

Electronic Supplementary Information

Excited-State Dependent Hydrogen Bond Natures and Their Critical Role in Determining the Photophysical Properties of Aromatic Thioketones

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1. Computational details

Aromatic thioketones of 2-hydroxy-pivalo-thiophenone (2HTP), 7-hydroxy-2,2,3,3-tetrahydro-1H-indene-1-thione(7HIT), and 7-hydroxy-2,2-dimethyl-3,3-dihydro-1H-indene-1-thione (DM-7HIT), and their non-H-bonded isomers (2HTP-iso, 7HIT-iso, and DM-7HIT-iso) were taken as representative systems in the present work. The five lowest-lying electronic states (S_0 , S_1 , T_1 , S_2 , and T_2) of these aromatic thioketones have been explored in order to understand the excited-state dependent H-bond interaction and its critical role in determining the photophysical properties. Multistate complete active space second-order perturbation theory (MS-CASPT2) developed by Roos and coworkers^{1,2} has been proved to afford high-accuracy treatment of excited states, but with less computational effort in comparison with multireference configuration interaction and coupled cluster theory. Therefore, the MS-CASPT2 method has been used to determine minimum-energy stationary and intersection structures, as well as their relative energies. The Cholesky decomposition technique was used to treat two-electron integrals and accelerate the MS-CASPT2 calculation.³ The imaginary shift of 0.2 a.u. was used to eliminate potential intruder state,⁴ and the ionization potential-electron affinity (IPEA) shift value was set to zero.⁵ As usual, 1s orbitals of C and O atoms as well as 1s, 2s, and 2p orbitals of S atom are kept frozen in the present MS-CASPT2 calculations.

The spin-orbit coupling (SOC) constant was calculated with atomic mean-field (AMFI) approximation.^{6,7} The equation can be expressed as follows:

$$\langle \Psi_I | H_{eff}^{so} | \Psi_J \rangle = \sqrt{|\langle \Psi_I | H_x^{so} | \Psi_J \rangle|^2 + |\langle \Psi_I | H_y^{so} | \Psi_J \rangle|^2 + |\langle \Psi_I | H_z^{so} | \Psi_J \rangle|^2}$$

where H_x^{so} , H_y^{so} , and H_z^{so} represent x, y, and z components of the SOC operator, respectively. After the MS-CASPT2 calculations, the CASSCF wavefunctions of Ψ_I and Ψ_J for the singlet and triplet states were used to construct the SOC matrix. Meanwhile, the MS-CASPT2 calculated energies were set as the diagonal elements of the matrix. Subsequently, the matrix was diagonalized to get the energies that contain both SOC

effects and electron correlation. The penalty function algorithm has been implemented to optimize the minimum-energy intersection structure of the S_1 , T_2 , and T_1 states (MEI- $S_1/T_2/T_1$),⁸ which was based on the MS-CASPT2 calculated energies and energy gradients. All the MS-CASPT2 calculations, together with cc-pVDZ, aug-cc-pVDZ, and cc-pVTZ basis sets,⁹ have been performed using OpenMolcas software.^{10,11}

The choice of the active space is crucial to the MS-CASPT2 calculation, which is to a certain extent dependent on an understanding of electronic structure. Since the σ orbitals are well separated from the non-bonding orbital (n) of the S atom and the conjugated π orbitals in energy, in principle, one non-bonding, four π and four π^* orbitals should be selected as the active orbitals. In addition, the lone-pair electrons of the O atom exhibit the conjugated interactions with the π electrons distributed in the aromatic ring, which should be included in the active space. Therefore, the active space of the MS-CASPT2 calculation is composed of twelve electrons distributed in ten orbitals, referred to as MS-PT2(12,10). These active orbitals are plotted in Figures S1 – S3 for 2HTP and 2HTP-iso, 7HIT and 7HIT-iso, and DM-7HIT and DM-7HIT-iso, respectively. It can be reasonably expected that the MS-PT2(12,10) calculations will provide a balanced description for the S_0 , $^{1,3}n\pi^*$, and $^{1,3}\pi\pi^*$ states of the aromatic thioketones under study.

The minimum-energy structures of 7HIT in the S_0 , S_1 , S_2 , T_1 , and T_2 states were firstly determined by the MS-PT2(12,10) optimizations with cc-pVDZ, aug-cc-pVDZ, and cc-pVTZ basis sets, referred to as MS-PT2(12,10)-DZ, MS-PT2(12,10)-augDZ, and MS-PT2(12,10)-TZ, respectively. The optimized minimum-energy structures of 7HIT in the S_0 , S_1 , S_2 , T_1 , and T_2 states are represented as $S_{0\text{-min}}$, $S_{1\text{-min}}$, $S_{2\text{-min}}$, $T_{1\text{-min}}$, and $T_{2\text{-min}}$, respectively. As shown in Figures S4 - S8, the MS-PT2(12,10)-DZ optimized bond lengths in the $S_{0\text{-min}}$, $S_{1\text{-min}}$, $T_{1\text{-min}}$, and $T_{2\text{-min}}$ structures are slightly elongated ($< 0.01\text{\AA}$) due to additional diffuse basis functions. However, the MS-PT2(12,10)-augDZ optimized bond lengths in the $S_{2\text{-min}}$ structure exhibit a little fluctuation ($< 0.01\text{\AA}$) with respect to those from the MS-PT2(12,10)-DZ optimizations, except that the C-S and S...H distances are elongated by $\sim 0.02\text{\AA}$. Unlike the effect of the diffuse basis

functions, the MS-PT2(12,10) optimized bond lengths of 7HIT in the ground and four excited states are generally shortened (~ 0.02 Å) as the size of basis set increases from cc-pVDZ to cc-pVTZ, with the maximum shrinkage of ~ 0.04 Å for the S...H distance in the $S_{1-\min}$ and $T_{1-\min}$ structures. It should be pointed out that the relative differences between the ground and excited states are closely relevant to the effect of basis set on the H-bond structures of the excited states. As plotted in Figures S9 – S12, the change in basis set from cc-pVDZ to aug-cc-pVDZ and to cc-pVTZ have a little influence on the relative differences of bond length, with the largest relative difference of 0.024 Å for the S...H distance. Overall, the MS-PT2(12,10) optimized $S_{0-\min}$, $S_{1-\min}$, $S_{2-\min}$, $T_{1-\min}$, and $T_{2-\min}$ structures exhibit a small dependent on the basis sets used herein, which is reflected by the MS-PT2(12,10)-DZ, MS-PT2(12,10)-augDZ, and MS-PT2(12,10)-TZ calculated relative energies of the excited states. As listed in Table S1, adiabatic excitation energies calculated at the MS-PT2(12,10)-DZ level are decreased by 0.0 - 0.07 eV (0.0 – 1.6 kcal/mol) as compared with those from the MS-PT2(12,10)-augDZ and MS-PT2(12,10)-TZ calculations. In addition, the vertical excitation energies from S_0 to S_1 and S_2 were calculated on the basis of the MS-PT2(12,10)-DZ, MS-PT2(12,10)-augDZ, and MS-PT2(12,10)-TZ optimized $S_{0-\min}$ structures. As listed in Table S2, the vertical excitation energies calculated with different basis sets are close to each other, and the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ absorption peaks are well reproduced by the MS-PT2(12,10)-DZ calculations.

The maxima of absorption and emission bands of pyranthione (PT), benzopyranthione (BPT), xanthione (XT) in inert media and the origins of these bands were determined experimentally.^{12,13} These experimental results have been used to ascertain the reliability of the MS-CASPT2 calculations. The stationary and intersection structures in the five lowest-lying states were optimized at the MS-PT2(10,8)-DZ, MS-PT2(12,10)-DZ, and MS-PT2(12,11)-DZ levels for PT, BPT, and XT, respectively. Then, the vertical excitation energies (VE), the emission energies (EE), and the adiabatic excitation energies (AE) were calculated at the same level of theory. The calculated results for PT, BPT, and XT as well the relevant experimental values are

listed in Table S3. The $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ absorption peaks for the three thioketones are well reproduced by the MS-PT2(10,8)-DZ, MS-PT2(12,10)-DZ, and MS-PT2(12,11)-DZ calculations for PT, BPT, and XT, respectively. The mean deviations are 0.04 and 0.08 eV for the first and second absorption bands, respectively. The calculated $S_2 \rightarrow S_0$ and $T_1 \rightarrow S_0$ emission energies are consistent with the fluorescent and phosphorescent maxima of the three thioketones in inert media (Table S3). In comparison with the $S_0 \rightarrow T_1$, $S_0 \rightarrow S_1$, and $S_0 \rightarrow S_2$ absorption band origins, the mean absolute deviations of the calculated adiabatic excitation energies (AE) are 0.10, 0.14, and 0.18 eV, respectively. The deviations between the calculated AE energy and the corresponding band origin can be improved, once the vibrational zero-point energy correction is included in the calculated AE energy. The above comparison makes it clear that the deviations in the calculated relative energies for the excited states of PT, BPT, and XT are within chemical accuracy (< 0.2 eV). Obviously, the excited-state properties of PT, BPT, and XT can be reliably described by the MS-CASPT2 calculations with the cc-pVDZ basis set.

The minimum-energy conical intersection between S_2 and S_1 states (MECI- S_2/S_1) of 7HIT was optimized at the MS-PT2(12,10)-DZ, MS-PT2(12,10)-augDZ, and MS-PT2(12,10)-TZ levels. As shown in Figure S13, the effect of basis set on the MECI- S_2/S_1 structure is almost the same as that on the minimum-energy structures of the ground and excited states. Recently, the extended multi-state complete active space second-order perturbation theory (XMS-CASPT2)¹⁴ was demonstrated to be well suited for the description of conical intersections of potential energy surfaces. For comparison, the MECI- S_2/S_1 structure was further optimized at the XMS-PT2(12,10)-DZ level. XMS-PT2(12,10)-DZ and MS-PT2(12,10)-DZ calculation adopt the same imaginary and IPEA shift values. It can be seen from Figure S13 that the XMS-PT2(12,10)-DZ optimized MECI- S_2/S_1 structure is nearly the same as that from MS-PT2(12,10)-DZ optimization, except for a slight fluctuation in the XMS-PT2(12,10)-DZ optimized bond parameters. From the above comparison and discussion, it can be concluded that the MS-PT2(12,10)-DZ calculation can accurately describe structures

and energies of 7HIT and the related aromatic thioketones in the five lowest-lying states.

2. Tables

Table S1. Adiabatic excitation energies (eV) determined at the various levels of theory for 7HIT, together with the relative energies of MECI-S₂/S₁ with respect to the S₀ minimum.

	S ₀ -min→S ₁ - min	S ₀ -min→S ₂ - min	S ₀ -min→T ₁ - min	S ₀ -min→T ₂ - min	MECI-S ₂ /S ₁
MS-PT2(12,10)-DZ	2.33	2.91	2.20	2.32	2.94/2.93
MS-PT2(12,10)- augDZ	2.28	2.84	2.16	2.30	2.85/2.84
XMS-PT2(12,10)- DZ	2.39	2.92	2.21	2.43	2.94/2.92
MS-PT2(12,10)-TZ	2.28	2.87	2.16	2.32	2.86/2.84

Table S2. The S₀→S₁ and S₀→S₂ vertical excitation energies (eV) calculated at various levels of theory, together with the energies (eV) corresponding to the absorption peaks.

	S ₁ (1nπ*)	S ₂ (1ππ*)
MS-PT2(12,10)-DZ	2.51	3.26
MS-PT2(12,10)-augDZ	2.45	3.18
MS-PT2(12,10)-TZ	2.42	3.17
Exp. ^a	2.58	3.26

a: Experimental values from Ref.¹⁵

Table S3. The vertical excitation (VE) and emission energies (EE, eV) as well as adiabatic excitation energies (AE, eV) calculated at the MS-PT2(10,8)-DZ, MS-PT2(12,10)-DZ, and MS-PT2(12,11)-DZ levels for PT, BPT, and XT, respectively, together with the maxima (eV) of the absorption and emission bands as well as their band origins (eV) in parentheses.^a

	S ₀ →S ₁		S ₀ →S ₂		S ₂ →S ₀	T ₂ →S ₀	T ₁ →S ₀	
	VE	AE	VE	AE	EE	AE	AE	EE
PT ^b	2.15 (2.19)	1.99 (2.21)	3.74 (3.76)	3.57 (3.45)	3.25 (3.34)	2.07	1.94 (2.13)	1.92 (1.97)
BPT ^c	2.11 (2.08)	1.97 (2.08)	3.55 (3.45)	3.34 (3.21)	2.98 (2.90)	2.05	1.93 (1.99)	1.90 (1.93)
XT ^d	2.04 (1.98)	1.89 (1.98)	3.39 (3.10)	3.26 (2.97)	2.87 (2.76)	2.02	1.84 (1.88)	1.80 (1.84)
MAE ^e	0.04	0.14	0.08	0.18	0.07	-	0.10	0.04

a: The relative energies in eV;

b: The experimental values for PT comes from Refs. ^{12, 13, 16-20}

- c: The experimental values for BPT comes from Refs. ^{12, 13, 16-19, 21, 22}
- d: The experimental values for XT comes from Refs. ^{12, 13, 16-18, 21, 23}
- e: MAE (Mean absolute error): an average of the absolute errors.

3. Figures

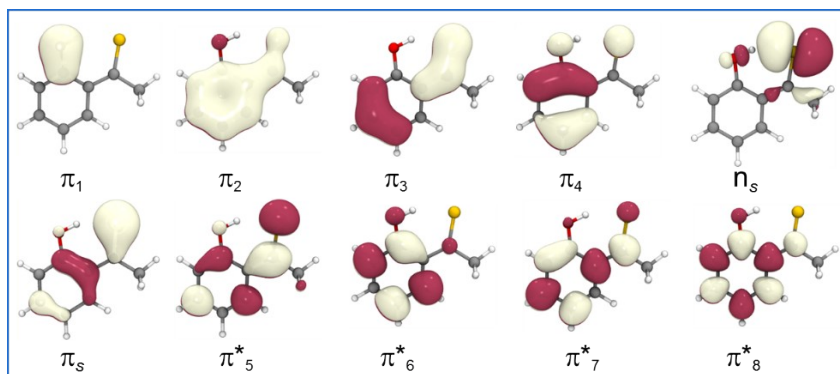


Figure S1. The active orbitals of the MS-PT2(12,10)-DZ calculations for 2HTP and 2HTP-iso.

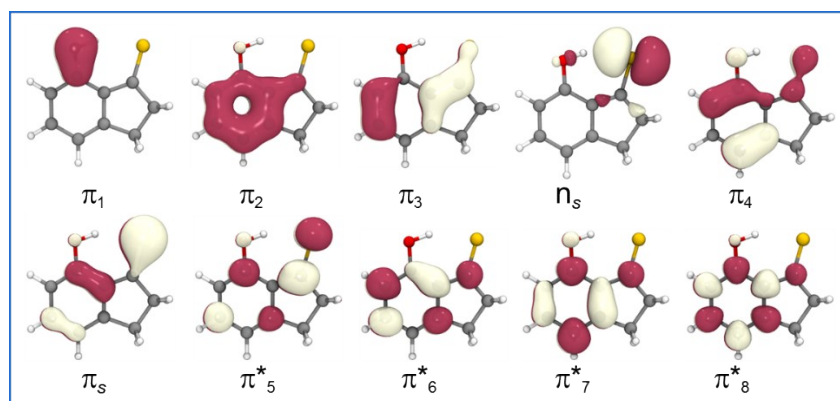


Figure S2. The active orbitals of the MS-PT2(12,10)-DZ calculations for 7HIT and 7HIT-iso.

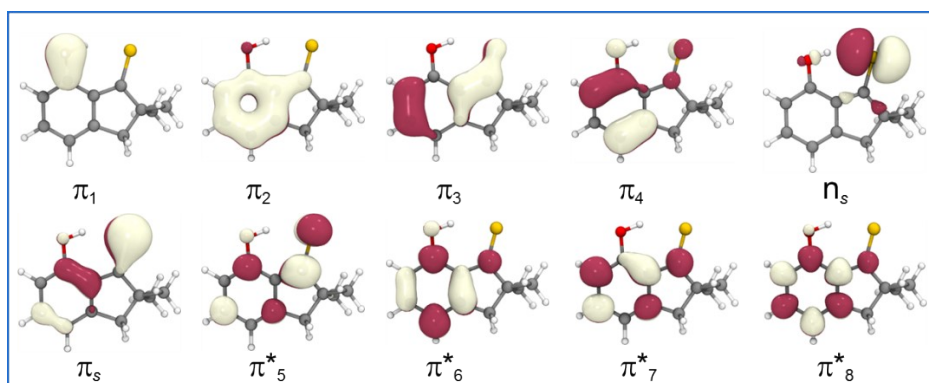


Figure S3. The active orbitals of the MS-PT2(12,10)-DZ calculations for DM-7HIT and DM-7HIT-iso.

7HIT-iso.

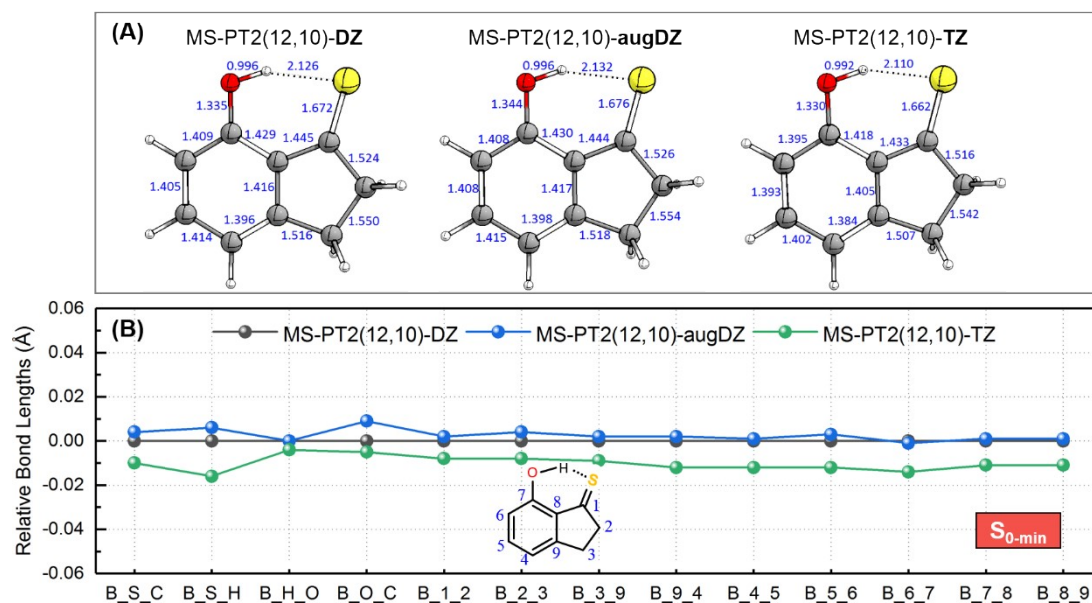


Figure S4. (A) The $S_{0-\min}$ structure of 7HIT optimized at the different levels of theory is shown, together with the selected bond lengths (Å); (B) The relative bond lengths (Å) in the MS-PT2(12,10)-augDZ and MS-PT2(12,10)-TZ optimized $S_{0-\min}$ structure are plotted, with all MS-PT2(12,10)-DZ optimized bond lengths set to zero. The 7HIT molecular structure is inserted, along with an atom numbering.

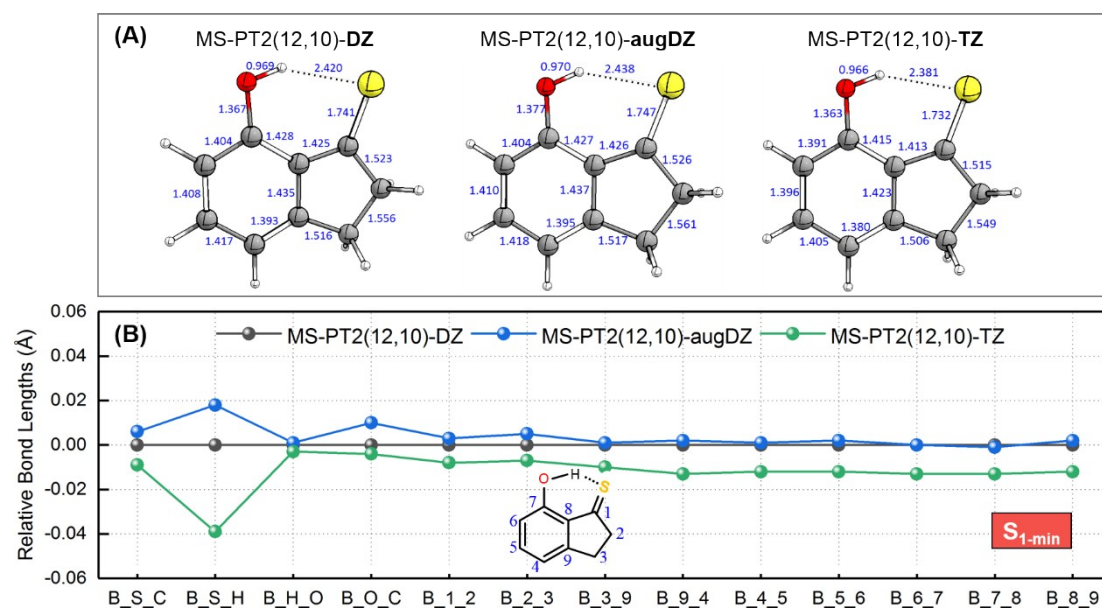


Figure S5. (A) The $S_{1-\min}$ structure of 7HIT optimized at the different levels of theory is shown, together with the selected bond lengths (Å); (B) The relative bond lengths (Å) in

the MS-PT2(12,10)-augDZ and MS-PT2(12,10)-TZ optimized $S_{1-\min}$ structure are plotted, with all MS-PT2(12,10)-DZ optimized bond lengths set to zero. The 7HIT molecular structure is inserted, along with an atom numbering.

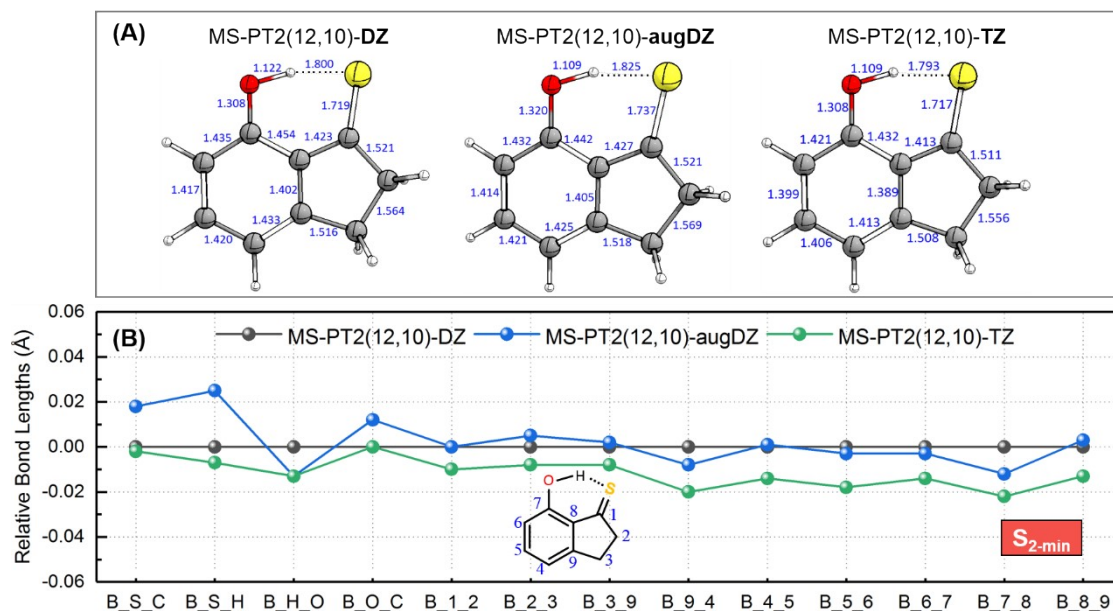


Figure S6. (A) The $S_{2-\min}$ structure of 7HIT optimized at the different levels of theory is shown, together with the selected bond lengths (Å); (B) The relative bond lengths (Å) in the MS-PT2(12,10)-augDZ and MS-PT2(12,10)-TZ optimized $S_{2-\min}$ structure are plotted, with all MS-PT2(12,10)-DZ optimized bond lengths set to zero. The 7HIT molecular structure is inserted, along with an atom numbering.

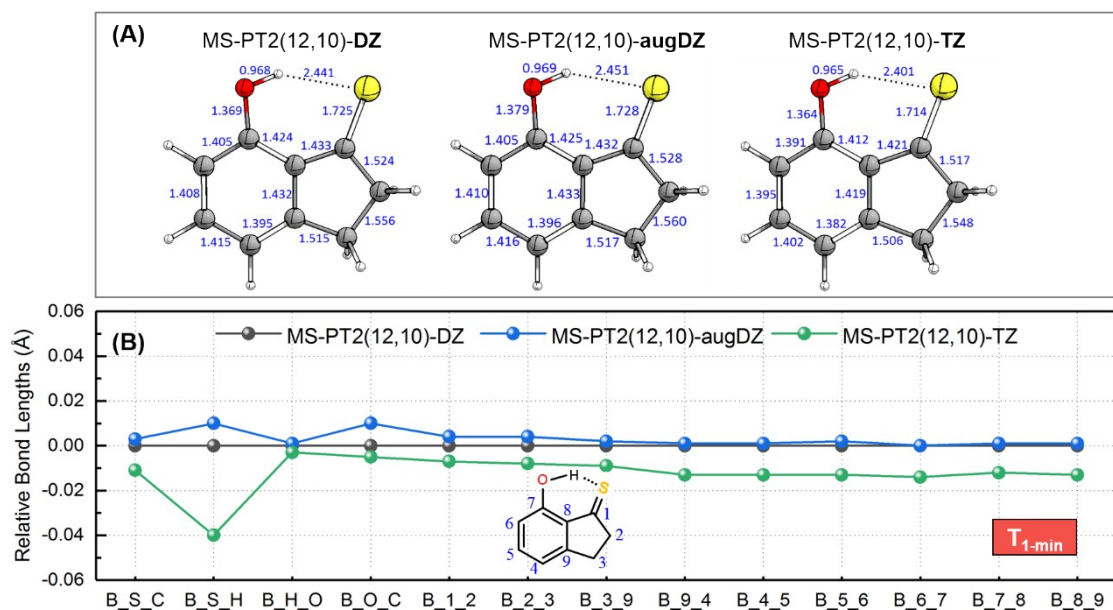


Figure S7. (A) The $T_{1-\min}$ structure of 7HIT optimized at the different levels of theory is shown, together with the selected bond lengths (Å); (B) The relative bond lengths (Å) in the MS-PT2(12,10)-augDZ and MS-PT2(12,10)-TZ optimized $T_{1-\min}$ structure are plotted, with all MS-PT2(12,10)-DZ optimized bond lengths set to zero. The 7HIT molecular structure is inserted, along with an atom numbering.

shown, together with the selected bond lengths (Å); (B) The relative bond lengths (Å) in the MS-PT2(12,10)-augDZ and MS-PT2(12,10)-TZ optimized $T_{1-\min}$ structure are plotted, with all MS-PT2(12,10)-DZ optimized bond lengths set to zero. The 7HIT molecular structure is inserted, along with an atom numbering.

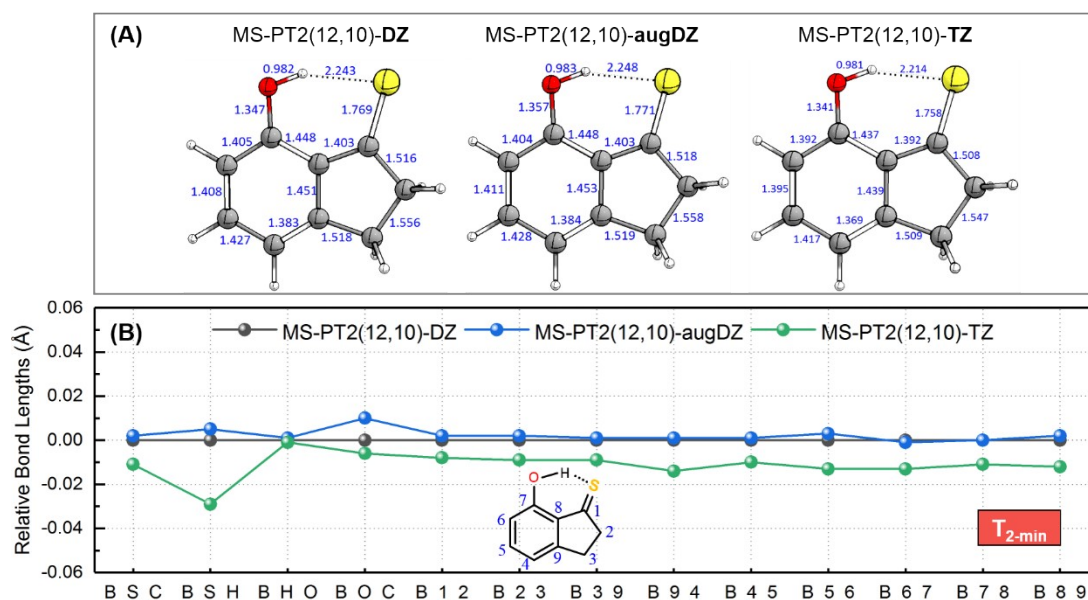


Figure S8. (A) The $T_{2-\min}$ structure of 7HIT optimized at the different levels of theory is shown, together with the selected bond lengths (Å); (B) The relative bond lengths (Å) in the MS-PT2(12,10)-augDZ and MS-PT2(12,10)-TZ optimized $T_{2-\min}$ structure are plotted, with all MS-PT2(12,10)-DZ optimized bond lengths set to zero. The 7HIT molecular structure is inserted, along with an atom numbering.

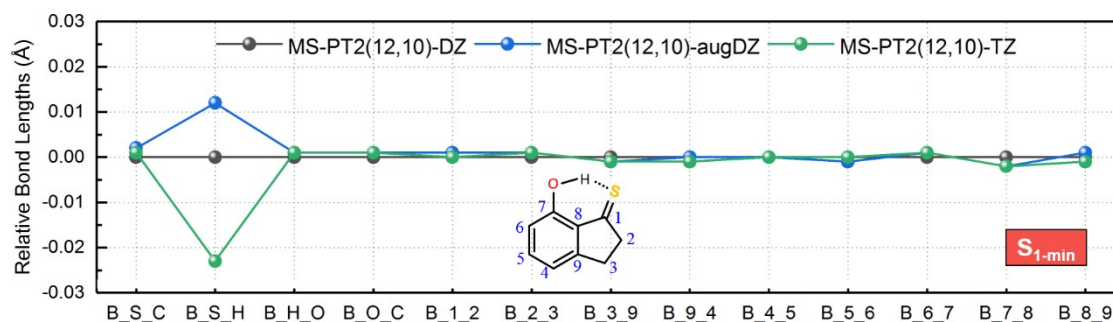


Figure S9. Relative to the bond-length differences (set to zero) obtained at the MS-PT2(12,10)-DZ level, the bond-length differences between $S_{1-\min}$ and $S_{0-\min}$ structures optimized at the MS-PT2(12,10)-TZ and MS-PT2(12,10)-augDZ level are plotted, together with the inserted molecular structure with an atom numbering.

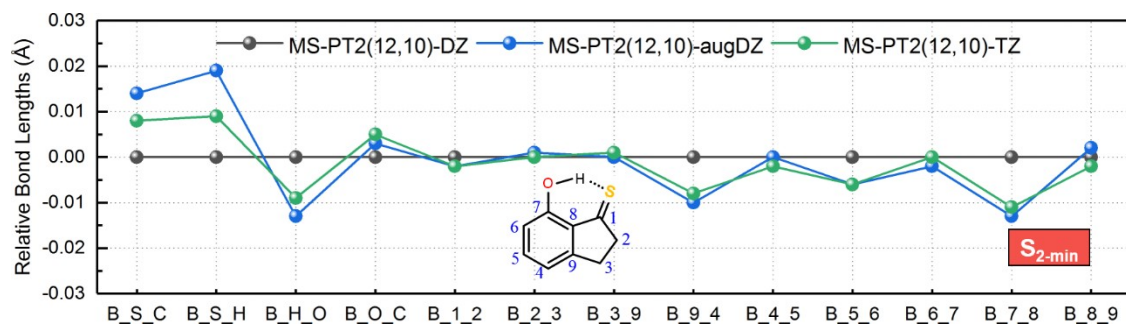


Figure S10. Relative to the bond-length differences (set to zero) obtained at the MS-PT2(12,10)-DZ level, the bond-length differences between $S_{2-\min}$ and $S_{0-\min}$ structures optimized at the MS-PT2(12,10)-TZ and MS-PT2(12,10)-augDZ level are plotted, together with the inserted molecular structure with an atom numbering.

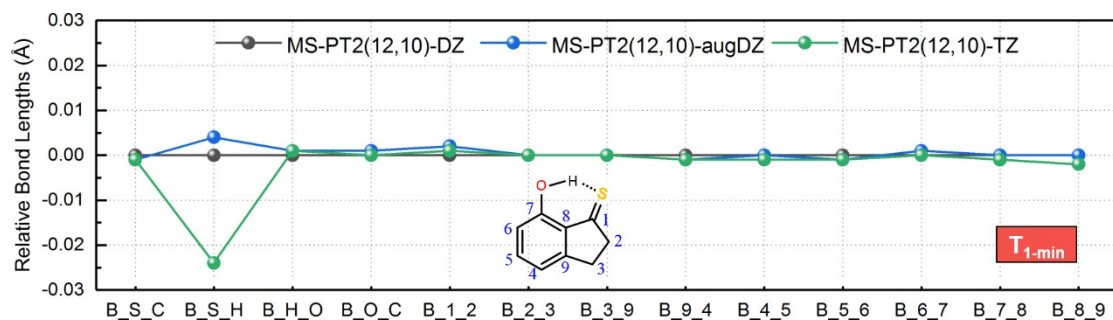


Figure S11. Relative to the bond-length differences (set to zero) obtained at the MS-PT2(12,10)-DZ level, the bond-length differences between $T_{1-\min}$ and $S_{0-\min}$ structures optimized at the MS-PT2(12,10)-TZ and MS-PT2(12,10)-augDZ level are plotted, together with the inserted molecular structure with an atom numbering.

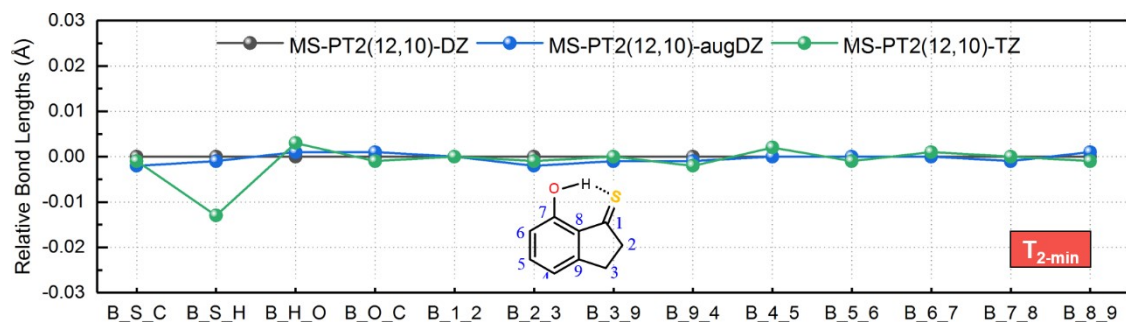


Figure S12. Relative to the bond-length differences (set to zero) obtained at the MS-PT2(12,10)-DZ level, the bond-length differences between $T_{2-\min}$ and $S_{0-\min}$ structures optimized at the MS-PT2(12,10)-TZ and MS-PT2(12,10)-augDZ level are plotted, together

with the inserted molecular structure with an atom numbering.

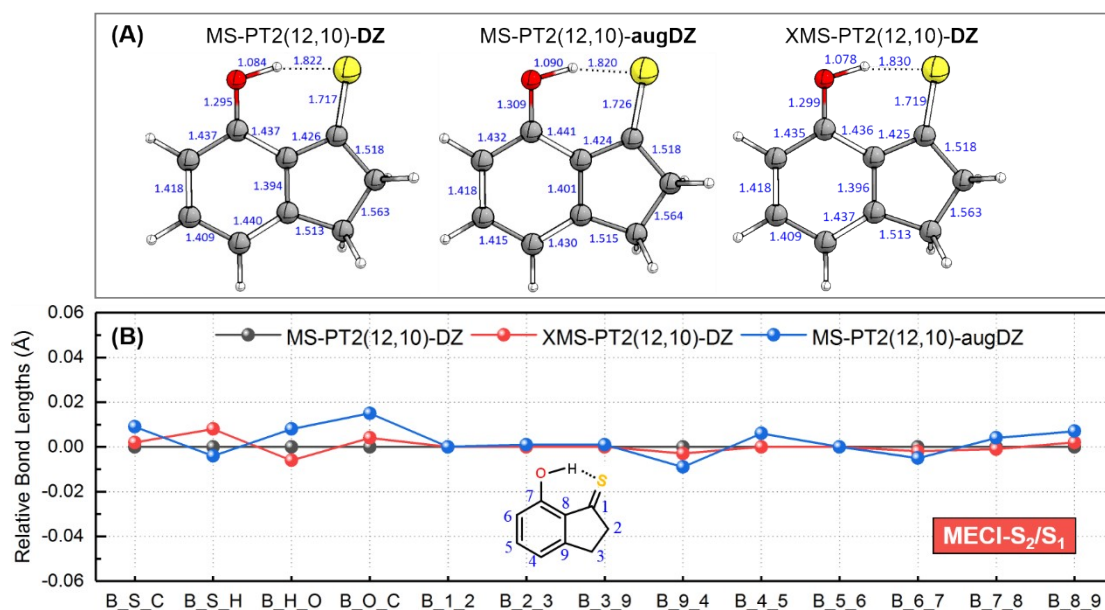


Figure S13. The MECI-S₂/S₁ structure of 7HIT optimized at the different levels of theory is shown, together with the selected bond lengths (Å); (B) The relative bond lengths (Å) in the MS-PT2(12,10)-augDZ and XMS-PT2(12,10)-DZ optimized MECI-S₂/S₁ structure are plotted, with all MS-PT2(12,10)-DZ optimized bond lengths set to zero. The 7HIT molecular structure is inserted, along with an atom numbering.

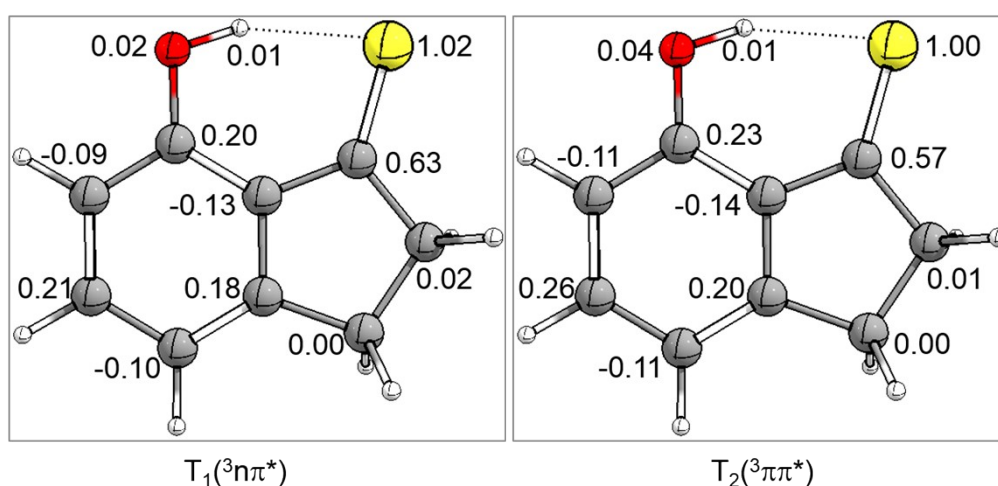


Figure S14. The MS-PT2(12,10)-DZ calculated Mulliken atomic spin populations in the T₁-min and T₂-min structures of 7HIT.

4. Cartesian coordinates and absolute energies in Hartrees

2HTP-S_{0-min} (MS-PT2(12,10)-DZ)

-781.3944867

C	-1.8370530100	-0.6135218800	2.4251912300
C	-0.4445351600	-0.5820415800	2.4161142500
C	0.2441625500	0.6536235200	2.4144400400
C	-0.4855647200	1.8376820300	2.4212604400
C	-1.9133460300	1.8567872900	2.4254778100
C	-2.5942219800	0.5822352100	2.4247698900
H	-2.3877729000	-1.5580832900	2.4274459100
H	0.1165205200	-1.5215376900	2.4112705200
H	1.3369834300	0.6801581300	2.4070418200
H	0.0577939800	2.7840845700	2.4228023500
C	-2.6162868400	3.1370687500	2.4240825200
C	-1.7880689900	4.4067055600	2.4098844200
H	-1.1393529900	4.4539208000	3.3010311100
H	-2.4490868000	5.2829831300	2.4010441600
H	-1.1381243700	4.4364317900	1.5189408600
S	-4.2910440600	3.3073445200	2.4399045200
O	-3.9181626100	0.4380243000	2.4230018500
H	-4.3148290100	1.3626398400	2.4325662700

2HTP-S_{1-min} (MS-PT2(12,10)-DZ)

-781.3097824

C	-1.8352505600	-0.6157228400	2.4264455700
C	-0.4328932100	-0.6037974900	2.4239181800
C	0.2510450700	0.6317002000	2.4143050800
C	-0.4703961700	1.8240970700	2.4083156200
C	-1.9081851200	1.8554842200	2.4165849300
C	-2.5752669200	0.5781810900	2.4244136300
H	-2.3966154900	-1.5541541500	2.4264841400
H	0.1204130900	-1.5471124700	2.4278502200
H	1.3445072800	0.6598036500	2.4106340700
H	0.0749568900	2.7701477100	2.3964640100
C	-2.5662202800	3.1271178600	2.4185574900
C	-1.7902627500	4.4302021400	2.4169040100
H	-1.1405063200	4.4995383500	3.3069870000
H	-2.4665069300	5.3002912400	2.4296251800
H	-1.1587597700	4.5109036600	1.5147778200
S	-4.3104043300	3.3875350600	2.4240705800
O	-3.9311596500	0.4114832800	2.4345316600
H	-4.3704838100	1.2788064500	2.4254008300

2HTP-S_{2-min} (MS-PT2(12,10)-DZ)

-781.29351438

C	-1.8310666600	-0.6425458200	2.4291159300
C	-0.4207831400	-0.6374258100	2.4185521800
C	0.2463786400	0.6021316800	2.4126778700
C	-0.4805314200	1.8239449000	2.4028729700
C	-1.8954877100	1.8751274100	2.4181240200
C	-2.5706013300	0.5732924900	2.4214898600
H	-2.4045804300	-1.5726438000	2.4434901400
H	0.1376772000	-1.5767274400	2.4169154300
H	1.3404966900	0.6375278200	2.4175749200
H	0.0804605200	2.7603779200	2.3877863100
C	-2.5976615000	3.1389808000	2.4184406300
C	-1.8169975300	4.4311504100	2.4207967700
H	-1.1635280100	4.5051243300	3.3103799800
H	-2.5047882700	5.2888143600	2.4294389700
H	-1.1731322100	4.5152428300	1.5248977700
S	-4.3387319700	3.2242821700	2.4134181300
O	-3.8877562100	0.4730487200	2.4351662100
H	-4.2813556700	1.5248020600	2.4251319600

2HTP-T_{1-min} (MS-PT2(12,10)-DZ)

-781.31455398

C	-1.8328394900	-0.6177037700	2.4177437000
C	-0.4304290100	-0.6028542900	2.4161198100
C	0.2488025100	0.6337294400	2.4206043400
C	-0.4787710300	1.8251932300	2.4229409500
C	-1.9126576200	1.8500844800	2.4248076100
C	-2.5750218500	0.5750372300	2.4240950300
H	-2.3934368900	-1.5567472300	2.4131580800
H	0.1248382300	-1.5450306300	2.4125230200
H	1.3419012100	0.6664848000	2.4255083300
H	0.0649549300	2.7721965300	2.4259606200
C	-2.5757431000	3.1311900200	2.4243842000
C	-1.7900675400	4.4288442200	2.4056763100
H	-1.1331828800	4.5031072400	3.2902607100
H	-2.4573908200	5.3061423100	2.4142005200
H	-1.1635044200	4.4946407300	1.4984461400
S	-4.2926310400	3.4142706700	2.4456952600
O	-3.9331706500	0.4012621700	2.4258237100
H	-4.3736395200	1.2646578200	2.4383216800

2HTP-T_{2-min} (MS-PT2(12,10)-DZ)

-781.31101337

C	-1.8360718500	-0.6285755600	2.4251661000
C	-0.4423026100	-0.6081005400	2.4212568700
C	0.2292112400	0.6448863400	2.4135247300
C	-0.4834430900	1.8370251500	2.4107108400
C	-1.9241927600	1.8770282000	2.4200001100
C	-2.5856706800	0.5675853800	2.4170153100
H	-2.3968049200	-1.5662285200	2.4259952700
H	0.1222103100	-1.5440763800	2.4224308400
H	1.3234711100	0.6792551700	2.4148346800
H	0.0672437000	2.7780964100	2.4078591300
C	-2.5767735400	3.1416110900	2.4241039200
C	-1.7760403700	4.4257958100	2.4108690700
H	-1.1304192300	4.5107131700	3.3044856200
H	-2.4508741100	5.2943790300	2.4023871800
H	-1.1227930600	4.4897786500	1.5215047400
S	-4.3322236800	3.3274328000	2.4593502200
O	-3.9158919700	0.4085186500	2.4207056000
H	-4.3306234500	1.3093801800	2.4240697400

2HTP-MECI-S₂/S₁ (MS-PT2(12,10)-DZ)

S₂: -781.29359371 S₁: -781.29364223

C	-1.8308598500	-0.6446686400	2.4306126500
C	-0.4196732800	-0.6394790900	2.4194649800
C	0.2442581100	0.6018282600	2.4100844300
C	-0.4828981500	1.8242978300	2.4018464100
C	-1.8980541700	1.8759500800	2.4172702300
C	-2.5702046700	0.5719786500	2.4184292600
H	-2.4035433000	-1.5743583200	2.4493299100
H	0.1404796100	-1.5770727000	2.4208224800
H	1.3390276400	0.6384712000	2.4109484200
H	0.0767864800	2.7604906000	2.3900116900
C	-2.5999615800	3.1413311800	2.4182222900
C	-1.8159920200	4.4314367000	2.4213925100
H	-1.1635982800	4.5058840100	3.3118291500
H	-2.5030208200	5.2890847600	2.4302445100
H	-1.1692660200	4.5150066900	1.5268965400
S	-4.3412444000	3.2244542600	2.4158790400
O	-3.8873444400	0.4733505800	2.4315577700
H	-4.2768798800	1.5265189400	2.4214277900

2HTP-MEI-S₁/T₂/T₁ (MS-PT2(12,10)-DZ)

S₁: -781.30605202 T₂: -781.30758539 T₁: -781.30850691

C	-1.8419499905	-0.6218567967	2.4258678247
C	-0.4411608289	-0.6005738084	2.4200148769

C	0.2405423561	0.6433237772	2.4135165277
C	-0.4674673364	1.8308876684	2.4093235799
C	-1.9084022804	1.8633637733	2.4194616111
C	-2.5807201506	0.5690818224	2.4205560678
H	-2.3974511209	-1.5618192346	2.4264185410
H	0.1217303987	-1.5400885170	2.4223922406
H	1.3308733246	0.6764574955	2.4150294804
H	0.0702335917	2.7767687957	2.4087787660
C	-2.5381162122	3.1150721440	2.4252531002
C	-1.7786150628	4.4264606699	2.4108833632
H	-1.1371193935	4.5091095581	3.3048410328
H	-2.4535164954	5.2981555622	2.4009962557
H	-1.1284393346	4.4900200114	1.5195602394
S	-4.3771720602	3.3496731758	2.4652482623
O	-3.9276102331	0.4179113695	2.4228929091
H	-4.3476026922	1.3025562536	2.4152437397

2HTP-iso-S_{0-min} (MS-PT2(12,10)-DZ)

-781.37378439

C	-1.7904619500	-0.6347029200	2.4115979500
C	-0.3907297300	-0.5877084700	2.4137537800
C	0.2565257500	0.6587047600	2.4219214800
C	-0.5148469600	1.8278601800	2.4266196800
C	-1.9377567500	1.8263365200	2.4242472000
C	-2.5719559900	0.5405694900	2.4139707900
H	-2.3050931500	-1.6038355600	2.4068852600
H	0.1848241100	-1.5184329500	2.4103921100
H	1.3482707400	0.7239900800	2.4247256700
H	0.0105683100	2.7835797500	2.4318003400
C	-2.6532724700	3.1276405900	2.4252861400
C	-1.7850954200	4.3763551900	2.4050946200
H	-1.1309967200	4.4174678500	3.2936234300
H	-2.4294336900	5.2645747500	2.3973630000
H	-1.1370715700	4.3947611600	1.5113119500
S	-4.3006342200	3.3229485300	2.4487644300
O	-3.9232577900	0.4477195100	2.4073489000
H	-4.1359334900	-0.4980184800	2.3589082500

2HTP-iso-S_{1-min} (MS-PT2(12,10)-DZ)

-781.31584827

C	-1.7929171500	-0.6445756900	2.4135685600
C	-0.3836980400	-0.6241251800	2.4110796300
C	0.2902151600	0.6135354600	2.4163232600
C	-0.4358022900	1.8084281000	2.4211628500

C	-1.8695857500	1.8266124800	2.4183822000
C	-2.5246123300	0.5484631200	2.4171715500
H	-2.3301052900	-1.6007198100	2.4155797100
H	0.1752022100	-1.5639774500	2.4070907300
H	1.3837359400	0.6442465900	2.4159805600
H	0.1044650000	2.7577726900	2.4257156800
C	-2.5817781500	3.0658704100	2.4139995300
C	-1.8476483600	4.3901214200	2.4129849800
H	-1.2164323900	4.4927647400	3.3135491900
H	-2.5515452100	5.2369507800	2.3984545100
H	-1.1954907300	4.4790958100	1.5261423800
S	-4.3325856100	3.2284060300	2.4090214200
O	-3.8933552700	0.5638658000	2.4245392500
H	-4.2044127400	-0.3529252700	2.3728689800

2HTP-iso-S_{2-min} (MS-PT2(12,10)-DZ)

-781.24556986

C	-1.7825228300	-0.6594891300	2.4125856200
C	-0.3660956100	-0.6444861300	2.4171347800
C	0.2447677100	0.6237480400	2.4191305800
C	-0.5253232900	1.8408790400	2.4171819000
C	-1.9579173800	1.8908907700	2.4167409000
C	-2.5597538500	0.5522852900	2.4086214900
H	-2.3324054800	-1.6100607000	2.4109021800
H	0.2133880300	-1.5698419300	2.4204238300
H	1.3367539300	0.7075739500	2.4223111400
H	0.0327203600	2.7782132600	2.4164466000
C	-2.6614341100	3.1409222300	2.4203363600
C	-1.7925544700	4.3880730100	2.4119640900
H	-1.1361504900	4.4389283100	3.3023358600
H	-2.4410136100	5.2737615800	2.4082826100
H	-1.1387045200	4.4285110400	1.5193270400
S	-4.3479985700	3.3413421100	2.4371743300
O	-3.8804455300	0.4479256300	2.3959371000
H	-4.1116612900	-0.4993663400	2.3767785900

2HTP-iso-T_{1-min} (MS-PT2(12,10)-DZ)

-781.32175702

C	-1.7925807900	-0.6454325300	2.4114931100
C	-0.3831706300	-0.6249459100	2.4104342400
C	0.2884794800	0.6115397300	2.4162452000
C	-0.4389783000	1.8090917800	2.4201839800
C	-1.8693283600	1.8255799200	2.4170637600
C	-2.5218301200	0.5497027300	2.4179447000

H	-2.3304898100	-1.6008878300	2.4125998100
H	0.1758655500	-1.5645585200	2.4079629400
H	1.3817795100	0.6435099500	2.4182535500
H	0.1027533700	2.7575391000	2.4237000600
C	-2.5880361900	3.0672155500	2.4105650400
C	-1.8520140100	4.3903905400	2.4140522200
H	-1.2189569800	4.4876238400	3.3141837100
H	-2.5508191000	5.2416364600	2.4027876100
H	-1.1992387900	4.4809679100	1.5275043600
S	-4.3115747800	3.2245219800	2.4006512000
O	-3.8944427400	0.5665060900	2.4273656400
H	-4.2037683300	-0.3501907900	2.3806238700

2HTP-iso-T_{2-min} (MS-PT2(12,10)-DZ)

-781.29434954

C	-1.7967110800	-0.6387429300	2.4165803800
C	-0.3912928800	-0.6019692700	2.4159120000
C	0.2589917900	0.6591563000	2.4172657400
C	-0.4896482300	1.8265268500	2.4200225500
C	-1.9473592900	1.8481198600	2.4210309200
C	-2.5787107900	0.5268728700	2.4148780700
H	-2.3135245100	-1.6074935700	2.4164217800
H	0.1843192500	-1.5320170900	2.4160600500
H	1.3519756700	0.7175249800	2.4169443900
H	0.0379186500	2.7817985300	2.4223079900
C	-2.5936056500	3.1048866000	2.4210090600
C	-1.7793557900	4.3818951700	2.4102106700
H	-1.1263884100	4.4588299200	3.3004206300
H	-2.4474529900	5.2540657200	2.4025490300
H	-1.1243603800	4.4426613500	1.5203777600
S	-4.3727355700	3.3169864100	2.4391480500
O	-3.9337637700	0.4393580100	2.4053754700
H	-4.1446470100	-0.5086497300	2.3571004500

2HTP-iso-MECI-S₂/S₁ (MS-PT2(12,10)-DZ)

S₂: -781.23542860 S₁: -781.23551549

C	-1.8322402700	-0.6053344600	2.6933309200
C	-0.4303908500	-0.6076619000	2.8806737300
C	0.1934089600	0.5717567300	2.4643260700
C	-0.6191981100	1.6927738300	1.9566988200
C	-1.9175268200	1.9413754300	2.5034569700
C	-2.5068283300	0.6139799400	2.2896366500
H	-2.4409435900	-1.5081460400	2.8193289300
H	0.1035511300	-1.4447025500	3.3343203100

H	1.2778235700	0.7027541600	2.5303395100
H	-0.1660327800	2.3867336500	1.2374484000
C	-2.6066103400	3.1524371800	2.7519471200
C	-1.8352566200	4.4273536800	2.4961576200
H	-0.7820048800	4.3252979200	2.8190847800
H	-2.3011980200	5.2681927600	3.0275106400
H	-1.8228917800	4.6738028000	1.4183570900
S	-4.1652730700	3.1286160800	3.3902388100
O	-3.6318364400	0.5328025500	1.5664464400
H	-3.7229027700	-0.3822217500	1.2543121900

2HTP-iso-MEI-S₁/T₂/T₁ (MS-PT2(12,10)-DZ)

S₁: -781.28512533 T₂: -781.28718289 T₁: -781.28798848

C	-1.8961926000	-0.5886783500	2.6972869700
C	-0.5079044400	-0.5514905100	2.9248250000
C	0.2524838700	0.6103936500	2.5128605300
C	-0.3648852600	1.7611291700	2.0761422900
C	-1.8261526000	1.8739072800	2.2688291000
C	-2.5254855800	0.5571022200	2.1938312400
H	-2.4518832900	-1.5308634300	2.7876631600
H	0.0119562500	-1.4309319300	3.3135025700
H	1.3465026700	0.5582747200	2.5273998600
H	0.2242000900	2.6249049000	1.7592911100
C	-2.5023797600	3.0485034500	2.5652387400
C	-1.8723615200	4.4091730600	2.3757442300
H	-0.8310649700	4.3857064400	2.0161252000
H	-1.9114501100	4.9775967100	3.3182908200
H	-2.4825263500	4.9768312200	1.6501397600
S	-4.0967964200	2.9511188600	3.3184484900
O	-3.7009245000	0.5677976300	1.5418420200
H	-4.0714864500	-0.3306651000	1.5861539200

7HIT-S_{0-min} (MS-PT2(12,10)-DZ)

-819.40121954

S	-2.6009615800	-0.7290534300	0.0176565300
O	-0.0576965900	-2.4249243300	-0.0042502700
H	-1.0117924300	-2.1406856100	0.0039745500
C	-1.3115133200	0.3348941700	0.0073466900
C	-1.4260462200	1.8547735800	-0.0061457500
C	0.0248912000	2.4009179300	0.0039434200
H	0.2367280100	3.0204061500	-0.8837272300
H	0.2235008700	3.0270787100	0.8902440700
C	0.8963657100	1.1605016800	0.0088780300

C	2.2889923900	1.0629644800	0.0058076200
C	2.8620236700	-0.2292233700	-0.0038063100
H	3.9520896000	-0.3297969100	-0.0091208600
C	2.0817297900	-1.3972117400	-0.0055942800
C	0.6758342800	-1.3095742500	0.0014103400
C	0.0930270700	-0.0052673500	0.0080568000
H	2.5458173900	-2.3870106800	-0.0135994600
H	2.9248756000	1.9532188800	0.0094931400
H	-1.9920741900	2.1656946600	-0.9001301600
H	-2.0112312200	2.1821874500	0.8696631100

7HIT-S_{1-min} (MS-PT2(12,10)-DZ)

-819.31569117

S	-2.7260325600	-0.6408893400	0.0138168600
O	-0.0063038800	-2.4892972900	0.0002142400
H	-0.9537010600	-2.2881320500	-0.0079085300
C	-1.3017097100	0.3605422700	0.0055614600
C	-1.4389121800	1.8769821700	-0.0019462900
C	0.0284593500	2.3958582100	0.0007720600
H	0.2332389400	3.0200152600	-0.8865793000
H	0.2311314800	3.0182606800	0.8898058700
C	0.8938076800	1.1513634900	0.0008162400
C	2.2837931700	1.0589954400	0.0007302300
C	2.8820183800	-0.2252642900	0.0006569900
H	3.9724490700	-0.3210655900	0.0022757000
C	2.0901528800	-1.3900520000	-0.0017612500
C	0.6880327400	-1.3114052200	0.0004616800
C	0.0698910700	-0.0240926200	0.0023508800
H	2.5489841100	-2.3834647700	-0.0062415000
H	2.9042726900	1.9612526900	0.0002659800
H	-1.9980228600	2.2153577300	-0.8948067900
H	-2.0069892800	2.2249252200	0.8816154500

7HIT-S_{2-min} (MS-PT2(12,10)-DZ)

-819.2943356

S	-2.5373195800	-0.8887086500	-0.0100643400
O	-0.0853061100	-2.3644017700	-0.0148908400
H	-1.1289665400	-1.9781330100	-0.0149962200
C	-1.3078690900	0.3322398600	-0.0126866200
C	-1.4524747700	1.8446702900	0.0148617900
C	0.0108087700	2.3951092400	-0.0108884700
H	0.2115726100	2.9973360100	-0.9145358600
H	0.2290616200	3.0409848400	0.8571585200
C	0.8924171300	1.1593314000	0.0036850800

C	2.3134040800	1.0404270300	0.0021938400
C	2.9161156500	-0.2415972900	0.0144169100
H	4.0026968500	-0.3383985800	0.0296271300
C	2.1077051900	-1.4079902500	0.0046441200
C	0.6844721300	-1.2952229100	-0.0079454700
C	0.0798222800	0.0125018200	-0.0130530300
H	2.5501942400	-2.4084029800	0.0103199900
H	2.9433179600	1.9371038600	-0.0100303800
H	-2.0409077400	2.2023804800	-0.8491872100
H	-1.9941846600	2.1706606800	0.9214710300

7HIT-T_{1-min} (MS-PT2(12,10)-DZ)

-819.32023124

S	-2.7255754700	-0.6250716800	0.0194303900
O	-0.0008395500	-2.4942179700	-0.0006301600
H	-0.9487104100	-2.2981812000	-0.0084062300
C	-1.3096007600	0.3594641000	0.0033716400
C	-1.4405829900	1.8781937400	-0.0031274600
C	0.0282148000	2.3918327900	0.0001282300
H	0.2343746100	3.0144463700	-0.8873394900
H	0.2324143500	3.0157020900	0.8870879400
C	0.8901860600	1.1459501300	0.0022024200
C	2.2823001900	1.0575395400	0.0030209500
C	2.8823835000	-0.2233869300	0.0009303700
H	3.9724692400	-0.3173669800	0.0023525900
C	2.0915221000	-1.3883335300	-0.0035502600
C	0.6883565600	-1.3111015300	0.0003502200
C	0.0698966800	-0.0279328900	0.0018549400
H	2.5499117700	-2.3813623500	-0.0079011000
H	2.8992109300	1.9618176000	0.0042614700
H	-1.9970358000	2.2221982100	-0.8948075400
H	-2.0043357300	2.2297005200	0.8808710600

7HIT-T_{2-min} (MS-PT2(12,10)-DZ)

-819.31580194

S	-2.6699601400	-0.7444641300	-0.0156249500
O	-0.0273151700	-2.4647497000	0.0132873100
H	-0.9776882000	-2.2162071800	0.0249467000
C	-1.2924430400	0.3649596900	-0.0012322900
C	-1.4341185200	1.8748061900	-0.0054997900
C	0.0270130500	2.4082800300	0.0092543800
H	0.2393096200	3.0448032900	-0.8666027200
H	0.2292582100	3.0169526500	0.9071934100
C	0.9007936200	1.1664740800	-0.0006960800

C	2.2792217600	1.0601953300	-0.0053766300
C	2.8786360800	-0.2344186100	-0.0077309300
H	3.9679884500	-0.3288786700	-0.0133124800
C	2.0857064200	-1.3981986800	-0.0029409600
C	0.6825808400	-1.3202188100	0.0040361700
C	0.0578329900	-0.0143846700	-0.0000361900
H	2.5426240200	-2.3918681000	-0.0035726800
H	2.9082347900	1.9565960400	-0.0085056100
H	-1.9908760000	2.2116529600	-0.8993990900
H	-2.0122387100	2.2185583300	0.8719124000

7HIT-MECI-S₂/S₁ (MS-PT2(12,10)-DZ)

S₂: -819.29320590 S₁: -819.29360288

S	-2.5366736100	-0.8770047700	0.0493462100
O	-0.0748849700	-2.3434770000	-0.0463967900
H	-1.1008125400	-1.9979812200	0.0146262100
C	-1.3173041500	0.3311692700	-0.0070289600
C	-1.4522104800	1.8430503100	-0.0004451100
C	0.0114908800	2.3908616000	-0.0048456600
H	0.2218091100	2.9925019100	-0.9021733900
H	0.2195662700	3.0343257800	0.8625700600
C	0.8828941200	1.1540667200	0.0168306200
C	2.3178870100	1.0358437300	0.0187244300
C	2.9145655800	-0.2402957900	0.0172994600
H	3.9961563400	-0.3407573500	0.0246735700
C	2.1056271900	-1.4042762700	-0.0146750000
C	0.6736244900	-1.2865141100	-0.0215749800
C	0.0736155900	0.0187314500	-0.0012171200
H	2.5400732700	-2.4001279600	-0.0172732600
H	2.9441103600	1.9289416000	0.0079913500
H	-2.0153134200	2.1864123900	-0.8800217900
H	-2.0096610100	2.1844197300	0.8836902200

7HIT-MEI-S₁/T₂/T₁ (MS-PT2(12,10)-DZ)

S₁: -819.31348459 T₂: -819.31517818 T₁: -819.31695051

S	-2.6855701972	-0.7161530412	-0.0188331335
O	-0.0177446799	-2.4546756241	0.0103266572
H	-0.9742783071	-2.2395948130	0.0306567678
C	-1.2751630909	0.3614100606	-0.0004524494
C	-1.4252096715	1.8671256582	-0.0049579674
C	0.0327020079	2.3989255193	0.0095154429
H	0.2340182870	3.0349601515	-0.8588907300
H	0.2243857557	3.0080874560	0.8995384578
C	0.9044032906	1.1652290329	-0.0003630163

C	2.2752338003	1.0557352624	-0.0059898394
C	2.8666372019	-0.2278175737	-0.0076401513
H	3.9479493964	-0.3246508173	-0.0129726392
C	2.0785383988	-1.3882520012	-0.0045160082
C	0.6887620591	-1.2996600004	0.0040191453
C	0.0659705946	-0.0099357108	-0.0016314836
H	2.5334276876	-2.3743741198	-0.0027707990
H	2.9029793211	1.9415822324	-0.0080677896
H	-1.9805083823	2.2016214873	-0.8909175690
H	-2.0019761097	2.2103205558	0.8640342157

7HIT-S_{0-min} (MS-PT2(12,10)-augDZ)

-819.48831488

S	-2.6030069500	-0.7297242400	0.0218109500
O	-0.0620329000	-2.4285022700	-0.0003232400
H	-1.0207958600	-2.1584524000	0.0060908300
C	-1.3104095000	0.3371217000	0.0070581600
C	-1.4294711500	1.8579447200	-0.0081375200
C	0.0244954300	2.4067668100	0.0052888000
H	0.2379685900	3.0281388700	-0.8779234800
H	0.2228303000	3.0245787300	0.8953365000
C	0.8968488600	1.1647847100	0.0067450200
C	2.2916586100	1.0649891800	0.0054710000
C	2.8645243500	-0.2292485500	-0.0046449400
H	3.9538128100	-0.3296749700	-0.0102150200
C	2.0834374400	-1.4003451000	-0.0068733800
C	0.6785099400	-1.3073342100	0.0001709200
C	0.0933293800	-0.0027948400	0.0066958700
H	2.5494863100	-2.3880049100	-0.0142737500
H	2.9288415500	1.9528739300	0.0080193200
H	-1.9901846600	2.1634232600	-0.9052744900
H	-2.0152825100	2.1833496000	0.8650784100

7HIT-S_{1-min} (MS-PT2(12,10)-augDZ)

-819.40458403

S	-2.7347914000	-0.6401269500	0.0020510100
O	-0.0072877300	-2.4935919600	0.0031882000
H	-0.9598268700	-2.3120445800	-0.0006999100
C	-1.3035619800	0.3610998700	0.0026933800
C	-1.4420427900	1.8811285200	-0.0028192600
C	0.0292614700	2.4018183000	0.0078725800
H	0.2360644000	3.0262390700	-0.8754642600
H	0.2295987200	3.0167287300	0.8989362600

C	0.8942174900	1.1551608200	0.0019084800
C	2.2855975200	1.0604043000	-0.0038727900
C	2.8847245400	-0.2251176900	-0.0036545100
H	3.9733894900	-0.3200236100	-0.0097911300
C	2.0926790000	-1.3921694300	0.0018937400
C	0.6912228200	-1.3072032600	0.0012353300
C	0.0703116300	-0.0218839300	0.0023051100
H	2.5522524600	-2.3829210400	0.0043600700
H	2.9085188300	1.9590686400	-0.0093409700
H	-1.9935897900	2.2171008800	-0.8978540600
H	-2.0121777800	2.2262233000	0.8771527200

7HIT-S_{2-min} (MS-PT2(12,10)-augDZ)

-819.38408908

S	-2.5541342000	-0.8778140000	0.0114050000
O	-0.0765753000	-2.3739506000	-0.0065838000
H	-1.1255747000	-2.0134173000	-0.0021212000
C	-1.3102117000	0.3348134000	-0.0054005000
C	-1.4555737000	1.8489842000	-0.0009627000
C	0.0137358000	2.3994975000	-0.0014965000
H	0.2243728000	3.0237279000	-0.8859279000
H	0.2243658000	3.0212838000	0.8847300000
C	0.8922399000	1.1612717000	-0.0031432000
C	2.3128131000	1.0440136000	-0.0010912000
C	2.9144662000	-0.2434641000	0.0016280000
H	4.0027501000	-0.3375170000	0.0027869000
C	2.1109749000	-1.4075091000	0.0021811000
C	0.6834493000	-1.2951798000	0.0012815000
C	0.0800056000	0.0148387000	-0.0028054000
H	2.5511781000	-2.4079632000	0.0024624000
H	2.9444665000	1.9379647000	-0.0004610000
H	-2.0211659000	2.1942065000	-0.8836095000
H	-2.0170227000	2.1861031000	0.8872283000

7HIT-T_{1-min} (MS-PT2(12,10)-augDZ)

-819.40882573

S	-2.7297752300	-0.6247381700	0.0094580700
O	-0.0052723500	-2.4962895500	0.0073200600
H	-0.9577159800	-2.3177846600	-0.0046147500
C	-1.3088380000	0.3590889700	0.0009551700
C	-1.4439101600	1.8811059600	-0.0048232300
C	0.0283128600	2.3981117000	0.0056713700
H	0.2371047200	3.0220946800	-0.8776907900
H	0.2288010600	3.0125266600	0.8978204900

C	0.8912771300	1.1508783300	0.0025600400
C	2.2846661700	1.0592866500	-0.0011399000
C	2.8850051000	-0.2235793400	-0.0044241400
H	3.9738182700	-0.3176617800	-0.0101168900
C	2.0942429600	-1.3908030200	-0.0006287400
C	0.6918498900	-1.3064724600	0.0028611600
C	0.0707483300	-0.0244360300	0.0022709300
H	2.5535481500	-2.3820922100	-0.0000059400
H	2.9042083600	1.9602787200	-0.0025049000
H	-1.9935347100	2.2216843600	-0.8996070900
H	-2.0099765500	2.2286911600	0.8767390500

7HIT-T_{2-min} (MS-PT2(12,10)-augDZ)

-819.40388351

S	-2.6705979000	-0.7451770300	-0.0169282400
O	-0.0309482900	-2.4689520100	0.0151862000
H	-0.9857722900	-2.2335693700	0.0245912700
C	-1.2924329000	0.3669073300	-0.0008265100
C	-1.4355331400	1.8776445700	-0.0057498900
C	0.0273988700	2.4134152700	0.0099970200
H	0.2410164800	3.0473204800	-0.8658304900
H	0.2292846000	3.0203154200	0.9076251000
C	0.9014487900	1.1710080400	0.0000149900
C	2.2807619500	1.0619606000	-0.0055050000
C	2.8801623400	-0.2340618700	-0.0089845400
H	3.9686230400	-0.3288986400	-0.0155151400
C	2.0872160400	-1.4006864800	-0.0033551600
C	0.6858751300	-1.3169352400	0.0043477900
C	0.0581773300	-0.0122790800	0.0011749400
H	2.5449353100	-2.3933203700	-0.0033057100
H	2.9107400400	1.9566011000	-0.0077665800
H	-1.9916410000	2.2103763200	-0.9001346100
H	-2.0141543400	2.2182209800	0.8710645400

7HIT-MECI-S₂/S₁ (MS-PT2(12,10)-augDZ)

S₂: -819.38342673 S₁: -819.38403909

S	-2.5434549200	-0.8774303500	0.0494614500
O	-0.0797712300	-2.3567992600	-0.0439568600
H	-1.1081907000	-1.9915341700	-0.0017355600
C	-1.3141825900	0.3323679300	-0.0057861800
C	-1.4520448600	1.8437896200	0.0016440000
C	0.0126177000	2.3928407300	-0.0084710300
H	0.2182498700	2.9993018900	-0.9068649600
H	0.2208929400	3.0365118600	0.8628566600

C	0.8872323600	1.1566710300	0.0091657300
C	2.3131276900	1.0377730600	0.0127262800
C	2.9156452300	-0.2426022100	0.0197693700
H	4.0004823000	-0.3397435400	0.0255296000
C	2.1087613800	-1.4084478000	-0.0098400400
C	0.6813090700	-1.2913484300	-0.0176330400
C	0.0747465000	0.0152919100	-0.0029155900
H	2.5468698500	-2.4064488900	-0.0096828500
H	2.9406817500	1.9355988000	0.0095956900
H	-2.0223054900	2.1896741400	-0.8767441900
H	-2.0061068300	2.1844237200	0.8929816000

7HIT-S_{0-min} (MS-PT2(12,10)-TZ)

-819.86092539

S	-2.5801856300	-0.7207471400	0.0217787400
O	-0.0548996700	-2.4040936000	-0.0013912500
H	-1.0079848600	-2.1285273000	0.0075875500
C	-1.2959832000	0.3349576100	0.0083041600
C	-1.4126809900	1.8462868100	-0.0078840400
C	0.0299861400	2.3897636900	0.0061305200
H	0.2405687200	3.0033616900	-0.8684740300
H	0.2231244800	3.0032416000	0.8848715500
C	0.8943751400	1.1557984300	0.0099053200
C	2.2745592000	1.0576469500	0.0056623900
C	2.8429984100	-0.2238152900	-0.0051583600
H	3.9190880700	-0.3223672900	-0.0110232700
C	2.0713290500	-1.3831988000	-0.0078491200
C	0.6788739700	-1.2942807900	0.0009336400
C	0.0971699900	-0.0006606200	0.0085490200
H	2.5322568100	-2.3592967700	-0.0169954100
H	2.9030005100	1.9360453600	0.0082419700
H	-1.9653098400	2.1490830700	-0.8956451400
H	-1.9957262700	2.1706924200	0.8525557400

7HIT-S_{1-min} (MS-PT2(12,10)-TZ)

-819.77725852

S	-2.7005329700	-0.6408572900	0.0108102600
O	-0.0111992500	-2.4613490100	0.0003311600
H	-0.9556587800	-2.2604810800	-0.0110767200
C	-1.2844780400	0.3568687100	0.0053630200
C	-1.4253950300	1.8652434200	-0.0014988300
C	0.0338889000	2.3834210900	0.0006738000
H	0.2334678700	2.9987017600	-0.8758934000

H	0.2320113700	2.9973943500	0.8785669100
C	0.8939816300	1.1468839700	0.0011165900
C	2.2707450900	1.0536077900	0.0002015200
C	2.8635348000	-0.2198215600	-0.0004717000
H	3.9393525900	-0.3133389000	-0.0018796300
C	2.0796290200	-1.3751867500	0.0001884800
C	0.6912437500	-1.2933366300	0.0010200600
C	0.0775437400	-0.0187690900	0.0027443200
H	2.5337347700	-2.3551874900	-0.0003144300
H	2.8850316700	1.9431368900	0.0002332200
H	-1.9780358700	2.1976935900	-0.8825705200
H	-1.9843052300	2.2052662200	0.8725558600

7HIT-S_{2-min} (MS-PT2(12,10)-TZ)

-819.75559915

S	-2.5180420000	-0.8679015000	-0.0023366000
O	-0.0713263000	-2.3536794000	-0.0535970000
H	-1.1189564000	-1.9890346000	-0.0444726000
C	-1.2899483000	0.3325071000	-0.0064496000
C	-1.4367983000	1.8364186000	0.0258663000
C	0.0195365000	2.3843297000	-0.0067800000
H	0.2107160000	2.9808343000	-0.8998725000
H	0.2299801000	3.0245316000	0.8500263000
C	0.8899985000	1.1535079000	0.0063026000
C	2.2975435000	1.0362138000	-0.0253493000
C	2.8897854000	-0.2375444000	0.0334143000
H	3.9626806000	-0.3294859000	0.0909345000
C	2.0967162000	-1.3897398000	0.0213894000
C	0.6799453000	-1.2841440000	-0.0146460000
C	0.0875371000	0.0198357000	-0.0207440000
H	2.5330296000	-2.3797018000	0.0332810000
H	2.9186381000	1.9204996000	-0.0926753000
H	-2.0215987000	2.1978065000	-0.8232650000
H	-1.9648766000	2.1546365000	0.9290736000

7HIT-T_{1-min} (MS-PT2(12,10)-TZ)

-819.78148633

S	-2.6985534900	-0.6236383900	0.0174868600
O	-0.0062573500	-2.4653036700	0.0007395900
H	-0.9507506200	-2.2691655400	-0.0063046200
C	-1.2918766500	0.3555157400	0.0034523400
C	-1.4271583600	1.8665951400	-0.0037496900
C	0.0334815300	2.3792386300	0.0006781300
H	0.2350541900	2.9936766700	-0.8755353400

H	0.2317095000	2.9929267200	0.8782221800
C	0.8903782100	1.1412996900	0.0022647200
C	2.2692749700	1.0516777600	0.0030417000
C	2.8637930000	-0.2184479600	-0.0004929800
H	3.9393108000	-0.3105387000	-0.0012985900
C	2.0812836600	-1.3737235300	-0.0033484700
C	0.6921687400	-1.2931309900	0.0005236300
C	0.0778720500	-0.0221835300	0.0018098000
H	2.5356559300	-2.3529221900	-0.0069102200
H	2.8788988300	1.9437207300	0.0056693800
H	-1.9756213000	2.2030976400	-0.8850483600
H	-1.9841035800	2.2111957800	0.8688999300

7HIT-T_{2-min} (MS-PT2(12,10)-TZ)

-819.77581710

S	-2.6456278700	-0.7391049500	-0.0130217300
O	-0.0272657300	-2.4400428100	0.0102349700
H	-0.9764079500	-2.1939800600	0.0192347500
C	-1.2771604900	0.3637966600	0.0009957400
C	-1.4209968900	1.8648075700	-0.0044676500
C	0.0319831800	2.3969934900	0.0091075500
H	0.2394903300	3.0238307200	-0.8572949200
H	0.2300523500	2.9971664900	0.8965715400
C	0.9000685100	1.1624467700	-0.0023385500
C	2.2646934400	1.0550488900	-0.0063755500
C	2.8599247000	-0.2307382000	-0.0074702700
H	3.9355164900	-0.3235392600	-0.0135309000
C	2.0759989700	-1.3850002200	-0.0007457500
C	0.6860456300	-1.3046985900	0.0032283600
C	0.0639024200	-0.0090659600	0.0002431000
H	2.5300692900	-2.3649454000	0.0007610600
H	2.8870148300	1.9397710900	-0.0089749000
H	-1.9710606500	2.1936870300	-0.8882819500
H	-1.9916804700	2.2034567700	0.8622250800

7HIT-MECI-S₂/S₁ (MS-PT2(12,10)-TZ)

S₂: -819.75590191 S₁: -819.75638587

S	-2.5318564800	-0.8676921800	0.0192421200
O	-0.0673673900	-2.3480911800	-0.0152783100
H	-1.1144959800	-1.9764637800	-0.0048740900
C	-1.3045825800	0.3319411100	-0.0014370500
C	-1.4427586900	1.8356605500	0.0022830600
C	0.0153127000	2.3777227400	-0.0031993400
H	0.2343095900	2.9810500900	-0.8855310500

H	0.2339873600	3.0003825300	0.8655597800
C	0.8845983100	1.1450020100	0.0056730800
C	2.2966714900	1.0310636400	-0.0035600700
C	2.8978424500	-0.2341851800	0.0203991100
H	3.9719196900	-0.3262392900	0.0553823600
C	2.0997272900	-1.3876908500	-0.0051850800
C	0.6870901600	-1.2757164500	-0.0034203800
C	0.0817613300	0.0166243300	-0.0031324300
H	2.5346369200	-2.3765442600	-0.0293207400
H	2.9121285300	1.9206680900	-0.0327487200
H	-2.0059583200	2.1853628500	-0.8655008700
H	-1.9884063800	2.1770353000	0.8847485800

7HIT-S_{0-min} (XMS-PT2(12,10)-DZ)

-819.40885187

S	-2.5801856300	-0.7207471400	0.0217787400
O	-0.0548996700	-2.4040936000	-0.0013912500
H	-1.0079848600	-2.1285273000	0.0075875500
C	-1.2959832000	0.3349576100	0.0083041600
C	-1.4126809900	1.8462868100	-0.0078840400
C	0.0299861400	2.3897636900	0.0061305200
H	0.2405687200	3.0033616900	-0.8684740300
H	0.2231244800	3.0032416000	0.8848715500
C	0.8943751400	1.1557984300	0.0099053200
C	2.2745592000	1.0576469500	0.0056623900
C	2.8429984100	-0.2238152900	-0.0051583600
H	3.9190880700	-0.3223672900	-0.0110232700
C	2.0713290500	-1.3831988000	-0.0078491200
C	0.6788739700	-1.2942807900	0.0009336400
C	0.0971699900	-0.0006606200	0.0085490200
H	2.5322568100	-2.3592967700	-0.0169954100
H	2.9030005100	1.9360453600	0.0082419700
H	-1.9653098400	2.1490830700	-0.8956451400
H	-1.9957262700	2.1706924200	0.8525557400

7HIT-S_{1-min} (XMS-PT2(12,10)-DZ)

-819.32100075

S	-2.7005329700	-0.6408572900	0.0108102600
O	-0.0111992500	-2.4613490100	0.0003311600
H	-0.9556587800	-2.2604810800	-0.0110767200
C	-1.2844780400	0.3568687100	0.0053630200
C	-1.4253950300	1.8652434200	-0.0014988300
C	0.0338889000	2.3834210900	0.0006738000

H	0.2334678700	2.9987017600	-0.8758934000
H	0.2320113700	2.9973943500	0.8785669100
C	0.8939816300	1.1468839700	0.00111165900
C	2.2707450900	1.0536077900	0.0002015200
C	2.8635348000	-0.2198215600	-0.0004717000
H	3.9393525900	-0.3133389000	-0.0018796300
C	2.0796290200	-1.3751867500	0.0001884800
C	0.6912437500	-1.2933366300	0.0010200600
C	0.0775437400	-0.0187690900	0.0027443200
H	2.5337347700	-2.3551874900	-0.0003144300
H	2.8850316700	1.9431368900	0.0002332200
H	-1.9780358700	2.1976935900	-0.8825705200
H	-1.9843052300	2.2052662200	0.8725558600

7HIT-S_{2-min} (XMS-PT2(12,10)-DZ)

-819.30150767

S	-2.5180420000	-0.8679015000	-0.0023366000
O	-0.0713263000	-2.3536794000	-0.0535970000
H	-1.1189564000	-1.9890346000	-0.0444726000
C	-1.2899483000	0.3325071000	-0.0064496000
C	-1.4367983000	1.8364186000	0.0258663000
C	0.0195365000	2.3843297000	-0.0067800000
H	0.2107160000	2.9808343000	-0.8998725000
H	0.2299801000	3.0245316000	0.8500263000
C	0.8899985000	1.1535079000	0.0063026000
C	2.2975435000	1.0362138000	-0.0253493000
C	2.8897854000	-0.2375444000	0.0334143000
H	3.9626806000	-0.3294859000	0.0909345000
C	2.0967162000	-1.3897398000	0.0213894000
C	0.6799453000	-1.2841440000	-0.0146460000
C	0.0875371000	0.0198357000	-0.0207440000
H	2.5330296000	-2.3797018000	0.0332810000
H	2.9186381000	1.9204996000	-0.0926753000
H	-2.0215987000	2.1978065000	-0.8232650000
H	-1.9648766000	2.1546365000	0.9290736000

7HIT-T_{1-min} (XMS-PT2(12,10)-DZ)

-819.32749021

S	-2.6985534900	-0.6236383900	0.0174868600
O	-0.0062573500	-2.4653036700	0.0007395900
H	-0.9507506200	-2.2691655400	-0.0063046200
C	-1.2918766500	0.3555157400	0.0034523400
C	-1.4271583600	1.8665951400	-0.0037496900
C	0.0334815300	2.3792386300	0.0006781300

H	0.2350541900	2.9936766700	-0.8755353400
H	0.2317095000	2.9929267200	0.8782221800
C	0.8903782100	1.1412996900	0.0022647200
C	2.2692749700	1.0516777600	0.0030417000
C	2.8637930000	-0.2184479600	-0.0004929800
H	3.9393108000	-0.3105387000	-0.0012985900
C	2.0812836600	-1.3737235300	-0.0033484700
C	0.6921687400	-1.2931309900	0.0005236300
C	0.0778720500	-0.0221835300	0.0018098000
H	2.5356559300	-2.3529221900	-0.0069102200
H	2.8788988300	1.9437207300	0.0056693800
H	-1.9756213000	2.2030976400	-0.8850483600
H	-1.9841035800	2.2111957800	0.8688999300

7HIT-T_{2-min} (XMS-PT2(12,10)-DZ)

-819.31938731

S	-2.6456278700	-0.7391049500	-0.0130217300
O	-0.0272657300	-2.4400428100	0.0102349700
H	-0.9764079500	-2.1939800600	0.0192347500
C	-1.2771604900	0.3637966600	0.0009957400
C	-1.4209968900	1.8648075700	-0.0044676500
C	0.0319831800	2.3969934900	0.0091075500
H	0.2394903300	3.0238307200	-0.8572949200
H	0.2300523500	2.9971664900	0.8965715400
C	0.9000685100	1.1624467700	-0.0023385500
C	2.2646934400	1.0550488900	-0.0063755500
C	2.8599247000	-0.2307382000	-0.0074702700
H	3.9355164900	-0.3235392600	-0.0135309000
C	2.0759989700	-1.3850002200	-0.0007457500
C	0.6860456300	-1.3046985900	0.0032283600
C	0.0639024200	-0.0090659600	0.0002431000
H	2.5300692900	-2.3649454000	0.0007610600
H	2.8870148300	1.9397710900	-0.0089749000
H	-1.9710606500	2.1936870300	-0.8882819500
H	-1.9916804700	2.2034567700	0.8622250800

7HIT-MECI-S₂/S₁ (XMS-PT2(12,10)-DZ)

S₂: -819.30030338 S₁: -819.30095294

S	-2.5368298400	-0.8751621100	0.0489466700
O	-0.0762875700	-2.3465186800	-0.0478513700
H	-1.0965833300	-2.0038979200	0.0137303500
C	-1.3148733900	0.3319697700	-0.0070954000
C	-1.4511273900	1.8437996200	0.0000250900
C	0.0121729200	2.3919073200	-0.0053895300

H	0.2205444000	2.9938942400	-0.9028294300
H	0.2181557400	3.0353199200	0.8626190400
C	0.8848201400	1.1557346200	0.0153805600
C	2.3167569900	1.0371540200	0.0184465600
C	2.9118783900	-0.2402795900	0.0167842700
H	3.9936356200	-0.3423478000	0.0232503800
C	2.1036176200	-1.4045823400	-0.0132916900
C	0.6737911400	-1.2864876400	-0.0212710800
C	0.0752173200	0.0183757800	-0.0019516800
H	2.5393456100	-2.4003575300	-0.0144127900
H	2.9428738200	1.9303457000	0.0091119300
H	-2.0149172200	2.1865116900	-0.8796236600
H	-2.0076309400	2.1845109400	0.8855218300

7HIT-iso-S_{0-min} (MS-PT2(12,10)-DZ)

-819.38410651

S	-2.6534292500	-0.7611338600	-0.0209915700
O	0.0052126800	-2.4119346200	0.0113254100
H	0.6291809700	-3.1542562000	0.0132771900
C	-1.3661647600	0.2801751300	-0.0044219800
C	-1.5147989100	1.8031601900	0.0001941400
C	-0.0866109000	2.3932691400	0.0051759000
H	0.1059057600	3.0282445400	-0.8765050200
H	0.1045339500	3.0137263000	0.8975686500
C	0.8193668900	1.1800605200	-0.0014232000
C	2.2220381200	1.1689011200	-0.0057609800
C	2.8744596200	-0.0763712900	-0.0045017500
H	3.9681238100	-0.1197975300	-0.0083224100
C	2.1447850500	-1.2800445100	0.0006145600
C	0.7368941700	-1.2740459500	0.0037591900
C	0.0647919300	-0.0187056400	0.0004102500
H	2.6754134400	-2.2395453800	0.0019227300
H	2.7925881300	2.1023584400	-0.0098256500
H	-2.0989815300	2.1072724700	-0.8841906500
H	-2.1035191600	2.1021171200	0.8830751800

7HIT-iso-S_{1-min} (MS-PT2(12,10)-DZ)

-819.31887958

S	-2.6572550500	-0.7254357500	0.0098617100
O	-0.1204461700	-2.3850350700	0.0143040000
H	0.4278249200	-3.1843615700	0.0185786600
C	-1.2734880000	0.3313643000	0.0044399800
C	-1.4319285900	1.8439806400	-0.0097635000
C	0.0265545800	2.3914753100	0.0136244800

H	0.2293831800	3.0398051900	-0.8558489800
H	0.2120052800	2.9974450000	0.9170332200
C	0.9111235000	1.1596801700	-0.0003947100
C	2.3039023800	1.0701338800	-0.0089532500
C	2.9061987000	-0.2097565400	-0.0106699100
H	3.9965065600	-0.3017529200	-0.0176657300
C	2.1162617600	-1.3840499600	-0.0029781300
C	0.7177012200	-1.3023882400	0.0049840600
C	0.0998914100	-0.0191184900	0.0022548000
H	2.6006388900	-2.3682943300	-0.0040194500
H	2.9237942000	1.9726614700	-0.0134283300
H	-1.9813969800	2.1705028300	-0.9125213900
H	-2.0203417600	2.1890541100	0.8605824800

7HIT-iso-S_{2-min} (MS-PT2(12,10)-DZ)

-819.25396647

S	-2.7162410000	-0.6745564200	-0.0127982400
O	-0.0514545800	-2.4012550700	0.0075742400
H	0.5392385300	-3.1739873600	0.0130012800
C	-1.3597602900	0.3286984600	-0.0059523900
C	-1.4373084100	1.8612502700	-0.0009757500
C	0.0263528000	2.3822494500	0.0041012100
H	0.2585996400	3.0109952300	-0.8757820300
H	0.2543537200	2.9975492800	0.8943968100
C	0.8679600700	1.1297553900	-0.0004695900
C	2.3011488600	1.0439163300	-0.0050854000
C	2.9495480500	-0.2169278600	-0.0035129700
H	4.0377933100	-0.2985796700	-0.0049483300
C	2.1335548100	-1.3799389000	-0.0000017400
C	0.6909370600	-1.2963905000	0.0017504300
C	0.0165512200	-0.0220346500	-0.0031646600
H	2.5892523100	-2.3783138700	0.0011652500
H	2.8903466100	1.9667967500	-0.0088058100
H	-1.9992673700	2.2097582300	-0.8847767100
H	-2.0023953300	2.2017349200	0.8836244400

7HIT-iso-T_{1-min} (MS-PT2(12,10)-DZ)

-819.32387477

S	-2.6367498600	-0.7305644300	-0.0016042000
O	-0.1230793300	-2.3832947100	-0.0009535000
H	0.4245650900	-3.1828031000	0.0038110500
C	-1.2795597800	0.3310146600	0.0009962500
C	-1.4354423600	1.8459882600	-0.0006744800
C	0.0255320400	2.3887801400	0.0027918600

H	0.2216878800	3.0233335400	-0.8787689600
H	0.2189995900	3.0078966000	0.8959050600
C	0.9094818400	1.1563631300	-0.0041239500
C	2.3045997400	1.0685541000	-0.0058264300
C	2.9072706500	-0.2095494000	-0.0018216500
H	3.9975139100	-0.3015906400	-0.0006126800
C	2.1168687600	-1.3817928200	0.0019815900
C	0.7165139000	-1.2999293600	-0.0004064200
C	0.0997467300	-0.0193281300	-0.0012345700
H	2.6007034400	-2.3658980600	0.0051467500
H	2.9229715000	1.9721073400	-0.0088270300
H	-1.9981992000	2.1841083400	-0.8905206200
H	-2.0042145500	2.1873245500	0.8840819300

7HIT-iso-T_{2-min} (MS-PT2(12,10)-DZ)

-819.30439593

S	-2.7302663600	-0.7003453100	0.0083039500
O	-0.0782749800	-2.4313277100	-0.0034660400
H	0.5125385800	-3.1999413500	-0.0020544200
C	-1.2876136800	0.3502501700	0.0065076100
C	-1.4213606000	1.8592902600	-0.0024467700
C	0.0334366300	2.3964281700	0.0018642800
H	0.2438436200	3.0222454700	-0.8825482000
H	0.2399023200	3.0174074500	0.8906361800
C	0.9037276900	1.1545590000	-0.0002063900
C	2.2887283600	1.0707650500	-0.0010719500
C	2.9007758700	-0.2111003400	-0.0012322300
H	3.9908352900	-0.3004222900	-0.0003628700
C	2.1094172500	-1.3828158200	-0.0007898900
C	0.7095475500	-1.3237570900	-0.0004138200
C	0.0644033000	-0.0303346500	0.0036973900
H	2.5975248400	-2.3650555000	-0.0019666900
H	2.9035076100	1.9764809400	-0.0001921700
H	-1.9913185300	2.1884738400	-0.8912488600
H	-2.0001447500	2.1999196900	0.8763309100

7HIT-iso-MECI-S₂/S₁ (MS-PT2(12,10)-DZ)

S₂: -819.22821220 S₁: -819.22854028

S	-2.8570274900	-0.5160304300	-0.5270470000
O	0.0668298400	-2.0493666400	0.8583579000
H	0.7321350100	-2.4959717000	1.4064508900
C	-1.4316281500	0.3276626300	-0.3912638300
C	-1.3588378300	1.8523099500	-0.1653724500
C	0.0001237000	2.0626173500	0.5737552900

H	0.4581666100	3.0645764100	0.4894984900
H	-0.1365571300	1.8408656900	1.6514883700
C	0.8344100500	0.9775870000	-0.0711904200
C	2.2673524500	1.0232610500	-0.4106421200
C	2.9562577600	-0.1929379100	-0.4606692900
H	3.9900392700	-0.2918522500	-0.7972400900
C	2.1321073600	-1.3192784200	-0.1774796100
C	0.6977014000	-1.1709667700	0.0641691300
C	-0.0643873100	-0.0530166900	-0.4766612700
H	2.5386198200	-2.3380419100	-0.1851870500
H	2.7394765300	1.9834934300	-0.6436204400
H	-1.3462974800	2.3750907700	-1.1429038100
H	-2.2292744000	2.2107184300	0.4048973600

7HIT-iso-MEI-S₁/T₂/T₁ (MS-PT2(12,10)-DZ)

S₁: -819.28855367 T₂: -819.28862514 T₁: -819.29077316

S	-2.3790295576	-0.7359341889	0.9677933703
O	0.0053249374	-2.2955798138	-0.8868934896
H	0.5923791194	-3.0650998124	-0.9847865946
C	-1.1996315330	0.3649716938	0.2602884165
C	-1.3381562988	1.8814888573	0.1785475410
C	-0.0061078169	2.3669137247	-0.4757226299
H	-0.1543020673	2.5387229880	-1.5596936392
H	0.3863388420	3.3038187074	-0.0453353666
C	0.9096233561	1.1776310885	-0.2642972357
C	2.2033817181	1.0619062000	0.2052749144
C	2.7478219932	-0.2390824828	0.5027923042
H	3.7624395244	-0.3144152942	0.8970104398
C	2.0266439499	-1.4272388011	0.2076511587
C	0.7156668026	-1.3226581241	-0.2587915251
C	0.0593775422	-0.0134481499	-0.1330716282
H	2.5296482741	-2.4078586217	0.2359617647
H	2.8245989868	1.9520480951	0.3675385547
H	-2.2267960336	2.1664836191	-0.4077299570
H	-1.4700102907	2.2980538023	1.1928063811

DM-7HIT-S_{0-min} (MS-PT2(12,10)-DZ)

-897.77344497

S	-2.6057521200	-0.7307478200	0.0185110400
O	-0.0717628700	-2.4403443200	-0.0026108600
H	-1.0249946000	-2.1515538300	0.0075266900
C	-1.3125988900	0.3317807200	0.0061806100
C	-1.4446416400	1.8607652600	-0.0009277600
C	0.0237333700	2.3827881500	0.0107283900

H	0.2312058300	3.0133088700	-0.8722203400
H	0.2222506900	3.0007702100	0.9046402900
C	0.8939188700	1.1454118900	0.0083837500
C	2.2870457500	1.0411936300	0.0023098900
C	2.8548794900	-0.2535367500	-0.0074800300
H	3.9447447100	-0.3585988300	-0.0140249100
C	2.0701079600	-1.4194224300	-0.0072482600
C	0.6650543800	-1.3262755300	-0.0008657500
C	0.0865692300	-0.0175054200	0.0047841200
H	2.5309820900	-2.4107123900	-0.0117098200
H	2.9269490300	1.9287324000	0.0029720200
C	-2.2101001200	2.3146781800	1.2515532600
H	-2.2750996400	3.4165930000	1.2717517100
H	-1.6927813600	1.9792521900	2.1667612300
H	-3.2291748600	1.8949510800	1.2509811300
C	-2.1933535200	2.3090703300	-1.2665820700
H	-2.2674490800	3.4102524900	-1.2906035900
H	-3.2104219800	1.8837574000	-1.2799565300
H	-1.6627722000	1.9772362000	-2.1756498100

DM-7HIT-S_{1-min} (MS-PT2(12,10)-DZ)

-897.68662347

S	-2.7244701000	-0.6916302300	0.0111825800
O	-0.0036895700	-2.5163404000	-0.0064937300
H	-0.9517611400	-2.3184604200	-0.0051669800
C	-1.3082107800	0.3375209500	0.0084632800
C	-1.4598029400	1.8657454100	0.0020071800
C	0.0196814000	2.3656594200	0.0090913600
H	0.2234116800	2.9982245900	-0.8736856800
H	0.2200316400	2.9841216600	0.9024142300
C	0.8858336300	1.1269747700	0.0040689300
C	2.2756011200	1.0373476700	-0.0003314900
C	2.8757659000	-0.2451078500	-0.0040959200
H	3.9653181400	-0.3384026000	-0.0091131800
C	2.0865347100	-1.4109618000	-0.0041559400
C	0.6849611500	-1.3353274800	-0.0020610300
C	0.0629816500	-0.0490849200	0.0021807800
H	2.5461000500	-2.4032574100	-0.0065789600
H	2.8941063100	1.9404798300	-0.0009741300
C	-2.2123064600	2.3429142300	1.2560076200
H	-2.2635389900	3.4463295100	1.2711832400
H	-1.6977772600	2.0015404200	2.1700422700
H	-3.2448536600	1.9521772800	1.2750826300
C	-2.1958020300	2.3318672400	-1.2659133600

H	-2.2438998100	3.4351588600	-1.2924465300
H	-3.2282061800	1.9415536000	-1.2932484700
H	-1.6694699800	1.9828023600	-2.1702542900

DM-7HIT-S_{2-min} (MS-PT2(12,10)-DZ)

-897.66651109

S	-2.5709871700	-0.8327127300	0.0232623000
O	-0.0958908500	-2.3824360500	-0.0156859900
H	-1.1071357300	-2.0110484800	-0.0036769300
C	-1.3158995000	0.3339576000	0.0103210900
C	-1.4590412800	1.8574640600	0.0034956600
C	0.0223357200	2.3805432700	0.0089576300
H	0.2320872000	3.0121097700	-0.8747493500
H	0.2294521300	3.0011879100	0.9011462400
C	0.8905709400	1.1422114300	0.0028575400
C	2.3165137300	1.0120783300	0.0021684000
C	2.9148375300	-0.2779968900	-0.0031392100
H	4.0033464100	-0.3770286600	-0.0028081200
C	2.0997522900	-1.4355297400	-0.0066551700
C	0.6685255700	-1.3154785500	-0.0060949200
C	0.0653880200	0.0040145600	0.0043660700
H	2.5290968800	-2.4422328700	-0.0140039900
H	2.9484751000	1.9069513500	0.0016997600
C	-2.2208038600	2.3241481500	1.2535518500
H	-2.3366427700	3.4233880100	1.2513834600
H	-1.6829553200	2.0279784000	2.1707673200
H	-3.2216051100	1.8605989600	1.2784588800
C	-2.2021454200	2.3100349500	-1.2634395300
H	-2.3206455400	3.4088972900	-1.2749190000
H	-3.2017894700	1.8449073100	-1.3013297500
H	-1.6483009600	2.0058373000	-2.1687299100

DM-7HIT-T_{1-min} (MS-PT2(12,10)-DZ)

-897.6931551

S	-2.6856744400	-0.6924564300	0.4754685200
O	-0.0766539100	-2.4859090200	-0.1850691400
H	-0.9984881700	-2.2552435500	-0.3841240700
C	-1.3243145600	0.3445256300	0.2392102100
C	-1.4667137800	1.8670189400	0.1060065600
C	0.0002417200	2.3476103100	0.3232174500
H	0.2465410200	3.2051772500	-0.3277183300
H	0.1343853500	2.6744914900	1.3722296300
C	0.8633905900	1.1341282800	0.0524673200
C	2.2479690200	1.0462952900	-0.1090829800

C	2.8324596300	-0.2325763500	-0.2748062300
H	3.9153481400	-0.3255166100	-0.4023464500
C	2.0356858900	-1.3957171800	-0.2939922400
C	0.6404614000	-1.3183367400	-0.1409637500
C	0.0432500500	-0.0403198300	0.0591696200
H	2.4817530100	-2.3827477700	-0.4491998900
H	2.8707428100	1.9468819700	-0.1029331900
C	-2.4278491500	2.4727308900	1.1364790500
H	-2.4170903000	3.5746776400	1.0619742100
H	-2.1365574900	2.1869198700	2.1610537300
H	-3.4648227300	2.1326038400	0.9651200800
C	-1.9293544600	2.2036615100	-1.3256427000
H	-2.0000174900	3.2990805300	-1.4560508100
H	-2.9208747300	1.7642468600	-1.5321745000
H	-1.2126834000	1.8067862100	-2.0650071200

DM-7HIT-T_{2-min} (MS-PT2(12,10)-DZ)
-897.68838144

S	-2.6669813600	-0.7636613900	0.2227006700
O	-0.0294172600	-2.4850050900	0.0729083300
H	-0.9783713600	-2.2431176200	0.1516591600
C	-1.2982392600	0.3513024900	0.1913808900
C	-1.4515453300	1.8677582000	0.0914756000
C	0.0177078300	2.3724250100	0.2387713500
H	0.2515003800	3.1792104500	-0.4773458700
H	0.1791763000	2.7795490400	1.2549586300
C	0.8878413100	1.1506049000	0.0409848600
C	2.2591834500	1.0464113800	-0.1186046200
C	2.8528258800	-0.2447519300	-0.2216745300
H	3.9347129000	-0.3396283800	-0.3522939400
C	2.0650284700	-1.4121923400	-0.1558318500
C	0.6713103300	-1.3354341700	0.0066782200
C	0.0499694200	-0.0332005900	0.0871256100
H	2.5187434900	-2.4050460000	-0.2299325500
H	2.8846452500	1.9433105500	-0.1626601400
C	-2.3630601400	2.4345175800	1.1864207500
H	-2.4051826600	3.5361304600	1.1190659100
H	-1.9890768300	2.1608588700	2.1877605600
H	-3.3884296300	2.0422664100	1.0806485500
C	-2.0101295600	2.2272892400	-1.2978284400
H	-2.1241103800	3.3212458800	-1.3983152800
H	-2.9990838800	1.7609247200	-1.4483568900
H	-1.3324788500	1.8700770000	-2.0924906000

DM-7HIT-MECI-S₂/S₁ (MS-PT2(12,10)-DZ)

S₂: -897.66550838 S₁: -897.66587332

S	-2.5564713900	-0.8639681800	-0.0089745100
O	-0.0992109900	-2.3774386300	0.0191150900
H	-1.1292139300	-1.9929923100	0.0037174300
C	-1.3068160100	0.3344401500	0.0006144300
C	-1.4583919500	1.8536588100	-0.0027775700
C	0.0221656800	2.3792758500	0.0041392200
H	0.2311320500	3.0092323500	-0.8797912800
H	0.2228884900	3.0021041400	0.8961560200
C	0.8967204200	1.1439224100	0.0046007600
C	2.3167605800	1.0167468300	-0.0045316300
C	2.9067446800	-0.2728991300	-0.0076933100
H	3.9947184400	-0.3759892000	-0.0140430700
C	2.0947384200	-1.4310883700	-0.0005617400
C	0.6684286800	-1.3124108200	0.0124019300
C	0.0770632300	0.0047342800	0.0057929400
H	2.5281555400	-2.4353272500	-0.0033671100
H	2.9518250200	1.9087673900	-0.0027598200
C	-2.2159297900	2.3140074300	1.2534053200
H	-2.3018072000	3.4155248300	1.2734095300
H	-1.6897403300	1.9833897700	2.1656015100
H	-3.2302566000	1.8790125200	1.2666657600
C	-2.2047127300	2.3152232200	-1.2639027400
H	-2.3202411600	3.4145786400	-1.2677430300
H	-3.2050164400	1.8532642500	-1.2979503800
H	-1.6569941800	2.0160756600	-2.1743193900

DM-7HIT-MEI-S₁/T₂/T₁ (MS-PT2(12,10)-DZ)

S₁: -897.68571951 T₂: -897.68747934 T₁: -897.68892427

S	-2.6956407155	-0.7554608662	0.1771802723
O	-0.0336036680	-2.4858732053	0.0563838343
H	-0.9766012006	-2.2577659866	0.1304735812
C	-1.2857678654	0.3454270014	0.1564041015
C	-1.4492320561	1.8691920030	0.0732782832
C	0.0242195393	2.3720738157	0.1946434439
H	0.2470845672	3.1487108506	-0.5573169677
H	0.1896096126	2.8229794038	1.1914525558
C	0.8954037400	1.1449625328	0.0296801259
C	2.2730353391	1.0446226466	-0.0959990997
C	2.8589497321	-0.2441351854	-0.1798981743
H	3.9436385449	-0.3421047551	-0.2851735251
C	2.0674249094	-1.4112595402	-0.1268653846
C	0.6709611299	-1.3287721407	0.0045435962

C	0.0642852729	-0.0350693159	0.0677214612
H	2.5224163269	-2.4045887076	-0.1876844501
H	2.8928063075	1.9384730253	-0.1288307324
C	-2.3356725191	2.4136457552	1.2025011647
H	-2.3866825013	3.5171464377	1.1496401951
H	-1.9325221176	2.1283326760	2.1899850517
H	-3.3655755547	2.0205597722	1.1210104467
C	-2.0493646366	2.2476775315	-1.2943079518
H	-2.1562388232	3.3457202344	-1.3746850902
H	-3.0471508513	1.7925909413	-1.4234949929
H	-1.3992447857	1.8947702573	-2.1134258076

DM-7HIT-iso-S_{0-min} (MS-PT2(12,10)-DZ)

-897.75708186

S	-2.6260787900	-0.6751701000	0.5709436500
O	-0.0912160800	-2.4250798900	-0.0533844700
H	0.4935907400	-3.1873605000	-0.1906043800
C	-1.3390539000	0.3176648400	0.2871487500
C	-1.4451564400	1.8480733100	0.1359473300
C	0.0112361900	2.3502238400	0.31113742600
H	0.2566779900	3.1742036100	-0.3820493800
H	0.1693005000	2.7266655600	1.3397479700
C	0.8687004800	1.1284524300	0.0786511400
C	2.2590252900	1.0721662500	-0.0974163600
C	2.8557596600	-0.1912078100	-0.2579897900
H	3.9385587500	-0.2712705500	-0.4009502200
C	2.0809784900	-1.3674531600	-0.2409880400
C	0.6844329800	-1.3150582600	-0.0621437300
C	0.0720669800	-0.0421036700	0.1002576200
H	2.5672975800	-2.3416413500	-0.3734611800
H	2.8622400200	1.9853423100	-0.1098478500
C	-2.4047518900	2.4786047000	1.1475038400
H	-2.4002071400	3.5773469900	1.0330366700
H	-2.1012936400	2.2333039200	2.1799122700
H	-3.4304998000	2.1074072500	0.9939664300
C	-1.9291314400	2.1273341700	-1.3007905600
H	-1.9959908600	3.2171495200	-1.4693427400
H	-2.9252869800	1.6796281900	-1.4566742400
H	-1.2304266600	1.6992933900	-2.0412359800

DM-7HIT-iso-S_{1-min} (MS-PT2(12,10)-DZ)

-897.69036682

S	-2.6549741300	-0.7579131800	0.2482564800
O	-0.1228017500	-2.3970181600	0.0384646500

H	0.4258313200	-3.1929630700	-0.0472870800
C	-1.2807970500	0.3273681400	0.2134167100
C	-1.4463915800	1.8489022900	0.1003918800
C	0.0191631500	2.3638632600	0.2470113900
H	0.2348484300	3.1783343100	-0.4681111200
H	0.1795006600	2.7674692200	1.2655420800
C	0.8984301800	1.1512874700	0.0347689400
C	2.2831073500	1.0699492400	-0.1201294500
C	2.8829681200	-0.2069352400	-0.2311162500
H	3.9668687100	-0.2948368100	-0.3578430300
C	2.0979133400	-1.3823041700	-0.1762626900
C	0.7060156900	-1.3092071700	-0.0204779400
C	0.0880667400	-0.0286035700	0.0756064800
H	2.5802706500	-2.3646092900	-0.2600663100
H	2.8975579400	1.9763554900	-0.1517163000
C	-2.3643814000	2.4185856100	1.1904036200
H	-2.3893779800	3.5217533300	1.1291642600
H	-2.0045320000	2.1294591700	2.1926162800
H	-3.3973372700	2.0440465300	1.0742626300
C	-1.9973851200	2.1948553600	-1.2967820600
H	-2.0887646400	3.2910518300	-1.4077365000
H	-2.9929428700	1.7426047900	-1.4493821700
H	-1.3200844900	1.8150196100	-2.0813835300

DM-7HIT-iso-S_{2-min} (MS-PT2(12,10)-DZ)

-897.62747395

S	-2.7087759400	-0.7058060500	0.0325437300
O	-0.0473214300	-2.4217304200	-0.0361513700
H	0.5481264900	-3.1926519400	-0.0507163700
C	-1.3610294500	0.3112640200	0.0174059800
C	-1.4597989000	1.8514805300	0.0137454100
C	0.0183691100	2.3539347600	0.0474819000
H	0.2479505100	3.0277115200	-0.8013613800
H	0.2336159700	2.9288394600	0.9702995700
C	0.8628149800	1.1102199000	-0.0026489300
C	2.2968720500	1.0282953000	-0.0233150000
C	2.9474237200	-0.2303455400	-0.0481646100
H	4.0362256200	-0.3096984900	-0.0651149000
C	2.1338024600	-1.3938155100	-0.0502406200
C	0.6899863100	-1.3146748100	-0.0310679500
C	0.0138726600	-0.0407562500	-0.0060457500
H	2.5945463800	-2.3903093300	-0.0691415300
H	2.8837738800	1.9535108400	-0.0185952600
C	-2.2385250000	2.3402539100	1.2432502200

H	-2.2914351500	3.4452026900	1.2541997900
H	-1.7475813800	2.0027958700	2.1733606500
H	-3.2619757700	1.9300319000	1.2263879000
C	-2.1650872000	2.3202407400	-1.2685698700
H	-2.2335915900	3.4243364900	-1.2913699300
H	-3.1817766000	1.8949385500	-1.3122808300
H	-1.6097096900	1.9832468600	-2.1622798700

DM-7HIT-iso-T_{1-min} (MS-PT2(12,10)-DZ)

-897.69564569

S	-2.6409603700	-0.7514420000	0.2852759700
O	-0.1231114800	-2.3965274100	0.0371413900
H	0.4256321400	-3.1915133100	-0.0571394400
C	-1.2849233200	0.3250521400	0.2464204200
C	-1.4486399800	1.8460524100	0.1131820500
C	0.0158503700	2.3583969600	0.2729496000
H	0.2332629400	3.1862987400	-0.4263356300
H	0.1730021000	2.7430682500	1.2994938000
C	0.8939405300	1.1481778400	0.0424205000
C	2.2799254100	1.0702357100	-0.1277977800
C	2.8798253800	-0.2036751500	-0.2524262000
H	3.9622561000	-0.2893082700	-0.3926224500
C	2.0967858000	-1.3784012700	-0.1949868000
C	0.7049444800	-1.3066150800	-0.0226682900
C	0.0886528500	-0.0295949500	0.0871318100
H	2.5769096000	-2.3606040600	-0.2905422000
H	2.8919586800	1.9783952600	-0.1611282500
C	-2.3805510600	2.4347965300	1.1805309800
H	-2.4006964300	3.5372086600	1.1038282700
H	-2.0378588400	2.1575750000	2.1921011600
H	-3.4138054600	2.0641838400	1.0524078000
C	-1.9749914600	2.1781820300	-1.2970604500
H	-2.0613279200	3.2735212200	-1.4226342500
H	-2.9691765600	1.7269189200	-1.4603906100
H	-1.2861315100	1.7861329600	-2.0655404000

DM-7HIT-iso-T_{2-min} (MS-PT2(12,10)-DZ)

-897.67612206

S	-2.7216987500	-0.7281926700	0.0757060600
O	-0.0828162400	-2.4482631800	0.0059458000
H	0.5098602900	-3.2145629100	-0.0342980400
C	-1.2917857400	0.3410691400	0.0744944000
C	-1.4404581600	1.8614509900	0.0407659100
C	0.0295848700	2.3737409600	0.1158579200

H	0.2531850700	3.0975801300	-0.6878352600
H	0.2156384500	2.8905183300	1.0753938900
C	0.8979087900	1.1388852300	0.0125912600
C	2.2812663200	1.0549623100	-0.0581719100
C	2.8922117200	-0.2278495700	-0.1132016200
H	3.9808060300	-0.3160581800	-0.1719166000
C	2.1009641500	-1.3977345900	-0.0910156800
C	0.7019642700	-1.3390908800	-0.0193876400
C	0.0573161500	-0.0435954900	0.0254755700
H	2.5868561500	-2.3801515500	-0.1322373800
H	2.8952852500	1.9612288700	-0.0676694700
C	-2.2756631300	2.3620009500	1.2283545800
H	-2.3806023500	3.4610315800	1.1875909400
H	-1.7942210500	2.0926935100	2.1846285800
H	-3.2838343900	1.9152472200	1.2086435700
C	-2.1066011600	2.2827756400	-1.2811799300
H	-2.2405618000	3.3792082700	-1.3118555000
H	-3.0978459200	1.8085619500	-1.3820586500
H	-1.4859868400	1.9810589400	-2.1430097900

DM-7HIT-iso-MECI-S₂/S₁ (MS-PT2(12,10)-DZ)

S₂: -897.60088384 S₁: -897.60117347

S	-2.8664229700	-0.7346800700	-0.1945832400
O	0.2375878900	-2.0220011100	1.0719488200
H	0.9794033500	-2.3893148100	1.5773174100
C	-1.4900477500	0.1913217100	-0.1259480300
C	-1.4938974600	1.7377729400	0.0685333500
C	-0.0255443500	2.0499512100	0.5558535600
H	0.3410130400	3.0712625300	0.3421343400
H	0.0273153000	1.9005232900	1.6531684000
C	0.7640924500	0.9809907400	-0.1386383000
C	2.1587023500	1.0399312200	-0.6216102100
C	2.8787629100	-0.1565130600	-0.6799765600
H	3.8717149100	-0.2572363500	-1.1257489900
C	2.1294137200	-1.2889757900	-0.2467739500
C	0.7176236400	-1.1889678800	0.1415063200
C	-0.1235169700	-0.1081448500	-0.3565663300
H	2.5595589500	-2.2958253700	-0.2814458300
H	2.5774873200	2.0054226500	-0.9182559100
C	-2.5137460000	2.2148406600	1.10111103200
H	-2.3230484400	3.2771674400	1.3405776700
H	-2.4396457300	1.6262840400	2.0301455000
H	-3.5358976300	2.1088638600	0.7185596800
C	-1.7539623100	2.4124822600	-1.2878777600

H	-1.7379343500	3.5129180700	-1.1857861600
H	-2.7425203100	2.0993084000	-1.6573705200
H	-0.9957195100	2.1191332500	-2.0386625500

DM-7HIT-iso-MEI-S₁/T₂/T₁ (MS-PT2(12,10)-DZ)

S₁: -897.66213104 T₂: -897.66180913 T₁: -897.66415205

S	-2.5900729200	-0.7986117900	-0.2464658500
O	0.1285025900	-2.3747123900	0.8537956200
H	0.6533759200	-3.1588703000	0.7819312100
C	-1.2739220100	0.3192092700	0.0608512400
C	-1.4149289300	1.8562641100	0.0950545400
C	0.0139056800	2.3438136400	0.4848833000
H	0.3141713200	3.2583893100	-0.0265487700
H	0.0561048900	2.5409542500	1.5599254600
C	0.9009548400	1.1724700800	0.1659345300
C	2.1437124300	1.0837876000	-0.3654439700
C	2.7003033300	-0.2202306400	-0.6746061600
H	3.6887873500	-0.2960321700	-1.1013830100
C	2.0029522200	-1.4090631300	-0.2973792900
C	0.7286179200	-1.3621568900	0.2229948200
C	0.0242974600	-0.0485125500	0.1869268900
H	2.5216878300	-2.3590744800	-0.3500367900
H	2.7367105500	1.9692570500	-0.5553633600
C	-2.4640030500	2.3055348500	1.1114320600
H	-2.5309691700	3.3969286700	1.1400433700
H	-2.2094570200	1.9612496500	2.1182999800
H	-3.4395362800	1.9017915500	0.8464139300
C	-1.7971870600	2.3598902800	-1.3034053300
H	-1.9168792400	3.4464979600	-1.3099542000
H	-2.7444686900	1.9148697200	-1.6141242100
H	-1.0318880000	2.1028713300	-2.0421650000

5. References

1. K. Andersson, P. A. Malmqvist, B. O. Roos, A. J. Sadlej and K. Wolinski, *J. Phys. Chem.*, 1990, **94**, 5483-5488.
2. K. Andersson, P. A. Malmqvist and B. O. Roos, *J. Chem. Phys.*, 1992, **96**, 1218-1226.
3. F. Aquilante, R. Lindh and T. B. Pedersen, *J. Chem. Phys.*, 2007, **127**, 114107.
4. N. Forsberg and P. A. Malmqvist, *Chem. Phys. Lett.*, 1997, **274**, 196-204.
5. G. Ghigo, B. O. Roos and P. A. Malmqvist, *Chem. Phys. Lett.*, 2004, **396**, 142-149.
6. C. M. Marian and U. Wahlgren, *Chem. Phys. Lett.*, 1996, **251**, 357-364.
7. C. M. Marian, *WIREs Comput. Mol. Sci.*, 2012, **2**, 187-203.
8. X.-Y. Liu, G. Cui and W.-H. Fang, *Theor. Chem. Acc.*, 2016, **136**.
9. T. H. Dunning, *J. Chem. Phys.*, 1989, **90**, 1007-1023.
10. I. F. Galvan, M. Vacher, A. Alavi, C. Angeli, F. Aquilante, J. Autschbach, J. J. Bao, S. I. Bokarev, N. A. Bogdanov, R. K. Carlson, L. F. Chibotaru, J. Creutzberg, N. Dattani, M. G. Delcey, S. S. Dong, A. Dreuw, L. Freitag, L. Manuel Frutos, L. Gagliardi, F. Gendron, A. Giussani, L. Gonzalez, G. Grell, M. Guo, C. E. Hoyer, M. Johansson, S. Keller, S. Knecht, G. Kovacevic, E. Kallman, G. Li Manni, M. Lundberg, Y. Ma, S. Mai, J. P. Malhado, P. A. Malmqvist, P. Marquetand, S. A. Mewes, J. Norell, M. Olivucci, M. Oppel, P. Quan Manh, K. Pierloot, F. Plasser, M. Reiher, A. M. Sand, I. Schapiro, P. Sharma, C. J. Stein, L. K. Sorensen, D. G. Truhlar, M. Ugandi, L. Ungur, A. Valentini, S. Vancoillie, V. Veryazov, O. Weser, T. A. Wesolowski, P.-O. Widmark, S. Wouters, A. Zech, J. P. Zobel and R. Lindh, *J. Chem. Theory Comput.*, 2019, **15**, 5925-5964.
11. F. Aquilante, J. Autschbach, A. Baiardi, S. Battaglia, V. A. Borin, L. F. Chibotaru, I. Conti, L. De Vico, M. Delcey, I. F. Galvan, N. Ferre, L. Freitag, M. Garavelli, X. Gong, S. Knecht, E. D. Larsson, R. Lindh, M. Lundberg, P. A. Malmqvist, A. Nenov, J. Norell, M. Odelius, M. Olivucci, T. B. Pedersen, L. Pedraza-Gonzalez, Q. M. Phung, K. Pierloot, M. Reiher, I. Schapiro, J. Segarra-Marti, F. Segatta, L. Seijo, S. Sen, D.-C. Sergentu, C. J. Stein, L. Ungur, M. Vacher, A. Valentini and V. Veryazov, *J. Chem. Phys.*, 2020, **152**, 214117.
12. A. Maciejewski, M. Szymanski and R. P. Steer, *J. Phys. Chem.*, 1986, **90**, 6314-6318.
13. A. Maciejewski and R. P. Steer, *Chem. Rev.*, 1993, **93**, 67-98.
14. T. Shiozaki, W. Gyorffy, P. Celani and H. J. Werner, *J. Chem. Phys.*, 2011, **135**.
15. Z.-Y. Liu, J.-W. Hu, C.-H. Huang, T.-H. Huang, D.-G. Chen, S.-Y. Ho, K.-Y. Chen, E. Y. Li and P.-T. Chou, *J. Am. Chem. Soc.*, 2019, **141**, 9885-9894.
16. A. Maciejewski and R. P. Steer, *J. Am. Chem. Soc.*, 1983, **105**, 6738-6740.
17. R. P. Steer and V. Ramamurthy, *Acc. Chem. Res.*, 1988, **21**, 380-386.
18. R. P. Brint, W. G. Doherty and A. A. Ruth, *I. Mol. Spectrosc.*, 2002, **216**, 151-158.
19. A. A. Ruth, F. J. Okeeffe, M. W. D. Mansfield and R. P. Brint, *J. Phys. Chem. A*, 1997, **101**, 7735-7741.
20. A. A. Ruth, W. G. Doherty and R. P. Brint, *Chem. Phys. Lett.*, 2002, **352**, 191-201.
21. A. Maciejewski, D. R. Demmer, D. R. James, A. Safarzadehamiri, R. E. Verrall and R. P. Steer, *J. Am. Chem. Soc.*, 1985, **107**, 2831-2837.
22. A. A. Ruth, T. Fernholz, R. P. Brint and M. W. D. Mansfield, *Chem. Phys. Lett.*, 1998, **287**, 403-411.
23. A. A. Ruth, F. J. Okeeffe, R. P. Brint and M. W. D. Mansfield, *Chem. Phys.*, 1997, **217**, 83-98.