	0.47010300
C	-1.94306900	4.76028800	1.24984200
C	-3.12352200	5.60546200	0.81112400
H	-0.99086000	5.28485000	1.08788700
H	-2.02376700	4.48280600	2.31179400
H	-3.14325800	6.54620100	1.38424100
H	-3.04449700	5.85002100	-0.26015900
H	-4.06890200	5.06919300	0.98745600
C	0.96654900	2.57327500	-0.57413400
O	1.07261500	2.96197800	-1.71197800
O	1.55153400	3.15836300	0.46269000
C	2.40018300	4.28362400	0.19799400
C	3.76955800	3.82821000	-0.26761700
H	2.45795600	4.81828800	1.15555600
H	1.91298900	4.92857000	-0.54801700
H	4.20946700	3.12874300	0.46245600
H	3.69585000	3.31970800	-1.24162800
H	4.43818300	4.69782400	-0.37118800
C	-4.40552000	-0.05458600	-0.26513100
C	-5.50846700	0.34602800	0.49865500
C	-4.62074600	-0.54907400	-1.55671100
C	-6.80216400	0.24298200	-0.01146800
H	-5.34121500	0.74489900	1.50249400
C	-5.91643000	-0.65957400	-2.06529400
H	-3.76952800	-0.84690100	-2.17367900
C	-7.01083700	-0.26561300	-1.29510100
H	-7.65323000	0.55454400	0.59959000

H	-6.06872000	-1.05708600	-3.07198000
H	-8.02430300	-0.35385600	-1.69432200
C	2.38241000	-0.01379900	-0.32742100
C	3.40311700	0.35341200	-1.20884200
C	2.69033000	-0.51360200	0.94032500
C	4.74306700	0.21786100	-0.82413100
H	3.14076000	0.73418500	-2.19711200
C	4.02719000	-0.66992600	1.31825400
H	1.88400000	-0.81971100	1.60524800
C	5.05788800	-0.28163200	0.44891900
O	5.79798900	0.53453600	-1.60379300
O	6.35975600	-0.42587200	0.82296500
O	4.42266100	-1.20968600	2.49172300
C	5.54594900	0.98544400	-2.91482400
H	4.96905900	1.92663600	-2.91115800
H	6.52651800	1.16339200	-3.37588600
H	4.99905300	0.22537500	-3.49989300
C	3.42654200	-1.58175100	3.41723100
H	2.81336100	-0.71199700	3.71209200
H	2.76786700	-2.36632600	3.00390300
H	3.95181400	-1.97450200	4.29784600
C	6.90385500	-1.68785600	0.48004300
H	7.95262100	-1.69029400	0.81048200
H	6.35732100	-2.50117700	0.98970400
H	6.86414300	-1.84609800	-0.61229500