

Aromaticity and Sterics Control Whether a Cationic Olefin Radical is Resistant to Disproportionation

Electronic Supplementary Information (ESI)

Julian Messelberger,[†] Annette Grünwald,[†] Stephen J. Goodner, Florian Zeilinger, Piermaria Pinter, Matthias E. Miehlich, Frank W. Heinemann, Max M. Hansmann and Dominik Munz^{*}

Contents

1. NMR Spectra	S2
2. Electrochemical Studies	S6
3. X-ray Crystallographic Data of Radical Cation 18^{rad}	S9
4. Computational Details	S13
5. References	S52

1. NMR Spectra

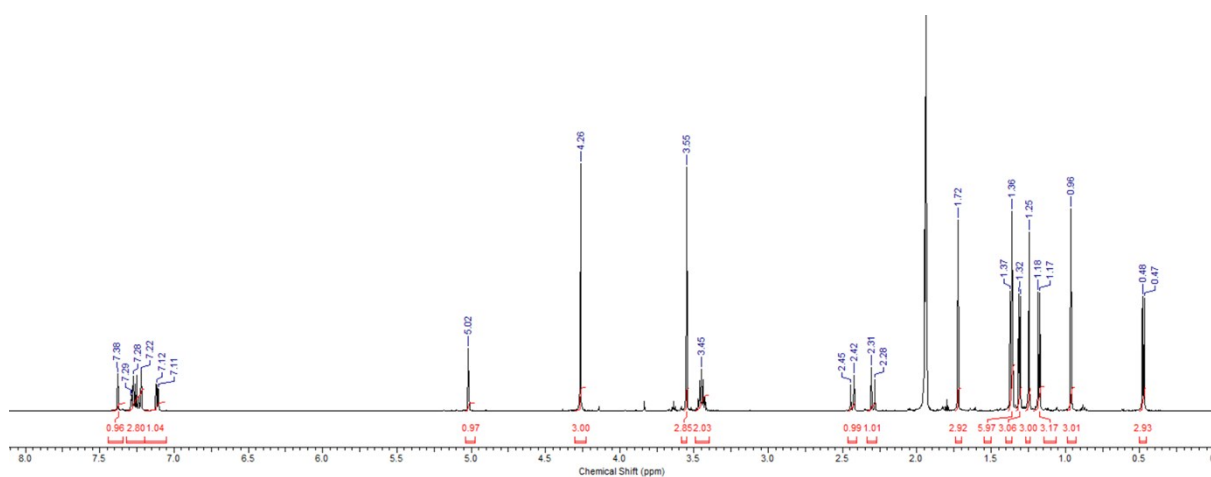


Figure S1. ^1H NMR spectrum of **17** (CD_3CN , 600.1 MHz).

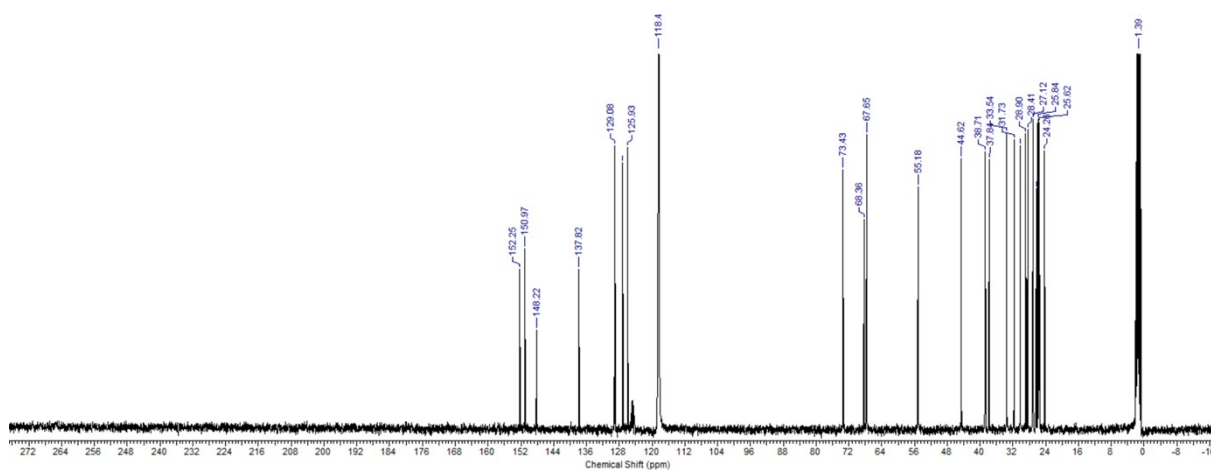


Figure S2. ^{13}C NMR spectrum of **17** (CD_3CN , 100.6 MHz).

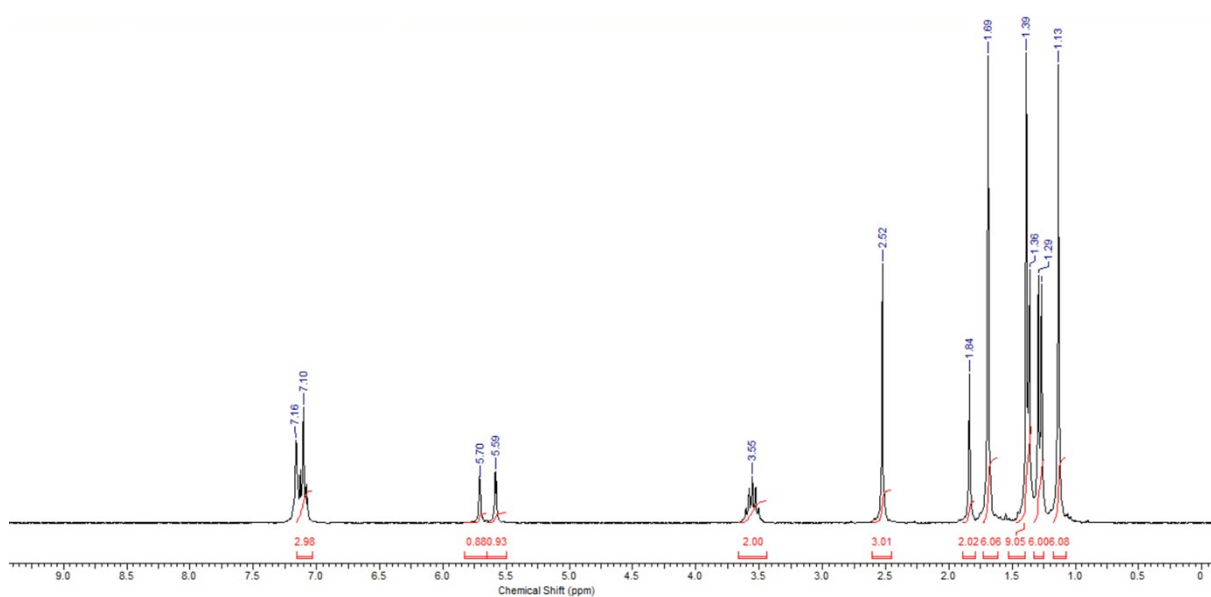


Figure S3. ^1H NMR spectrum of **18** (C_6D_6 , 269.7 MHz).

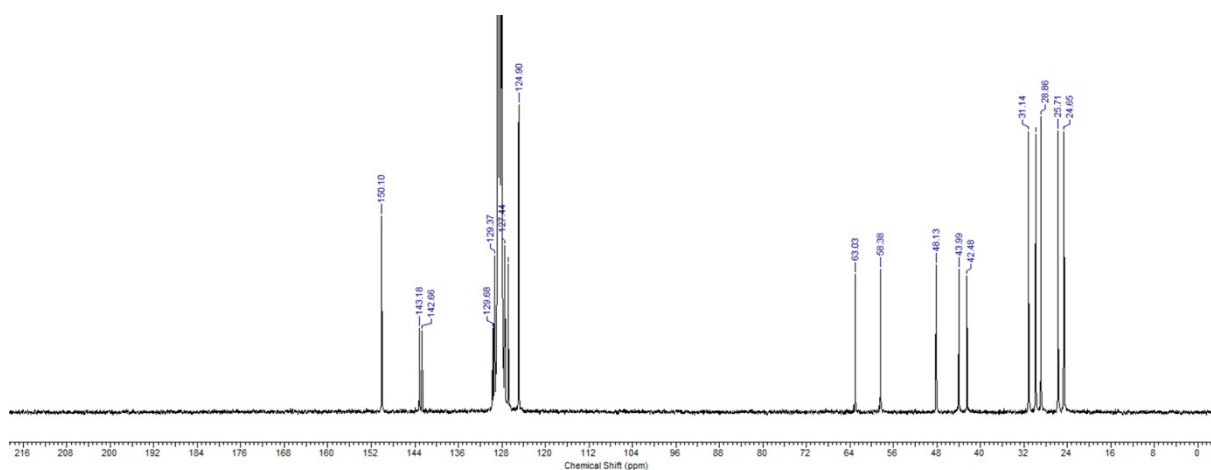


Figure S4. ¹³C NMR spectrum of **18** (C₆D₆, 67.8 MHz).

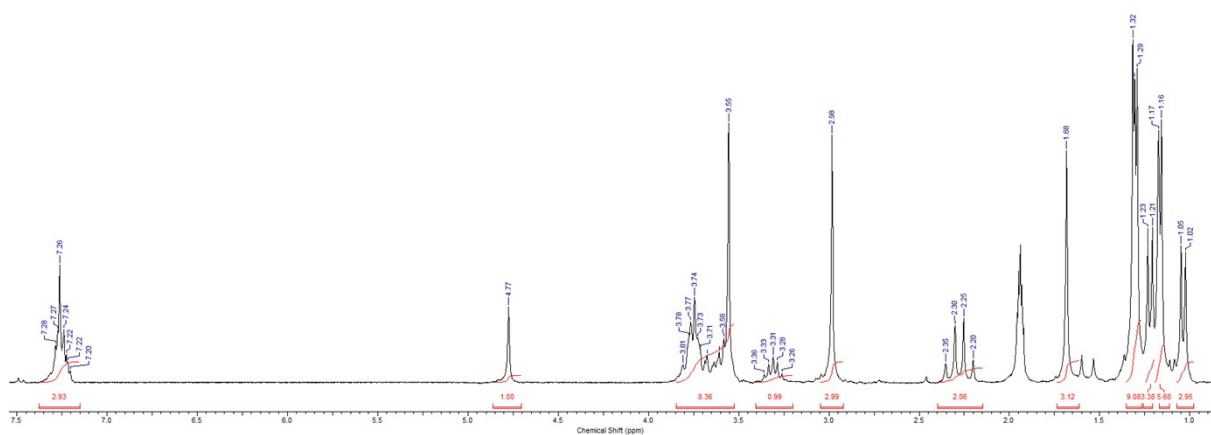


Figure S5. ¹H NMR spectrum of **21** (CD₃CN, 269.7 MHz).

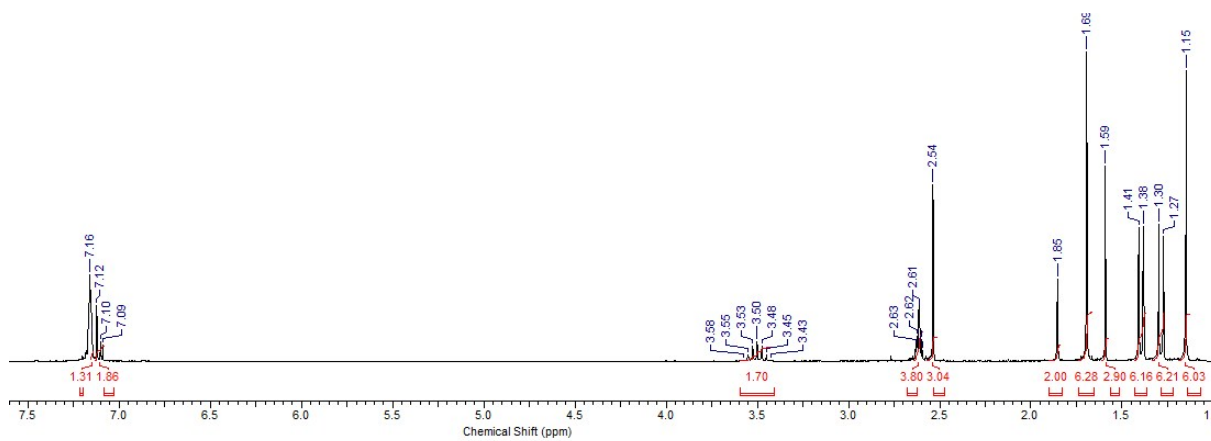


Figure S6. ¹H NMR spectrum of **22** (C₆D₆, 269.7 MHz).

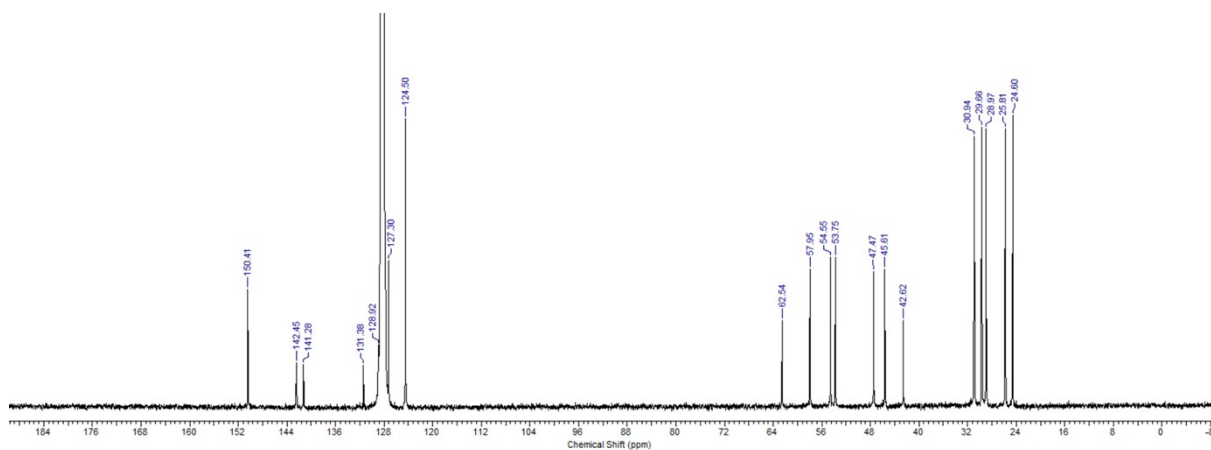


Figure S7. ^{13}C NMR spectrum of **22** (C_6D_6 , 100.6 MHz).

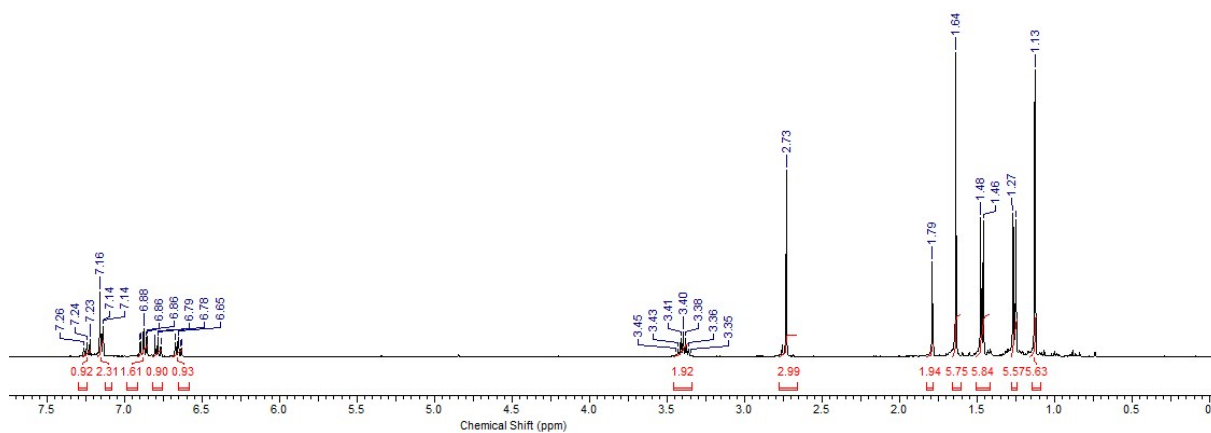


Figure S8. ^1H NMR spectrum of **25** (C_6D_6 , 399.8 MHz).

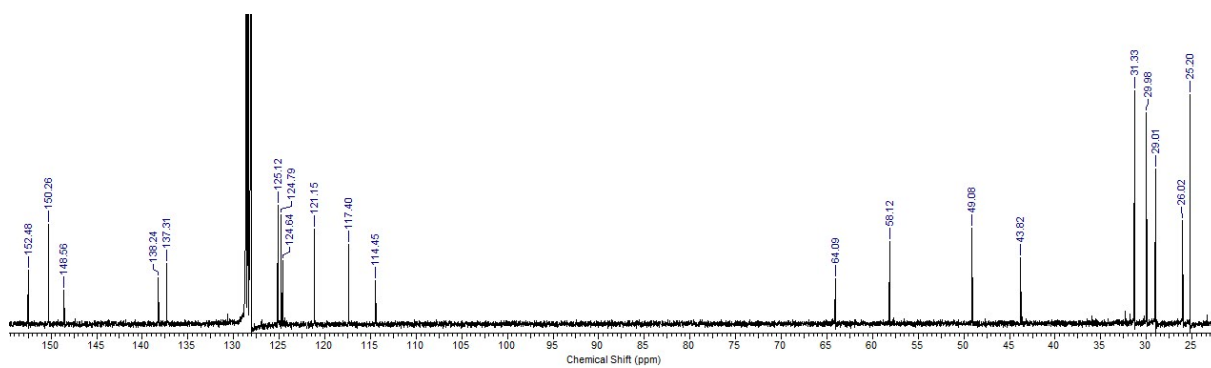


Figure S9. ^{13}C NMR spectrum of **25** (C_6D_6 , 100.6 MHz).

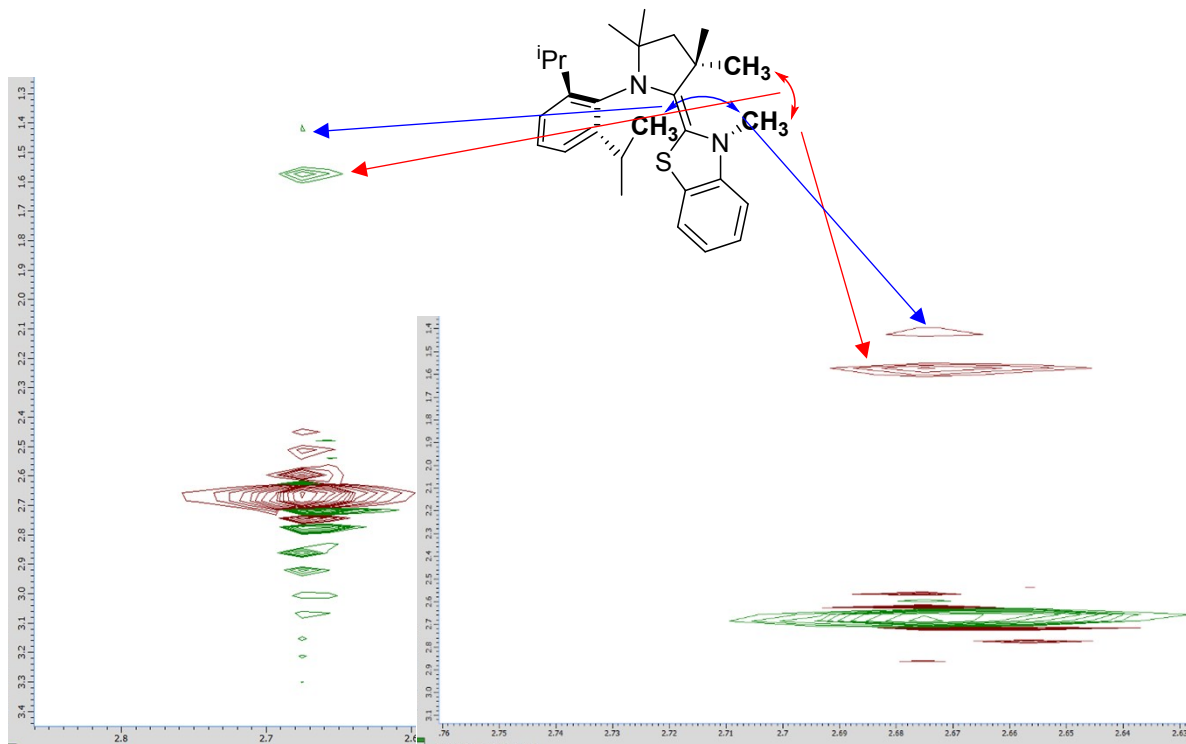


Figure S10. ROESY (left) and NOESY (right) spectra of **21** (C_6D_6 , 399.8 MHz), which indicate strong coupling of the *N*-methyl substituent with the methyl groups of the CAAC (calculated distance: 2.20 Å) and weak coupling with one *i*Pr group of the Dipp substituent (calculated distance: 2.68 Å).

2. Electrochemical Studies

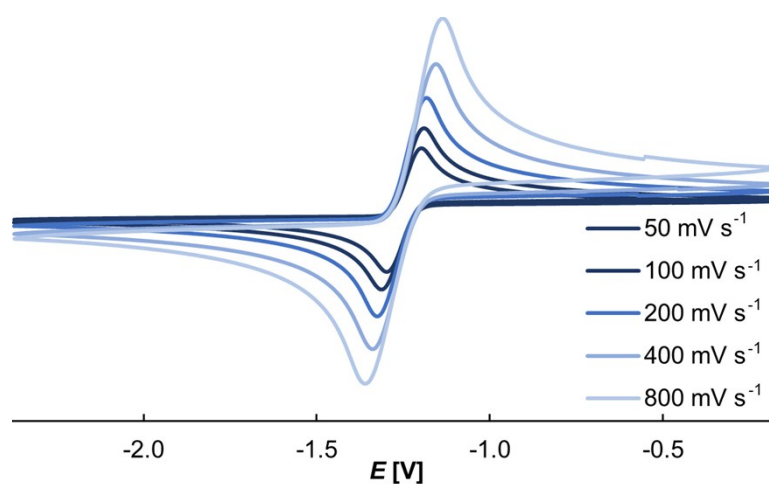


Figure S11. Cyclic voltammogram of **9** at various scan rates ($n\text{Bu}_4\text{PF}_6$ 0.1 M in DMF, vs. Fc/Fc⁺).

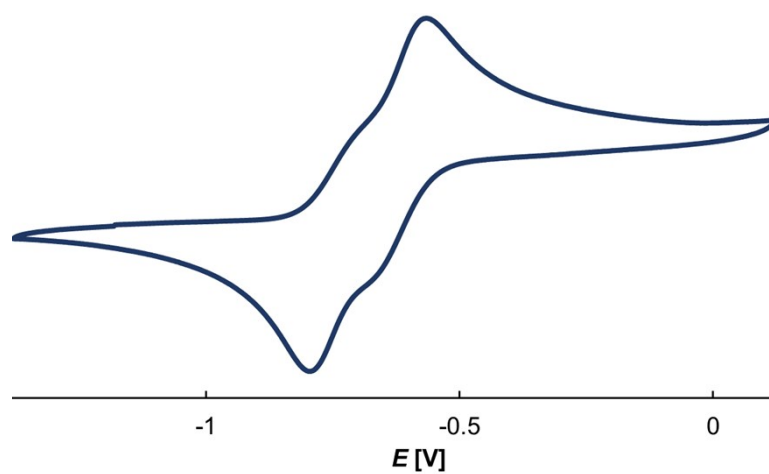


Figure S12. Cyclic voltammogram of Ph^h**9** at 50 mV s⁻¹ ($n\text{Bu}_4\text{PF}_6$ 0.1 M in CH₂Cl₂, vs. Fc/Fc⁺).

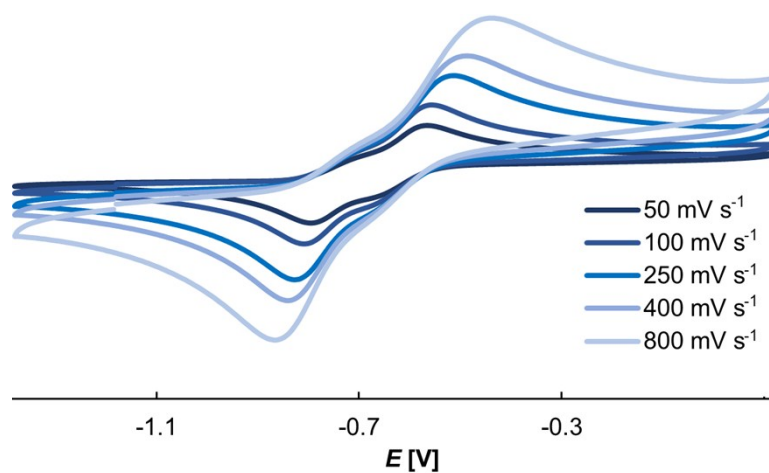


Figure S13. Cyclic voltammogram of Ph^h**9** at various scan rates ($n\text{Bu}_4\text{PF}_6$ 0.1 M in CH₂Cl₂, vs. Fc/Fc⁺).

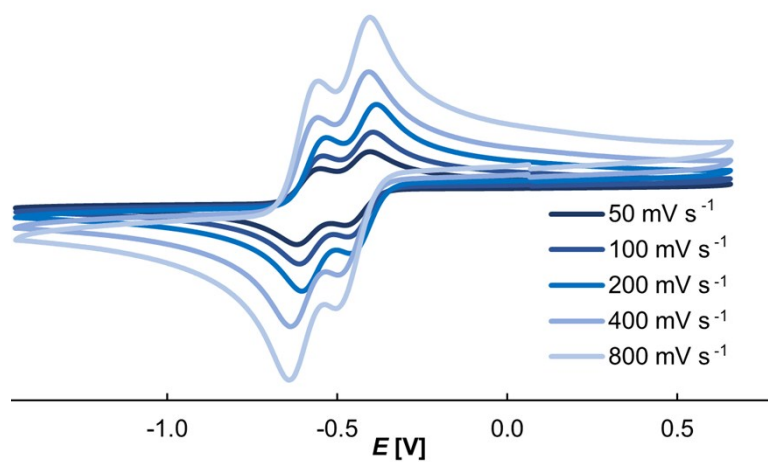


Figure S14. Cyclic voltammogram of **13** at various scan rates ($n\text{Bu}_4\text{PF}_6$ 0.1 M in MeCN, vs. Fc/Fc⁺).

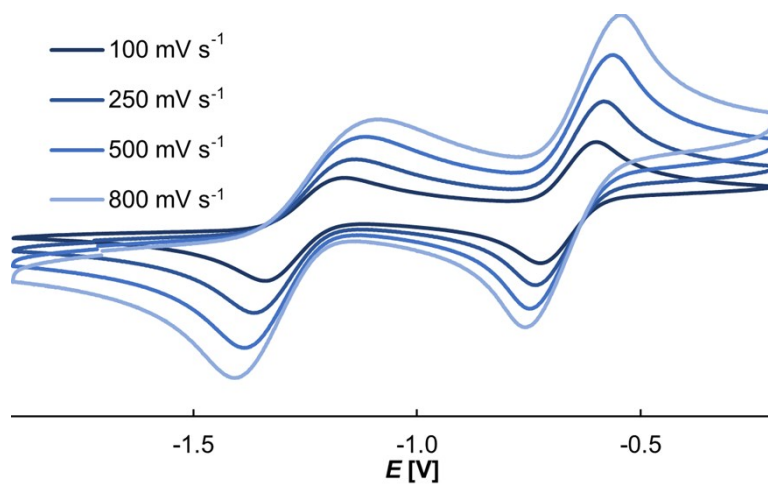


Figure S15. Cyclic voltammogram of **18** at various scan rates ($n\text{Bu}_4\text{PF}_6$ 0.1 M in THF, vs. Fc/Fc⁺).

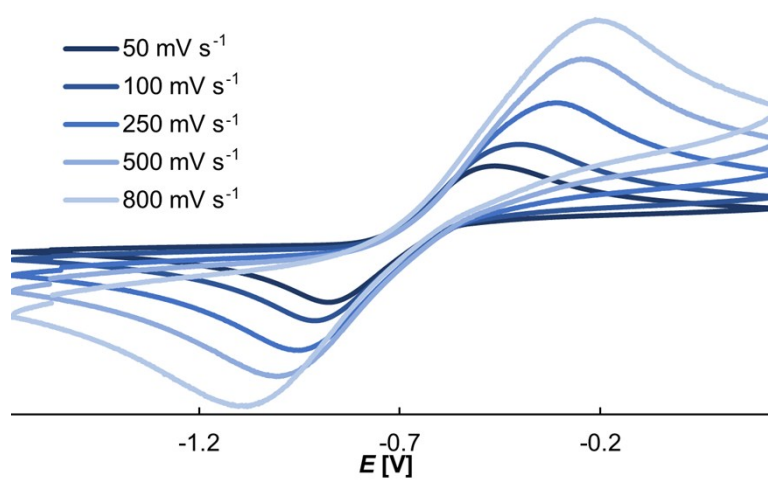


Figure S16. Cyclic voltammogram of **22** at various scan rates ($n\text{Bu}_4\text{PF}_6$ 0.1 M in THF, vs. Fc/Fc⁺).

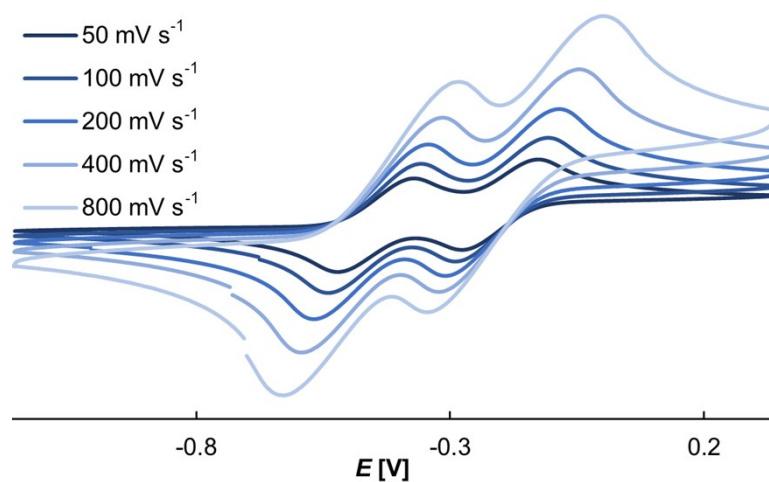


Figure S17. Cyclic voltammogram of **25** at various scan rates ($n\text{Bu}_4\text{PF}_6$ 0.1 M in THF, vs. Fc/Fc^+).

	THF			DMF			MeCN			DCM		
	$E_{1,2}$	$E_{2,3}$	ΔE	$E_{1,2}$	$E_{2,3}$	ΔE	$E_{1,2}$	$E_{2,3}$	ΔE	$E_{1,2}$	$E_{2,3}$	ΔE
1	0.71 ¹	0.45 ¹	0.26	0.58 ²	0.19 ²	0.39	0.71 ³	0.32 ³	0.39	irrev., n.a. ¹	irrev., n.a. ¹	–
3	0.98 (irrev., peak pot.) ⁴	0.64 (irrev., peak pot.) ⁴	0.34	0.88 ⁴	0.65 ⁴	0.23	0.89 ⁵	0.55 ⁵	0.34	1.11 ⁶	0.68 ⁶	0.43
4	–	–	–	0.84 ⁷	0.42 ⁷	0.42	0.81 ⁷	0.40 ⁷	0.41	–	–	–
Pr- teth 8	–	–	–	-1.20 ⁸ / -1.08 ⁹	-1.20 ⁸ / -1.08 ⁹	0	-1.37 (irrev.) ⁸	-1.18 ⁸	0.19	–	–	–
9	-0.61 (irrev.)	-0.61 (irrev.)	0	-0.71	-0.71	0	–	–	–	–	–	–
Ph 9	-1.28 (quasi rev.)	-1.28 (quasi rev.)	0	-1.28 (irrev.)	-1.28 (irrev.)	0	broad, undefined signal	broad, un- defined signal	–	-1.19	-1.09	0.10
10	–	–	–	-0.84 ¹⁰	-0.84 ¹⁰	0	-0.90 ¹⁰	-0.90 ¹⁰	0	–	–	–
Pr- teth 10	–	–	–	-0.62 ⁸	-0.84 ⁸	0.22	-0.64 ⁸	-0.93 ⁸	0.29	–	–	–

Table S1. Potentials of homodimers **1**, **3**, **4**, **9**, Ph**9**, and **10** in different solvents vs. SCE in [V].

3. X-ray Crystallographic Data of Radical Cation **18^{rad}**

CCDC-1964614 and CCDC-1964615 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK (fax: ++33-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

Single crystals of **18^{rad}** were obtained by slow diffusion of diethyl ether into a tetrahydrofuran solution of **18^{rad}**. In the crystallization flask two different types of crystals were observed: red prisms and orange needles. A specimen of both crystal types was investigated by small molecule single crystal X-ray diffraction and it turned out that they represented different polymorphs of the same compound. For the preparation the sample was coated with protective perfluoropolyalkylether oil. A suitable single each crystal was selected, mounted on a MiTeGen micro mount and transferred to the cold nitrogen gas stream of the diffractometer. Intensity data were collected at 100 K on a Bruker Kappa Photon 2 *I* μ S Duo diffractometer equipped with QUAZAR focusing Montel optics using MoK α radiation ($\lambda = 0.71073 \text{ \AA}$). Data were corrected for Lorentz and polarization effects; semiempirical absorption corrections were performed on the basis of multiple scans using SADABS.¹¹ The structure was solved by direct methods (*SHELXT*)¹² and refined by full-matrix least-squares procedures on F^2 using *SHELXL 2014/6*.¹³ *OLEX2* was used to prepare material for publication.¹⁴

Polymorph A, CCDC-1964614

The triflate anion was disordered. Two alternative orientations were refined and resulted in site occupancies of 49.2(2) and 50.8(2) % for the atoms, S1, C26, O1 – O3, F1 – F3 and S1A, C26A, O1A – O3A, F1A – F3A, respectively. Similarity restraints were applied to the anisotropic displacement parameters of the atoms C26 and C26A (see Fig. S18). Treatment of hydrogen atoms: All hydrogen atoms were placed in positions of optimized geometry, their isotropic displacement parameters were tied to those of their corresponding carrier atoms by a factor of 1.2 or 1.5.

Identification code	18^{rad}
Empirical formula	C ₂₆ H ₃₉ N ₃ F ₃ O ₃ S
Formula weight/g mol ⁻¹	530.66
Temperature/K	100.15
Crystal system	Monoclinic
Space group	P2 ₁ /n
<i>a</i> /Å	11.3959(4)
<i>b</i> /Å	8.8582(3)
<i>c</i> /Å	26.7626(10)
α /°	90
β /°	91.5800(10)

$\gamma/^\circ$	90
Volume/ \AA^3	2700.58(17)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.305
μ/mm^{-1}	0.173
F(000)	1132.0
Crystal size/ mm^3	0.17 \times 0.15 \times 0.11
Radiation	MoK α , $\lambda = 0.71073 \text{ \AA}$
2 Θ range for data collection/ $^\circ$	4.76 \leq 2 Θ \leq 57.4
Index ranges	-15 \leq h \leq 15, -11 \leq k \leq 11, -36 \leq l \leq 36
Reflections collected	44464
Independent reflections	6963
Data/restraints/parameters	6963 / 0 / 408
Goodness-of-fit on F ²	1.051
Final R indexes [$I \geq 2\sigma(I)$]	R ₁ = 0.0416, wR ₂ = 0.1005
Final R indexes [all data]	R ₁ = 0.0538, wR ₂ = 0.1100
Largest diff. Peak/hole/ $\text{e}\text{\AA}^{-3}$	0.41 / -0.29

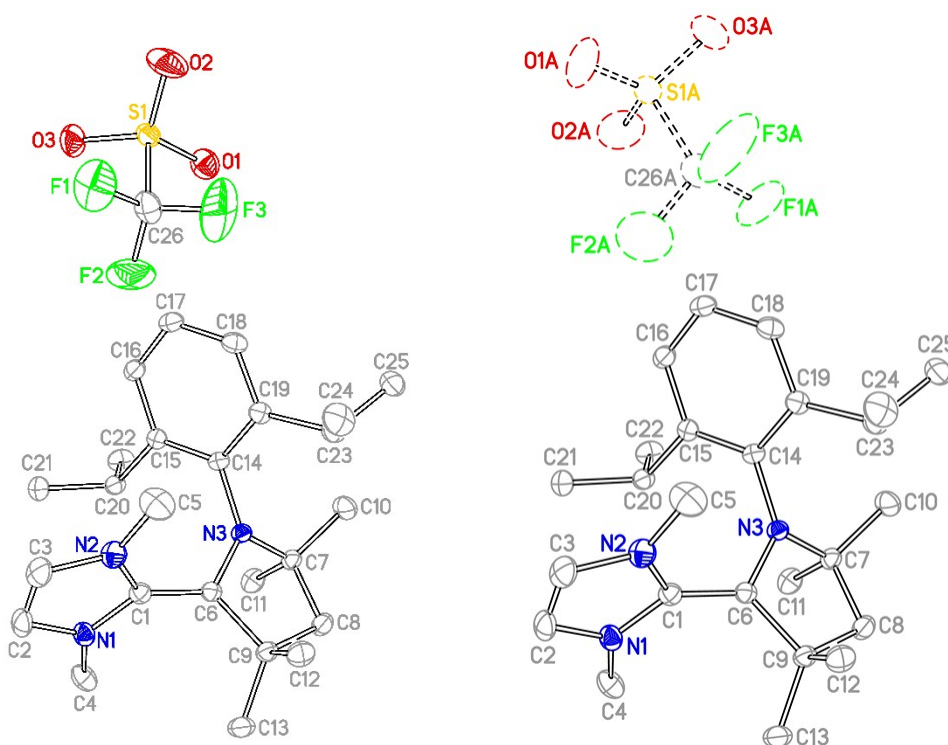


Figure S18. Thermal ellipsoid representation of the molecular structure of **18^{rad}** with the applied numbering scheme (left and right pictures display the alternative orientations of the disordered triflate anion; 50% probability ellipsoids, hydrogen atoms are omitted for clarity).

Polymorph B, CCDC-1964615

In this crystal structure the cation was disordered. Two alternative orientations were refined for the substituted pyrrolidine moiety and resulted in site occupancies of 47.4(5) and 52.6(5) % for the affected atoms, C8, C10, C11 and C8A, C10A, C11A, respectively (see Figure S19). Treatment of hydrogen atoms: All hydrogen atoms were placed in positions of optimized geometry, their isotropic displacement parameters were tied to those of their corresponding carrier atoms by a factor of 1.2 or 1.5.

Identification code	18^{rad}
Empirical formula	C ₂₆ H ₃₉ N ₃ F ₃ O ₃ S
Formula weight/g mol ⁻¹	530.66
Temperature/K	100.15
Crystal system	Monoclinic
Space group	P2 ₁ /n
a/Å	14.9305(9)
b/Å	11.6700(7)
c/Å	16.4062(9)
α/°	90
β/°	109.508(2)
γ/°	90
Volume/Å ³	2694.4(3)
Z	4
ρ _{calc} /g/cm ³	1.308
μ/mm ⁻¹	0.173
F(000)	1132.0
Crystal size/mm ³	0.24×0.07×0.05
Radiation	MoKα, λ = 0.71073 Å
2θ range for data collection/°	4.37 ≤ 2θ ≤ 55.75
Index ranges	-19 ≤ h ≤ 19, -15 ≤ k ≤ 15, -21 ≤ l ≤ 21
Reflections collected	94277
Independent reflections	6421
Data/restraints/parameters	6421 / 0 / 365
Goodness-of-fit on F ²	1.083

Final R indexes [$I \geq 2\sigma(I)$]

$R_1 = 0.0577$, $wR_2 = 0.1268$

Final R indexes [all data]

$R_1 = 0.0642$, $wR_2 = 0.1305$

Largest diff. Peak/hole/ $e\text{\AA}^{-3}$

0.68 / -0.65

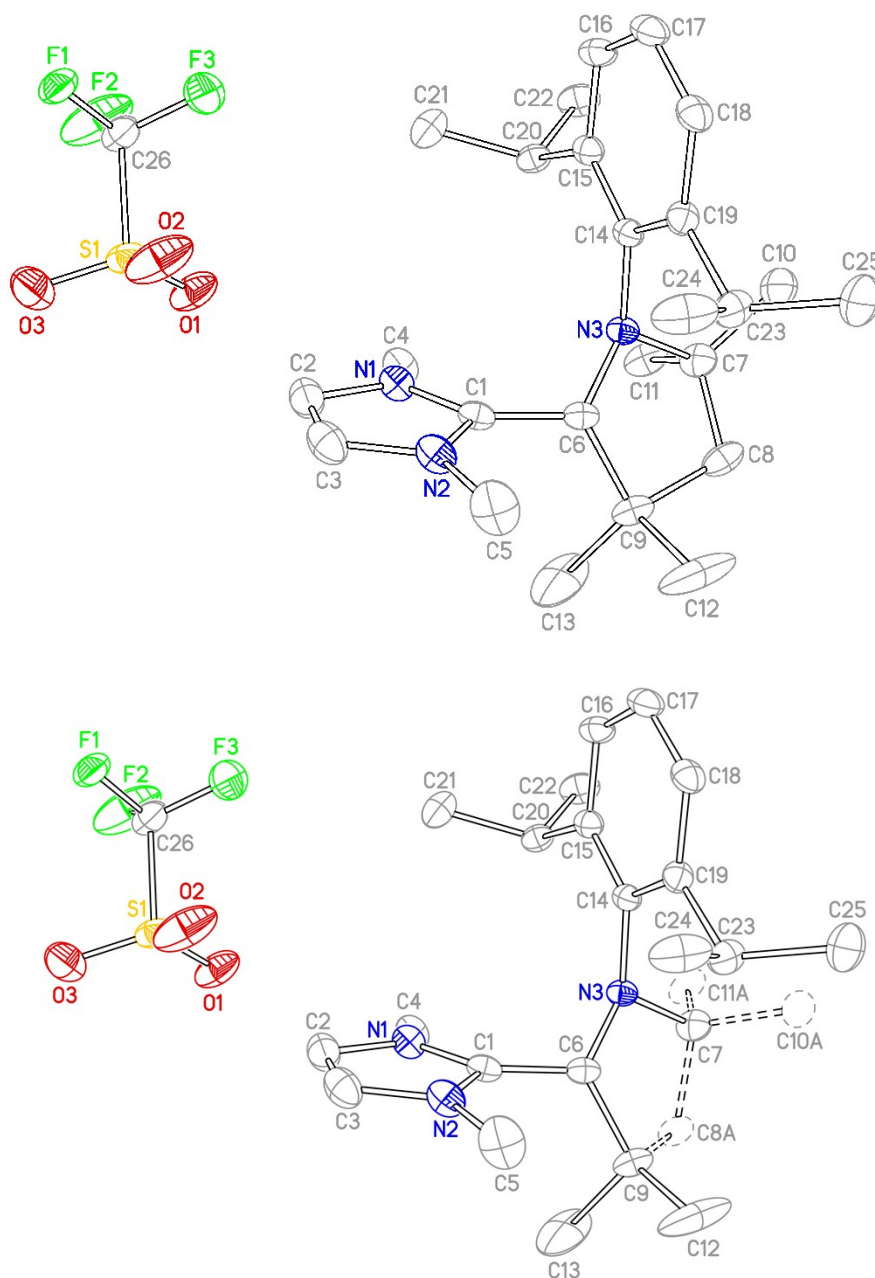


Figure S19. Thermal ellipsoid representation of the molecular structure of **18^{rad}** in crystals with the applied numbering scheme (top and bottom pictures display the alternative orientations of the disordered cation; 50% probability ellipsoids, hydrogen atoms are omitted for clarity).

4. Computational Details

	$\Delta\mu^\circ$ (calc.) [eV]	ΔE (exp.) [V]	ΔE (fit) [V]	Root- mean- square devia- tion (RMSD) [V]	RMSD (aver- aged) [V]	Mean absol- ute de- viation (MAD) [V]	MAD (aver- aged) [V]	RMSD (fit) [V]	RMSD (fit, a- ver- aged) [V]	MAD (fit) [V]	MAD (fit, a- ver- aged) [V]
Homodimers					0.10		0.09		0.09		0.07
1	0.36	0.39 ³	0.39	0.09	0.10	0.07	0.09	0.07	0.09	0.06	0.07
2	0.45	0.45 ¹⁵	0.46								
3	0.38	0.33 ⁵	0.40								
4	0.31	0.41 ⁷	0.34								
5	0.02	0.07 ¹⁶	0.10								
6	-0.33	0 ¹⁷	-								
7	0.22	0.30 ¹⁸	0.27								
8	-0.22	0 ¹⁹	-								
9	-0.96	0	-								
Ph9	-0.09	0.10	0.08								
10	-0.05	0 ¹⁰	0.04								
11	0.03	0.13 ²⁰	0.10								
12	0.02	n. a.	n. a.								
13	0.06	0.14	0.12								
Tethered homodimers											
Et-teth6	0.18	0.23 ¹⁷	0.15	0.08		0.06		0.05		0.04	
Pr-teth6	0.05	0 ⁹	0.06								
Et-teth8^c	0.41	(0.36) ^a	-								
Pr-teth8^c	0.27	0.19 ⁸	0.18								
Et-teth10^c	0.43	(0.91) ^b	-								
Pr-teth10^c	0.37	0.29 ⁸	0.32								
Heterodimers											
14	0.19	0.34 ²¹	0.30	0.15		0.14		0.14		0.10	
18	0.42	0.60	0.60								
22	-0.31	0	-								
25	0.17	0.26	0.29								

Table S2. Calculated $\Delta\mu^\circ$ and experimentally determined ΔE as well as the fitted ΔE values for all dimers. Fit parameters: $\Delta E(\text{homodimers}) = 0.8509 \Delta\mu^\circ + 0.0775$; $\Delta E(\text{tethered homodimers}) = 0.7098 \Delta\mu^\circ + 0.0225$; $\Delta E(\text{heterodimers}) = 1.2611 \Delta\mu^\circ + 0.0753$. For the the RMSD and MAD values, only dimers which form a radical cation with (borderline) stability towards disproportionation were taken into account. [a] To the best of our knowledge, Et-teth8 and its electrochemical properties has not been reported. Therefore, the potential of the ethylene-propylene linked dimer $\text{Et,Pr-teth8}^{\text{rad}}$ is used. [b] Hünig and coworkers questioned the precision of $E_{2,3}$.^{8, 22} [c] Two conformers of comparable energy ($\Delta G < 1 \text{ kcal mol}^{-1}$) were calculated for $\text{Et-teth8}^{\text{rad}}$, $\text{Pr-teth8}^{\text{rad}}$, $\text{Et-teth10}^{\text{rad}}$, and $\text{Pr-teth10}^{\text{rad}}$; given values relate to the average.

Additional Correlations

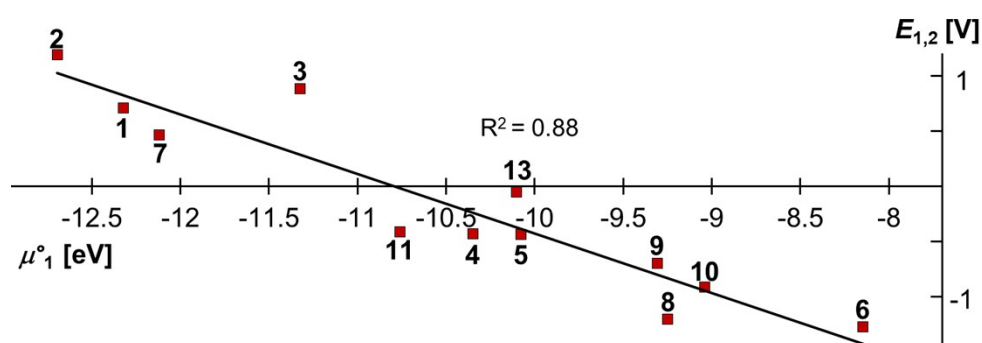


Figure S20. When approximating the electron affinity to the respective LUMO energies, the correlation is worse in comparison to the data depicted in Fig. 6. The experimentally determined potentials are referenced vs. SCE.

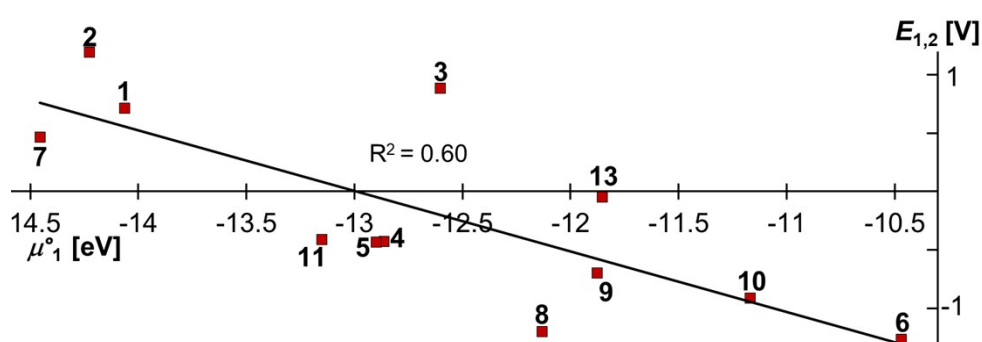


Figure S21. No satisfying correlation between experimental halfwave potentials of the first oxidation step for the homodimers and the chemical potential μ^o_1 was obtained when predicting the latter with Eq. 1. The experimentally determined potentials are referenced vs. SCE.

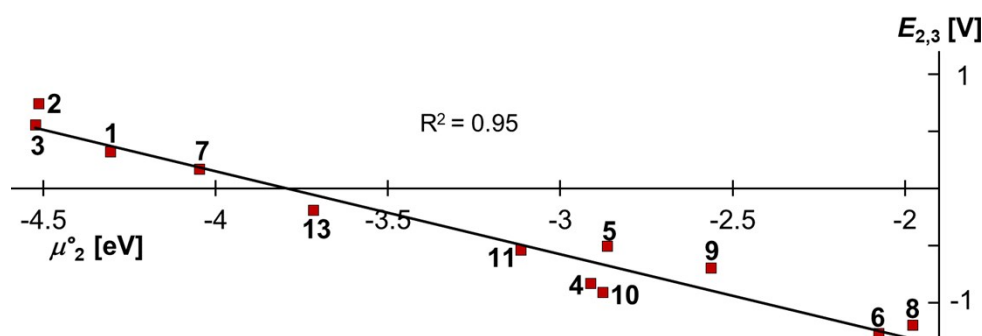


Figure S22. When using Eq. 2 instead of Eq. 1 for the prediction of the chemical potential μ^o_2 , the correlation with experimental halfwave potentials of the second oxidation step for the homodimers is slightly better. The experimentally determined potentials are referenced vs. SCE.

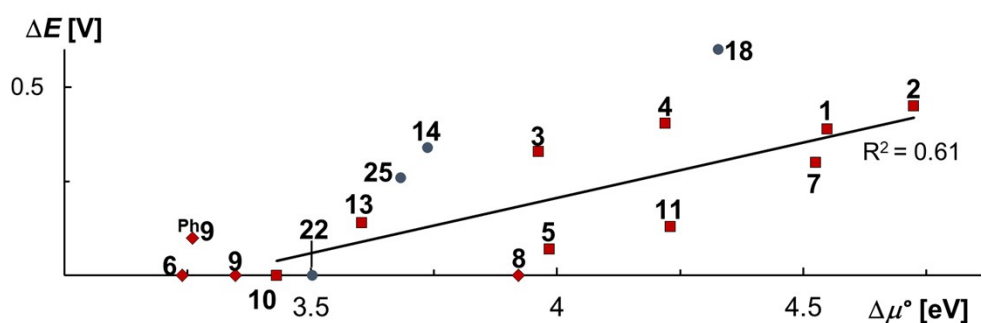


Figure S23. The separation of the halfwave potentials of the homodimer (ΔE) obtained by experiments does not correlate linearly with the difference of the calculated chemical potentials in the gas phase ($\Delta\mu^\circ = \mu^\circ_1 - \mu^\circ_2$), if both μ°_1 and μ°_2 are calculated with Eq. 2. Heterodimers are given in blue circles, homodimers are given in red squares and diamonds. Heterodimers and homodimers given in red diamonds are not included in the linear correlation.

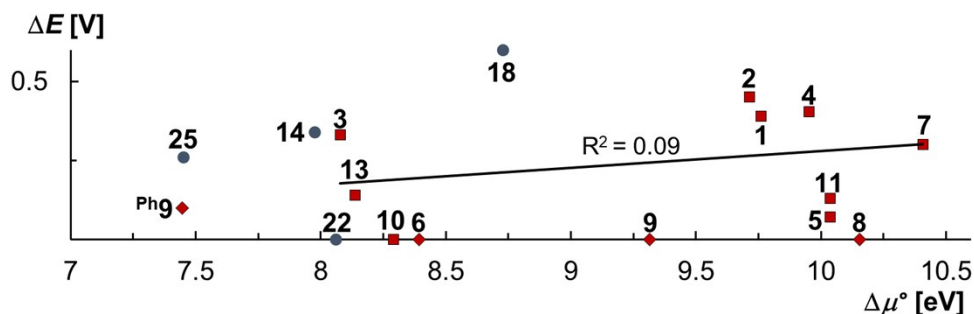


Figure S24. The separation of the halfwave potentials of the homodimer (ΔE) obtained by experiments does not correlate linearly with the difference of the calculated chemical potentials in the gas phase ($\Delta\mu^\circ = \mu^\circ_1 - \mu^\circ_2$), if μ°_1 is calculated with Eq. 1 and μ°_2 with Eq. 2. Heterodimers are given in blue circles, homodimers are given in red squares and diamonds. Heterodimers and homodimers given in red diamonds are not included in the linear correlation.

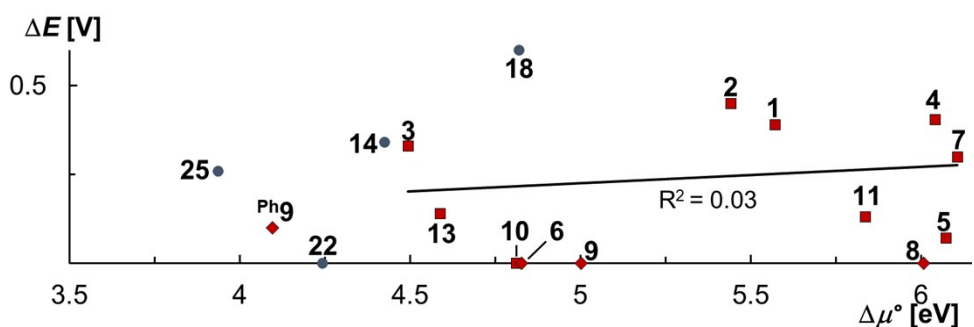


Figure S25. The separation of the halfwave potentials of the homodimer (ΔE) obtained by experiments does not correlate linearly with the difference of the calculated chemical potentials in the gas phase ($\Delta\mu^\circ = \mu^\circ_1 - \mu^\circ_2$), if both μ°_1 and μ°_2 are calculated with Eq. 1. Heterodimers are given in blue circles, homodimers are given in red squares and diamonds. Heterodimers and homodimers given in red diamonds are not included in the linear correlation.

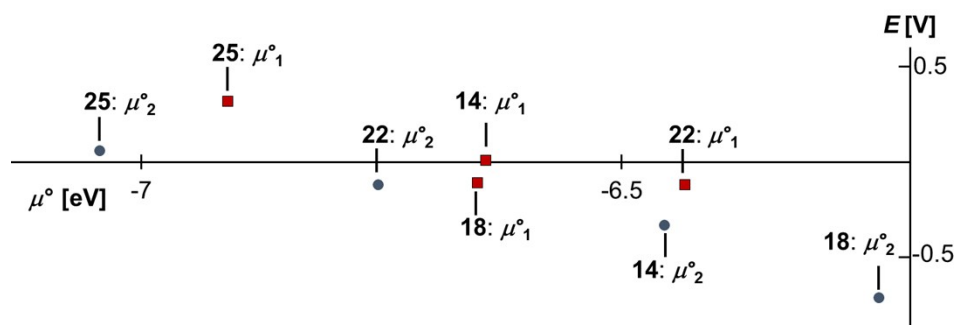


Figure S26. The calculated chemical potentials of the heterodimers are plotted against their respective experimental halfwave potential ($\Delta E_{1,2}$ vs. μ°_1 ; $\Delta E_{2,3}$ vs. μ°_2). The experimentally determined potentials are referenced vs. SCE.

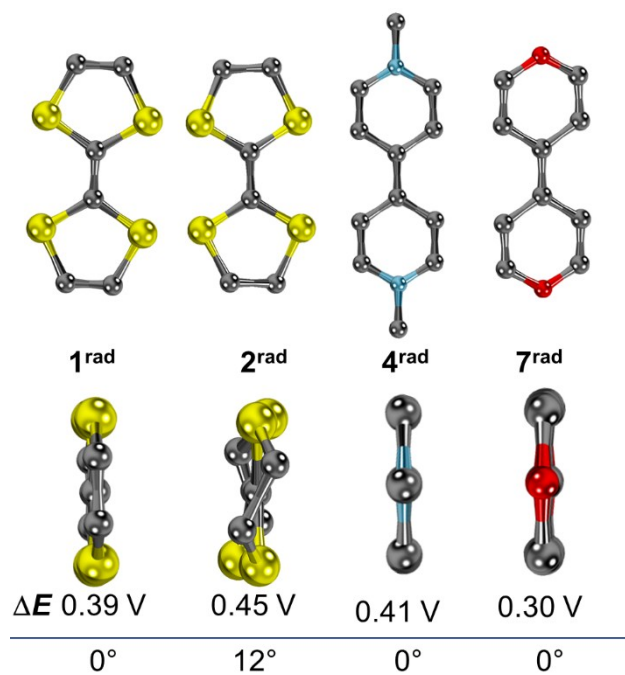


Figure S27. Geometry optimized structures (B3LYP-D3BJ/def2-SVP) of radical cations **1^{rad}**, **2^{rad}**, **4^{rad}**, and **7^{rad}**. Unsubstituted homodimer radicals and their corresponding ΔE from literature.^{3, 7, 15, 18} Homodimeric radicals are stable if the dihedral angle (bottom) is small enough.

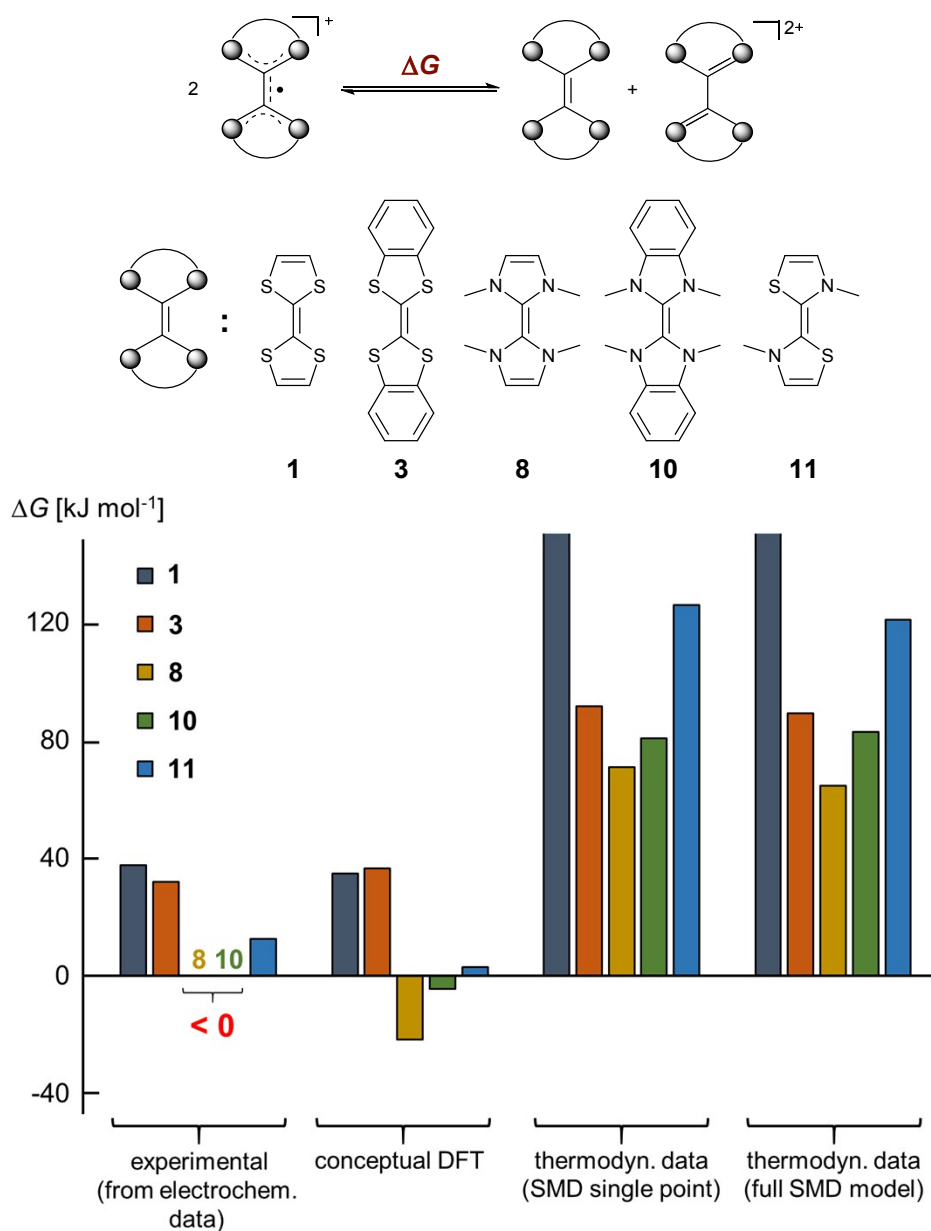


Figure S28. Results obtained from conceptual DFT are much better in agreement with the experiment than directly modelling ΔG of the disproportionation reaction using implicit solvation models (B3LYP-D3BJ(SMD=THF)/def2-TZVPP//B3LYP-D3BJ/def2-SVP or B3LYP-D3BJ(SMD=THF)/def2-TZVPP//B3LYP-D3BJ(SMD=THF)/def2-SVP). The experimental Gibbs free energy was obtained from electrochemical data ($\Delta G = -\Delta E z F$; ΔE [V]; Separation of potentials $E_{1,2}$ and $E_{2,3}$; $z = 1$; Number of electrons; $F = 96485.3399$ C mol⁻¹; Faraday constant).

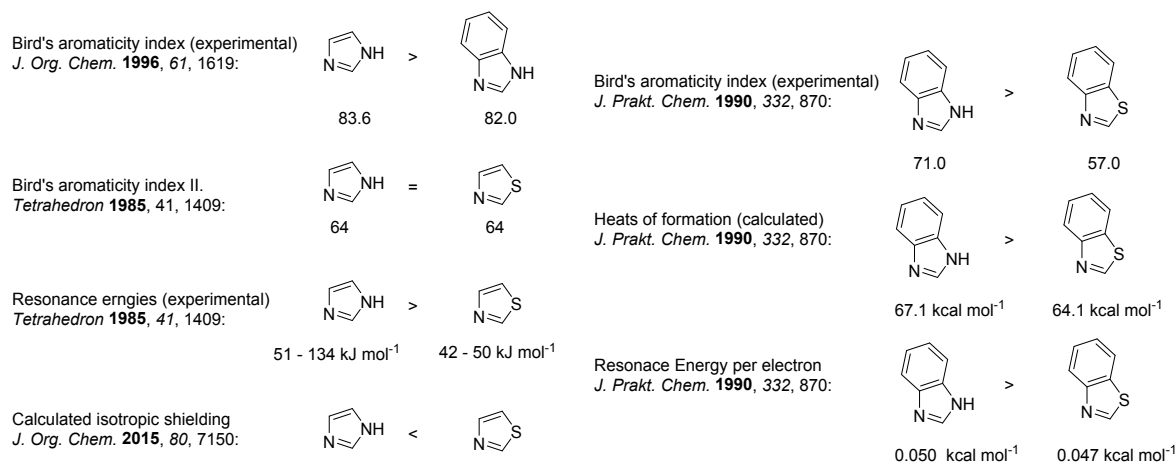


Figure S29. Benzimidazole is less aromatic than imidazole and although ambiguous reports exist in the literature, benzimidazole is likely to be (slightly) more aromatic than benzothiazole.

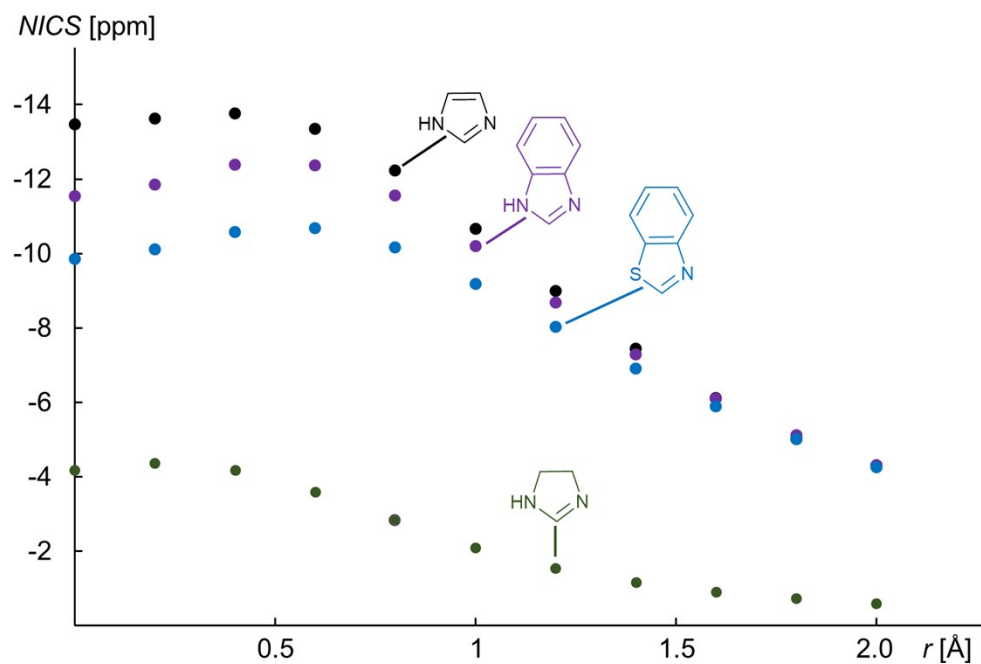


Figure S30. The isotropic NICS scan of imidazole, benzimidazole, benzothiazole, and imidazoline. Imidazole is more aromatic than benzimidazole, followed by benzothiazole. Imidazoline is the least aromatic heterocycle in comparison to the other three heterocycles.

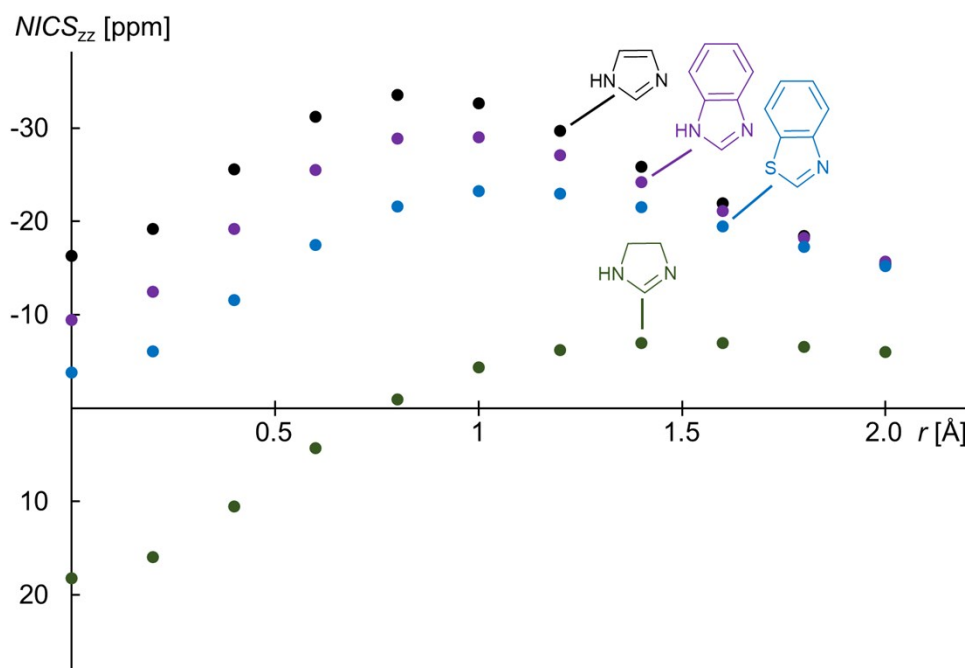


Figure S31. The out-of-plane $NICS$ (i.e., $NICS_{zz}$) scan of imidazole, benzimidazole, benzothiazole, and imidazoline. Imidazole is more aromatic than benzimidazole, followed by benzothiazole. Imidazoline is the least aromatic heterocycle in comparison to the other three heterocycles.

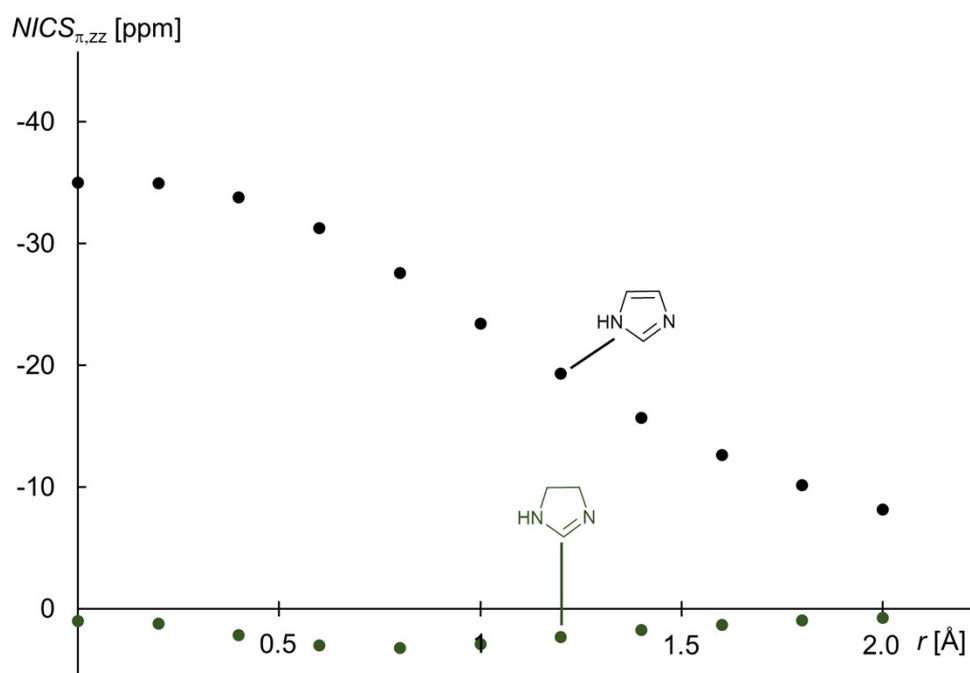


Figure S32. Subtracting the “ σ -only” contributions²³ from $NICS_{zz}$, i.e. $NICS_{\pi,zz}$, indicates non-aromatic character of imidazoline.

Energies

Denominator	Nimag	ΔE (B3LYP- D3BJ/def2- SVP)	ΔG (B3LYP- D3BJ/def2- SVP)	ΔE (B3LYP- D3BJ/def2- TZVPP//B3LYP- D3BJ/def2-SVP)	ΔE [biscation vertical energies] (B3LYP- D3BJ/def2- TZVPP//B3LY P-D3BJ/def2- SVP)
1	0	-1822.789600	-1822.741973	-1823.606757	
1 ^{rad}	0	-1822.565984	-1822.518158	-1823.38244	
1 ^{biscat}	0	-1822.164066	-1822.114563	-1822.985241	-1823.374235
2	0	-1825.232814	-1825.139238	-1826.052047	
2 ^{rad}	0	-1825.000443	-1824.906364	-1825.818269	
2 ^{biscat}	0	-1824.586739	-1824.492087	-1825.408132	-1825.811066
3	0	-2129.730226	-2129.594652	-2130.869751	
3 ^{rad}	0	-2129.508300	-2129.372303	-2130.647117	
3 ^{biscat}	0	-2129.134174	-2128.996848	-2130.276476	-2130.640498
4	0	-574.430192	-574.232851	-575.058077	
4 ^{rad}	0	-574.263817	-574.064043	-574.887853	
4 ^{biscat}	0	-574.043063	-574.096830	-574.559457	-574.877796
5	0	-574.412471	-574.213940	-575.038863	
5 ^{rad}	0	-574.236470	-574.035630	-574.860156	
5 ^{biscat}	0	-573.908529	-573.705587	-574.532212	-574.843101
6	0	-842.008724	-841.674691	-842.932149	
6 ^{rad}	0	-841.862930	-841.527554	-842.908717	
6 ^{biscat}	0	-841.593676	-841.256157	-842.511464	-842.758788
Et-teth 6	0	-840.830766	-840.514582	-841.747673	
Et-teth 6 ^{rad}	0	-840.686911	-840.368975	-841.598708	
Et-teth 6 ^{biscat}	0	-840.402337	-840.080617	-841.314086	-841.589660
Pr-teth 6	0	-880.082982	-879.738952	-881.042691	
Pr-teth 6 ^{rad}	0	-879.942446	-879.596333	-880.896768	
Pr-teth 6 ^{biscat}	0	-879.667654	-879.317786	-880.622109	-880.882202
7	0	-535.588758	-535.466569	-536.185663	
7 ^{rad}	0	-535.372319	-535.247917	-535.965438	
7 ^{biscat}	0	-534.978539	-534.853787	-535.572019	-535.952089
8	0	-608.838430	-608.620822	-609.508833	
8 ^{rad}	0	-608.683224	-608.465752	-609.347164	
8 ^{biscat}	0	-608.382694	-608.163009	-609.046287	-609.324578
Et-teth 8	0	-606.437181	-606.256073	-607.097234	
Et-teth 8 ^{rad}	0	-606.279479	-606.098106	-606.932417	
(isomer 1) Et-teth 8 ^{rad}	0	-606.279910	-606.097385	-606.933046	
(isomer 2) Et-teth 8 ^{biscat}	0	-605.958791	-605.773045	-606.612236	-606.922893
(isomer 1) Et-teth 8 ^{biscat}	0	-605.956945	-605.771248	-606.610479	-606.922856
(isomer 2) Pr-teth 8	0	-684.984026	-684.747727	-685.728554	
(isomer 1) Pr-teth 8 ^{rad}	0	-684.829957	-684.591822	-685.568174	
(isomer 2) Pr-teth 8 ^{rad}	0	-684.829739	-684.591725	-685.567670	

Pr-teth 8 biscat (isomer 1)	0	-684.520476	-684.278109	-685.258471	-685.557100
Pr-teth 8 biscat (isomer 2)	0	-684.519842	-684.277599	-685.257792	-685.558413
9	0	-611.268144	-611.004402	-611.942104	
9 ^{rad}	0	-611.095983	-610.830591	-611.766812	
9 biscat	0	-610.774444	-610.509942	-611.445070	-611.724676
Ph 9	0	-1377.328830	-1376.865068	-1378.808140	
Ph 9 ^{rad}	0	-1377.150497	-1376.685663	-1378.627366	
Ph 9 biscat	0	-1376.846886	-1376.379709	-1378.325102	-1378.609025
10	0	-915.793272	-915.487344	-916.784082	
10 ^{rad}	0	-915.626563	-915.318718	-916.612438	
10 biscat	0	-915.326268	-915.016696	-916.312401	-916.594534
Et-teth 10	0	-913.396100	-913.126340	-914.374964	
Et-teth 10 ^{rad} (isomer 1)	0	-913.226168	-912.954601	-914.201111	
Et-teth 10 ^{rad} (isomer 2)	0	-913.226219	-912.955352	-914.201853	
Et-teth 10 biscat (isomer 1)	0	-912.911708	-912.637841	-913.887654	-914.194915
Et-teth 10 biscat (isomer 2)	0	-912.909990	-912.636093	-913.886278	-914.194707
Pr-teth 10	0	-991.935867	-991.611909	-992.998924	
Pr-teth 10 ^{rad} (isomer 1)	0	-991.767538	-991.440423	-992.827109	
Pr-teth 10 ^{rad} (isomer 2)	0	-991.766666	-991.438802	-992.826285	
Pr-teth 10 biscat (isomer 1)	0	-991.460568	-991.129842	-992.520661	-992.821455
Pr-teth 10 biscat (isomer 2)	0	-991.46055	-991.129651	-992.520627	
11	0	-1215.815013	-1215.684344	-1216.558107	
11 ^{rad}	0	-1215.631185	-1215.498415	-1216.370870	
11 biscat	0	-1215.274832	-1215.140283	-1216.017428	-1216.350061
12	0	-1218.247043	-1218.069708	-1218.994091	
12 ^{rad}	0	-1218.049160	-1217.871070	-1218.792220	
12 biscat	0	-1217.684918	-1217.505533	-1218.430747	-1218.773824
13	0	-1522.762679	-1522.541869	-1522.541760	
13 ^{rad}	0	-1522.570101	-1522.346859	-1523.631923	
13 biscat	0	-1522.232273	-1522.007412	-1523.295969	-1523.616215
14	0	-1292.380667	-1291.792235	-1293.783326	
14 ^{rad}	0	-1292.209116	-1291.617717	-1293.608015	
14 biscat	0	-1291.898464	-1291.306219	-1293.298806	-1293.593083
18	0	-1138.908530	-1138.365291	-1140.151698	
18 ^{rad}	0	-1138.741644	-1138.195562	-1139.979345	
18 biscat	0	-1138.428107	-1137.880082	-1139.667377	-1139.965217
22	0	-1140.121040	-1139.554425	-1141.182343	
22 ^{rad}	0	-1139.941321	-1139.372056	-1139.372088	
22 biscat	0	-1139.625391	-1139.054861	-1140.867853	-1141.159557
25	0	-1595.879798	-1595.334262	-1597.317407	
25 ^{rad}	0	-1595.688924	-1595.141632	-1597.125676	
25 biscat	0	-1595.357802	-1594.808195	-1596.796837	-1597.110000
25 [(E) isomer]	0	-1595.874054	-1595.327809		

Table S3. Electronic (ΔE) and Gibbs free energies (ΔG). All Energies are given in [Hartree].

XYZ Coordinates

1				S	-5.93404	3.04766	-2.10995
C	-6.63415	1.67920	-1.19825	H	-7.44390	1.23990	-1.64375
C	-5.98446	1.31447	-0.08230	C	-4.75934	3.51231	-0.86090
S	-6.15988	3.18275	-1.97583	S	-4.59841	2.34366	0.48101
H	-7.43968	1.10821	-1.66188	H	-6.23155	0.58242	0.62690
C	-4.90238	3.58210	-0.77861	C	-4.06176	4.66439	-0.93674
S	-4.70648	2.36579	0.50949	S	-4.43223	5.91265	-2.16176
H	-6.18944	0.40577	0.48572	C	-3.10681	7.06106	-1.63454
C	-4.15961	4.71029	-0.84440	C	-2.88787	6.87381	-0.13913
S	-4.35507	5.92697	-2.13205	S	-2.72713	5.07301	0.15847
C	-3.09028	6.98756	-1.52874	H	-1.96039	7.35388	0.20722
C	-2.44052	6.62216	-0.41302	H	-2.18673	6.84382	-2.19773
S	-2.90147	5.10846	0.35284	H	-3.73684	7.27270	0.43687
H	-1.64165	7.19781	0.05633	H	-3.44805	8.08022	-1.87585
H	-2.89179	7.90135	-2.09086	H	-7.50218	2.47294	-0.33928
				H	-5.24965	0.42519	-0.86767
1^{rad}				2^{rad}			
C	-6.62751	1.68854	-1.20450	C	-6.82764	1.79467	-1.07746
C	-5.97438	1.32121	-0.08092	C	-5.74635	1.14543	-0.23030
S	-6.15150	3.18765	-1.94400	S	-6.04159	3.15552	-2.03266
H	-7.42770	1.11918	-1.68133	H	-7.26024	1.09086	-1.80343
C	-4.92157	3.56781	-0.77135	C	-4.93538	3.59065	-0.76583
S	-4.72900	2.38736	0.49517	S	-4.78591	2.49465	0.57219
H	-6.16657	0.40976	0.48883	H	-6.17147	0.52430	0.57197
C	-4.14891	4.73080	-0.84357	C	-4.20624	4.79156	-0.81969
S	-4.34159	5.91131	-2.10994	S	-4.61283	6.03106	-1.96612
C	-3.09694	6.97792	-1.53340	C	-3.10383	7.02811	-1.64485
C	-2.44379	6.61060	-0.40983	C	-2.77263	6.89203	-0.16859
S	-2.91917	5.11107	0.32919	S	-2.88768	5.10731	0.26303
H	-1.64382	7.18024	0.06703	H	-1.74801	7.22067	0.05885
H	-2.90442	7.88943	-2.10296	H	-2.29929	6.64625	-2.29155
				H	-3.47964	7.44216	0.47061
1^{bisecat}				H	-3.33457	8.06714	-1.92293
C	-6.49837	1.59509	-1.28748	H	-7.63156	2.23075	-0.46525
C	-6.09173	1.41180	0.00490	H	-5.04795	0.54109	-0.82940
S	-5.87076	2.97376	-2.09460				
H	-7.17040	0.93163	-1.84270	2^{bisecat}			
C	-4.95454	3.55522	-0.77352	C	-6.76930	1.71615	-1.18212
S	-5.04216	2.60777	0.64748	C	-5.80946	1.18318	-0.13346
H	-6.39239	0.58166	0.65351	S	-5.91765	3.08322	-2.09605
C	-4.14498	4.76205	-0.85096	H	-7.04396	0.94700	-1.92031
S	-4.56094	6.09378	-1.83933	C	-4.99813	3.58269	-0.76123
C	-3.20278	7.05696	-1.42453	S	-4.96364	2.63470	0.64540
C	-2.33337	6.52226	-0.51565	H	-6.33238	0.63796	0.66827
S	-2.70145	4.94366	0.04818	C	-4.22348	4.84329	-0.81903
H	-1.42914	7.01255	-0.13800	S	-4.72874	6.10915	-1.82861
H	-3.10385	8.04468	-1.88886	C	-3.18334	7.10326	-1.60361
				C	-2.65302	6.83512	-0.20449
2				S	-2.83090	5.02312	0.13341
C	-6.83798	1.90257	-1.00692	H	-1.58460	7.08727	-0.11233
C	-5.78792	1.13201	-0.21768	H	-2.49649	6.78587	-2.40566

H	-3.21559	7.35282	0.58974	C	5.78940	6.04969	-3.80930
H	-3.45042	8.16184	-1.75089	H	5.54584	5.87942	-5.93814
H	-7.68414	2.15946	-0.75474	H	6.93534	7.14151	4.91760
H	-5.00755	0.54812	-0.54571	H	5.78482	7.14152	-3.80774

3

S	1.50609	2.36207	0.85758
S	-0.84172	3.62411	2.19487
C	1.76830	2.97178	2.49918
C	0.66002	3.56959	3.12939
C	0.77165	4.05673	4.43422
C	1.99260	3.94557	5.10656
C	3.09373	3.35262	4.48110
C	2.98600	2.86256	3.17577
C	-0.08141	3.13509	0.66669
H	-0.08761	4.52628	4.91871
H	2.08363	4.33631	6.12265
H	4.04670	3.27601	5.00922
H	3.84634	2.40466	2.68275
C	-0.66831	3.31320	-0.53812
S	-2.26047	4.07393	-0.73960
S	0.08422	2.79126	-2.05886
C	-2.03064	4.43207	-2.45963
C	-0.91813	3.83163	-3.07993
C	-2.89824	5.23510	-3.20525
C	-0.66664	4.04326	-4.43746
C	-2.64544	5.44198	-4.56501
H	-3.76098	5.70206	-2.72487
C	-1.53338	4.85360	-5.17682
H	0.20300	3.58184	-4.91112
H	-3.32116	6.07197	-5.14749
H	-1.32816	5.03470	-6.23454

3^{rad}

C	6.45151	4.63292	1.24738
S	6.57883	3.15783	2.15898
C	6.78493	3.92821	3.72244
C	6.93075	3.21634	4.91910
C	7.06663	3.93038	6.10736
C	6.26400	4.63292	-0.13703
S	6.13683	3.15784	-1.04868
C	5.93307	3.92822	-2.61243
C	5.78932	3.21632	-3.80936
C	5.65546	3.93038	-4.99783
H	6.93551	2.12451	4.91771
H	7.17810	3.38671	7.04752
H	5.78469	2.12450	-3.80786
H	5.54578	3.38671	-5.93820
S	6.57875	6.10805	2.15893
C	6.78489	5.33774	3.72241
C	7.06658	5.33570	6.10734
S	6.13697	6.10803	-1.04863
C	5.93312	5.33774	-2.61240
C	5.65550	5.33570	-4.99780
C	6.93065	6.04968	4.91904
H	7.17801	5.87942	7.04747

3^{biscat}

C	-5.80267	1.27941	-1.23457
C	-6.61428	1.72209	-0.15040
S	-4.62611	2.42930	-1.79360
C	-4.99407	3.65357	-0.66164
S	-6.24772	3.31357	0.44801
C	-4.26539	4.90364	-0.63288
S	-4.96884	6.34173	-0.03634
C	-3.57011	7.35044	-0.25498
C	-2.44241	6.70459	-0.84026
S	-2.64921	5.01162	-1.17685
C	-7.61707	0.89622	0.37923
H	-8.23989	1.22690	1.21272
C	-5.98711	0.00908	-1.80063
C	-7.79171	-0.35952	-0.19134
H	-5.36682	-0.33554	-2.63100
H	-8.56471	-1.02293	0.20279
C	-6.98736	-0.79693	-1.26916
H	-7.15495	-1.78928	-1.69434
C	-1.25524	7.41192	-1.08417
H	-0.38866	6.92272	-1.53369
C	-1.21743	8.75715	-0.73435
C	-3.51960	8.70919	0.09088
H	-0.30563	9.33122	-0.91449
H	-4.37900	9.21145	0.54033
C	-2.33516	9.39627	-0.15091
H	-2.26760	10.45250	0.11983

4

N	-4.06998	6.25679	-5.23731
C	-5.21860	5.95117	-4.51517
C	-2.96464	6.69306	-4.51350
H	-6.08111	5.65540	-5.11588
H	-2.09715	6.97906	-5.11201
C	-5.26265	5.99314	-3.16176
C	-2.95511	6.75041	-3.15981
H	-6.20127	5.70820	-2.68694
H	-2.03546	7.08937	-2.68298
C	-4.11327	6.38281	-2.35001
C	-4.12201	6.40470	-0.96332
C	-5.28042	6.03764	-0.15360
C	-2.97288	6.79495	-0.15149
H	-6.19927	5.69641	-0.63037
H	-2.03344	7.07761	-0.62606
C	-5.27207	6.09822	1.19994
C	-3.01813	6.84014	1.20178
H	-6.13977	5.81283	1.79842
H	-2.15591	7.13654	1.80259
N	-4.16768	6.53713	1.92361
C	-4.13179	6.43617	-6.66890
H	-3.13049	6.30066	-7.10555

H	-4.79756	5.68296	-7.11667
H	-4.50556	7.43865	-6.96207
C	-4.10718	6.36187	3.35577
H	-5.10946	6.49564	3.79063
H	-3.73098	5.36126	3.65215
H	-3.44420	7.11819	3.80248

4^{rad}

C	7.87283	-0.96625	2.57725
H	7.27525	-1.75433	2.11748
C	9.23832	-0.94591	2.49834
H	9.71568	-1.75343	1.94606
C	10.00956	0.08671	3.12639
C	5.72553	-0.11604	3.41569
N	7.17471	0.00516	3.24720
C	7.86811	1.03417	3.82847
H	7.26742	1.79362	4.33022
C	9.23455	1.09945	3.78081
H	9.70841	1.95170	4.26522
H	5.30269	0.86322	3.67358
H	5.48977	-0.83007	4.22038
H	5.26825	-0.46829	2.48092
C	13.57848	-0.96620	2.57683
H	14.17601	-1.75429	2.11700
C	12.21299	-0.94588	2.49811
H	11.73560	-1.75340	1.94587
C	11.44180	0.08670	3.12631
C	15.72591	-0.11593	3.41493
H	15.96188	-0.82988	4.21963
H	16.14876	0.86337	3.67266
H	16.18301	-0.46823	2.48009
N	14.27670	0.00522	3.24669
C	13.58334	1.03417	3.82814
H	14.18408	1.79364	4.32981
C	12.21689	1.09942	3.78069
H	11.74308	1.95159	4.26526

4^{biscat}

N	-0.03870	-0.02512	-5.68325
C	-1.14846	0.34239	-5.00612
C	1.08222	-0.38868	-5.01669
H	-2.01668	0.63082	-5.60086
H	1.94063	-0.68150	-5.62456
C	-1.16776	0.35286	-3.61839
C	1.12085	-0.38850	-3.63211
H	-2.08178	0.67644	-3.11845
H	2.04073	-0.70887	-3.14092
C	-0.01957	-0.01443	-2.89781
C	-0.00891	-0.00745	-1.41124
C	-1.13993	-0.40248	-0.67349
C	1.12991	0.39442	-0.69412
H	-2.05160	-0.74978	-1.16170
H	2.03586	0.73553	-1.19710
C	-1.10156	-0.38898	0.71110
C	1.11057	0.39637	0.69357
H	-1.95266	-0.69725	1.32157

H	1.97129	0.71151	1.28567
N	0.00992	0.00812	1.37419
C	-0.02725	-0.02959	-7.16776
H	0.70820	0.70580	-7.52222
H	0.24396	-1.03360	-7.52081
H	-1.02371	0.23539	-7.53701
C	-0.00118	0.01864	2.85871
H	0.99018	0.30636	3.22476
H	-0.75051	0.74340	3.20593
H	-0.25297	-0.98663	3.22228

5

C	5.51509	1.77375	14.68949
C	5.22310	2.94105	15.49411
N	5.95233	0.62180	5.42345
C	5.05820	2.85607	6.84220
C	5.68218	0.53309	6.78347
C	5.21030	1.57850	7.50297
H	5.07338	3.89853	4.99538
H	4.79753	3.74294	17.42357
H	5.90353	-0.43844	17.23539
H	4.96730	1.45067	18.55856
C	5.37581	1.74251	13.30326
N	5.31474	0.51260	12.57398
C	5.32323	2.94278	12.49412
C	5.50681	0.50860	11.20167
C	5.44514	2.91010	11.13997
C	5.60243	1.64181	10.46611
H	5.23237	3.90281	13.00040
H	5.54991	-0.48652	10.74999
H	5.43474	3.83706	10.56285
H	5.78442	1.58245	9.39268
C	4.51772	-0.58235	13.11217
H	3.43726	-0.35681	13.04074
H	4.72521	-1.49513	12.53447
H	4.75972	-0.76124	14.16767
C	7.14508	-0.06648	14.94583
H	7.33056	-0.94860	15.57561
H	7.02659	-0.39449	13.90274
H	8.02934	0.59500	15.00086

5^{rad}

C	5.45108	1.70150	14.76775
C	5.98512	0.59283	15.46689
N	5.04166	2.80523	15.52138
C	6.17794	0.62123	16.83231
C	5.26102	2.84123	16.87541
C	5.81929	1.79112	17.55282
H	6.32715	-0.26503	14.88890
H	6.63645	-0.22684	17.34389
H	4.94115	3.75418	17.37943
H	5.97952	1.87091	18.62831
C	5.43469	1.76349	13.32348
N	4.98265	0.66736	12.58273
C	5.97716	2.85833	12.60928
C	5.17200	0.62239	11.22443

C	6.13868	2.82190	11.23993
C	5.73907	1.65770	10.53166
H	6.35012	3.71051	13.17639
H	4.82037	-0.28423	10.73023
H	6.60296	3.65885	10.71544
H	5.87372	1.57103	9.45318
C	4.19273	-0.40152	13.20307
H	3.60614	0.01593	14.03194
H	3.50684	-0.81739	12.45440
H	4.82576	-1.21287	13.59135
C	4.27167	3.89944	14.92069
H	3.61021	4.32948	15.68327
H	4.92126	4.69518	14.52719
H	3.66002	3.50425	14.09923

5^{biscat}

C	5.65521	1.69775	14.79352
C	6.47568	0.80132	15.46832
N	4.89735	2.59263	15.50164
C	6.52486	0.80797	16.86975
C	4.93777	2.60885	16.85482
C	5.74289	1.72761	17.56739
H	7.08822	0.10387	14.89324
H	7.17165	0.10609	17.40272
H	4.30793	3.34915	17.35210
H	5.74909	1.77703	18.65863
C	5.64162	1.75094	13.29704
N	4.84104	0.88352	12.60191
C	6.47563	2.62395	12.60836
C	4.85042	0.87461	11.24802
C	6.49308	2.62440	11.20621
C	5.66576	1.73517	10.52176
H	7.12206	3.29908	13.17293
H	4.18707	0.15728	10.76088
H	7.14983	3.30868	10.66263
H	5.64388	1.69393	9.43036
C	3.96252	-0.07394	13.32052
H	3.32184	0.46786	14.02811
H	3.33162	-0.59393	12.59097
H	4.57624	-0.80798	13.85903
C	4.03481	3.57476	14.79759
H	3.41945	4.10153	15.53559
H	4.66056	4.30070	14.26151
H	3.37835	3.05333	14.08941

6

N	-0.03241	11.56805	4.21084
N	-0.98328	11.24916	1.48064
N	1.18193	8.13276	6.34810
N	-2.87393	7.63271	0.37874
C	-1.04831	12.61291	4.17020
C	0.22628	12.02652	1.23580
C	0.89252	11.63336	5.23643
H	1.21919	12.64408	5.50308
C	1.36737	10.54187	5.88136
H	2.16210	10.65368	6.61738

C	0.79249	9.23578	5.57851
C	-0.07583	9.15014	4.52222
H	-0.55706	8.20533	4.28782
C	-0.35807	10.28428	3.65937
C	-0.90165	10.14642	2.39381
C	-1.41902	8.88529	1.89154
H	-1.12724	7.97886	2.41356
C	-2.27253	8.82098	0.82167
C	-2.59653	10.06761	0.13621
H	-3.37367	10.10676	-0.62619
C	-1.91186	11.19065	0.45587
H	-2.05697	12.12656	-0.09327
C	1.23796	8.26738	7.79202
H	1.58502	9.26660	8.08277
H	1.93942	7.53019	8.21428
H	0.24702	8.10113	8.26834
C	0.76061	6.82103	5.91663
H	-0.32538	6.63469	6.07071
H	1.31366	6.05907	6.48709
H	0.98144	6.68232	4.84769
C	-2.67102	6.44938	1.18107
H	-1.62382	6.07482	1.15260
H	-3.32292	5.64292	0.81289
H	-2.92980	6.65234	2.23143
C	-2.87239	7.36002	-1.04854
H	-3.12130	8.26057	-1.62367
H	-3.62420	6.59008	-1.28306
H	-1.88665	6.99152	-1.40884
H	-1.40860	12.77056	3.14472
H	-0.61782	13.55165	4.55111
H	-1.91906	12.34518	4.79671
H	-0.01517	12.87531	0.57855
H	1.00181	11.41102	0.74359
H	0.64537	12.40914	2.17636

6^{rad}

N	-0.52121	10.97022	3.92166
N	-0.54260	8.30989	1.43090
N	1.19692	8.18445	6.54691
N	-4.34282	9.85192	0.53738
C	-0.77907	12.03450	2.94984
C	0.84743	7.87920	1.57414
C	-0.10220	11.32675	5.17340
H	-0.21914	12.38226	5.42494
C	0.45242	10.45550	6.05972
H	0.75776	10.83334	7.03187
C	0.62379	9.07149	5.68807
C	0.13243	8.69876	4.42740
H	0.11583	7.65137	4.14264
C	-0.46354	9.61717	3.53432
C	-1.13225	9.22544	2.31857
C	-2.42295	9.71220	2.00811
H	-2.90401	10.33089	2.75953
C	-3.10579	9.37170	0.83191
C	-2.44201	8.43867	-0.04460
H	-2.89757	8.08775	-0.96686

C	-1.22009	7.94479	0.30200
H	-0.70518	7.22928	-0.34065
C	1.68773	8.61986	7.84936
H	2.45199	9.40921	7.75352
H	2.15119	7.76904	8.36194
H	0.87469	9.00055	8.49050
C	1.33393	6.79214	6.15521
H	0.35091	6.30970	6.01056
H	1.87100	6.24068	6.93497
H	1.90487	6.69321	5.21505
C	-5.03550	10.68880	1.50134
H	-5.24645	10.13866	2.43549
H	-5.98851	11.02705	1.07825
H	-4.44489	11.58516	1.75932
C	-4.98715	9.52446	-0.72836
H	-4.34400	9.78814	-1.58366
H	-5.91435	10.10217	-0.81775
H	-5.24474	8.45367	-0.80355
H	-0.36618	11.74344	1.97432
H	-0.27898	12.95143	3.28597
H	-1.85131	12.24227	2.81752
H	1.21463	7.52963	0.60114
H	0.96193	7.06276	2.30205
H	1.46391	8.72545	1.90794

6biscat

N	-1.01289	11.10144	4.49750
N	-0.15731	10.57721	1.41185
N	1.62126	8.43280	6.33355
N	-3.21533	7.97375	0.26833
C	-1.95048	12.05398	3.87630
C	0.99316	11.42031	1.78447
C	-0.64720	11.26207	5.80373
H	-1.09172	12.11305	6.32228
C	0.21882	10.41657	6.44330
H	0.46031	10.62931	7.48299
C	0.78485	9.29602	5.75294
C	0.38987	9.16311	4.37814
H	0.77268	8.35293	3.76205
C	-0.47820	10.05174	3.79234
C	-0.86565	9.87874	2.35852
C	-1.87911	9.01893	2.00855
H	-2.39692	8.49667	2.81035
C	-2.24872	8.81969	0.63350
C	-1.50579	9.59502	-0.31425
H	-1.71197	9.54024	-1.38099
C	-0.49932	10.42533	0.09874
H	0.08390	11.00516	-0.61826
C	1.99418	8.58813	7.74593
H	2.57957	9.50824	7.90456
H	2.60778	7.73367	8.04933
H	1.09929	8.61168	8.38589
C	2.22024	7.34072	5.56046
H	1.44580	6.68972	5.12545
H	2.84103	6.72885	6.22328
H	2.86057	7.73379	4.75408

C	-3.95500	7.19966	1.26994
H	-3.27693	6.56507	1.86218
H	-4.67038	6.54682	0.75919
H	-4.51822	7.86128	1.94785
C	-3.56424	7.81341	-1.14967
H	-3.89381	8.76944	-1.58549
H	-4.38673	7.09662	-1.23803
H	-2.70777	7.42760	-1.72451
H	-2.71731	11.51248	3.30943
H	-1.41663	12.74166	3.20408
H	-2.43858	12.63994	4.66342
H	1.41156	11.87417	0.87877
H	1.76625	10.81030	2.27068
H	0.68276	12.22333	2.46538

Et-teth6

N	0.28794	11.40607	4.04185
N	-1.08068	11.17059	1.59116
N	1.20738	8.05449	6.43221
N	-2.84005	7.55662	0.31937
C	-0.19988	12.58217	3.36073
H	0.46826	13.42937	3.57776
H	-1.21662	12.85306	3.70671
C	-0.24630	12.31617	1.85176
H	-0.65110	13.19096	1.32115
H	0.78633	12.14198	1.49008
C	1.13179	11.50037	5.11635
H	1.52679	12.50164	5.31141
C	1.47186	10.44087	5.89162
H	2.20158	10.57132	6.68820
C	0.87877	9.13634	5.60381
C	0.06334	9.02654	4.50917
H	-0.42815	8.08390	4.28697
C	-0.20229	10.13288	3.60934
C	-0.88756	10.01982	2.41785
C	-1.42884	8.78135	1.89166
H	-1.13974	7.86504	2.39810
C	-2.25527	8.73893	0.80026
C	-2.57522	9.99813	0.12925
H	-3.31074	10.04409	-0.67170
C	-1.95942	11.13435	0.54080
H	-2.13881	12.09533	0.04973
C	1.15422	8.23969	7.87059
H	1.80843	7.50883	8.37222
H	0.12652	8.10359	8.27346
H	1.49320	9.24441	8.15206
C	0.79350	6.73437	6.01892
H	-0.30201	6.56486	6.11746
H	1.30290	5.98422	6.64323
H	1.07227	6.55895	4.96924
C	-2.65183	6.36005	1.10520
H	-1.60105	5.99410	1.10064
H	-3.28640	5.55592	0.70338
H	-2.94212	6.54159	2.15114
C	-2.79353	7.30935	-1.11150
H	-3.02073	8.22118	-1.67772

H	-3.53938	6.54610	-1.38374
H	-1.79738	6.94401	-1.44590

Et-teth6rad

N	0.20838	11.37211	4.07429
N	-0.90585	11.08444	1.52094
N	0.97375	8.10036	6.55334
N	-2.68692	7.52752	0.25549
C	-0.20052	12.54991	3.31574
H	0.45679	13.38871	3.58206
H	-1.23724	12.82838	3.57634
C	-0.09980	12.25544	1.83208
H	-0.46840	13.10952	1.24930
H	0.95220	12.06901	1.55043
C	0.75988	11.53537	5.31039
H	0.99404	12.56507	5.58842
C	1.01559	10.49991	6.15443
H	1.48577	10.71157	7.11108
C	0.72038	9.15095	5.72900
C	0.18821	8.99112	4.44296
H	-0.02682	7.99579	4.06901
C	-0.12040	10.09147	3.60239
C	-0.78671	9.95758	2.34647
C	-1.36771	8.74918	1.88344
H	-1.25939	7.86732	2.50489
C	-2.11719	8.68039	0.70010
C	-2.27276	9.90605	-0.05041
H	-2.85414	9.95184	-0.96685
C	-1.65007	11.03662	0.38139
H	-1.71164	11.97075	-0.17996
C	1.31796	8.31284	7.95416
H	1.16469	7.37669	8.50530
H	0.66566	9.07161	8.41111
H	2.36854	8.62711	8.09043
C	0.88130	6.74153	6.04505
H	-0.15826	6.46000	5.79638
H	1.25400	6.04196	6.80239
H	1.49635	6.61721	5.13840
C	-2.40975	6.27345	0.93576
H	-1.33630	6.01406	0.88785
H	-2.97994	5.46715	0.46109
H	-2.71174	6.31546	1.99590
C	-3.41347	7.49503	-1.00772
H	-4.22671	8.23691	-1.02501
H	-3.87184	6.50685	-1.13229
H	-2.74996	7.67936	-1.87126

Et-teth6biscat

N	-0.11000	11.34479	4.20920
N	-0.72134	10.99261	1.48709
N	1.18515	8.09639	6.45688
N	-2.73427	7.57669	0.24768
C	-0.52968	12.49701	3.39408
H	-0.03482	13.39635	3.78165
H	-1.62016	12.63438	3.48422
C	-0.12401	12.25764	1.95195

H	-0.50121	13.07086	1.31833
H	0.97277	12.21435	1.84567
C	0.40287	11.52565	5.45965
H	0.46894	12.55886	5.80608
C	0.81767	10.48277	6.23924
H	1.22288	10.70978	7.22281
C	0.74339	9.13827	5.74712
C	0.17711	8.98643	4.43623
H	0.10881	8.00177	3.98279
C	-0.25194	10.07450	3.70661
C	-0.85526	9.93518	2.35569
C	-1.51669	8.79248	1.96058
H	-1.65253	7.99903	2.69025
C	-2.03426	8.64818	0.62835
C	-1.76007	9.73572	-0.26451
H	-2.07106	9.71286	-1.30654
C	-1.14423	10.86426	0.19716
H	-0.96804	11.72453	-0.45121
C	1.75195	8.30084	7.79825
H	2.08951	7.33790	8.19506
H	0.99702	8.71491	8.48531
H	2.61955	8.97754	7.76209
C	1.09713	6.73356	5.92500
H	0.05117	6.45643	5.71649
H	1.49178	6.03205	6.66704
H	1.69328	6.62760	5.00492
C	-3.11507	6.54727	1.21911
H	-2.23191	6.02799	1.62492
H	-3.74553	5.80351	0.72115
H	-3.69217	6.98935	2.04704
C	-3.20488	7.44852	-1.13872
H	-3.91966	8.24808	-1.39097
H	-3.71215	6.48532	-1.25628
H	-2.36007	7.48142	-1.84316

Pr-teth6

N	-0.05535	11.51801	4.25292
N	-1.06265	11.22115	1.50932
N	1.23421	8.07942	6.31531
N	-2.83487	7.57326	0.36024
C	-0.87719	12.67256	3.92602
H	-0.84388	13.38510	4.76463
H	-1.92017	12.32314	3.84169
C	-0.44707	13.35323	2.62124
H	0.42889	14.00265	2.79238
H	-1.26471	13.99988	2.25945
C	-0.08951	12.30187	1.57060
H	0.00363	12.76016	0.57382
H	0.88963	11.85445	1.81102
C	0.87036	11.59480	5.26391
H	1.18557	12.60689	5.53642
C	1.36736	10.50366	5.89935
H	2.15109	10.62396	6.64494
C	0.81954	9.19180	5.57017
C	-0.05153	9.10494	4.51619
H	-0.50969	8.15264	4.26743

C	-0.36793	10.24338	3.66914
C	-0.93741	10.11678	2.41540
C	-1.43581	8.85425	1.89621
H	-1.15400	7.95321	2.43166
C	-2.25530	8.77333	0.80129
C	-2.57128	10.00617	0.08866
H	-3.29721	10.02521	-0.72233
C	-1.93735	11.14840	0.45299
H	-2.08975	12.08417	-0.09236
C	1.29906	8.18653	7.76108
H	2.00752	7.44471	8.16315
H	0.31261	8.00515	8.24152
H	1.64312	9.18135	8.06950
C	0.82400	6.77066	5.86444
H	-0.25996	6.57216	6.01886
H	1.38549	6.00484	6.42124
H	1.04209	6.64997	4.79271
C	-2.66054	6.40666	1.19295
H	-1.61412	6.02906	1.20734
H	-3.30194	5.59376	0.82024
H	-2.95301	6.63265	2.22960
C	-2.78689	7.27253	-1.06022
H	-3.01016	8.16330	-1.66053
H	-3.53513	6.50232	-1.30552
H	-1.79188	6.89110	-1.37965

Pr-teth6rad

N	-0.42956	11.40789	4.36548
N	-0.63414	11.01938	1.41164
N	1.22743	8.14420	6.40058
N	-2.82218	7.62676	0.28977
C	-1.16985	12.51760	3.76015
H	-1.40944	13.24348	4.54768
H	-2.12466	12.11318	3.38840
C	-0.39840	13.18274	2.62158
H	0.38244	13.84936	3.02164
H	-1.09525	13.80726	2.03917
C	0.26290	12.13437	1.72695
H	0.60457	12.58285	0.78485
H	1.15092	11.71221	2.22386
C	0.09460	11.54260	5.61718
H	0.03640	12.54494	6.04509
C	0.63847	10.50794	6.31598
H	1.03349	10.70604	7.30870
C	0.66896	9.18801	5.72936
C	0.13889	9.06113	4.43601
H	0.21158	8.11753	3.90225
C	-0.38203	10.16206	3.71627
C	-0.87287	10.01924	2.37249
C	-1.57758	8.86270	1.96424
H	-1.79991	8.13176	2.73668
C	-2.07100	8.69832	0.66122
C	-1.78789	9.76043	-0.27590
H	-2.12368	9.72045	-1.30849
C	-1.09916	10.85945	0.13926
H	-0.87138	11.67518	-0.54909

C	1.83160	8.34479	7.71257
H	2.64009	9.09407	7.68132
H	2.26902	7.39997	8.05559
H	1.08836	8.66691	8.46161
C	1.23897	6.82203	5.79809
H	0.21784	6.48689	5.54612
H	1.66844	6.10224	6.50418
H	1.84351	6.79751	4.87405
C	-3.22445	6.65054	1.28879
H	-2.35344	6.15169	1.74756
H	-3.84372	5.88019	0.81541
H	-3.81394	7.12240	2.09570
C	-3.34151	7.51228	-1.06731
H	-4.04289	8.32804	-1.31537
H	-3.88220	6.56354	-1.16472
H	-2.52949	7.51310	-1.81213

Pr-teth6biscat

N	-0.67749	11.24116	4.39490
N	-0.39710	10.79684	1.42125
N	1.44775	8.26419	6.38874
N	-3.04691	7.78873	0.28052
C	-1.33669	12.33459	3.64963
H	-1.69955	13.07280	4.37521
H	-2.22227	11.91245	3.15255
C	-0.38572	12.97786	2.63364
H	0.31850	13.65812	3.13836
H	-0.98868	13.59444	1.94789
C	0.43451	11.94110	1.85447
H	0.89160	12.38971	0.96359
H	1.25596	11.54103	2.46628
C	-0.28688	11.41257	5.68920
H	-0.55933	12.36514	6.14729
C	0.39622	10.45322	6.38614
H	0.66611	10.66950	7.41776
C	0.74062	9.20866	5.76258
C	0.28261	9.04828	4.40843
H	0.49461	8.13933	3.85047
C	-0.39798	10.05338	3.76274
C	-0.85498	9.89279	2.35038
C	-1.71268	8.87878	1.99326
H	-2.05693	8.20852	2.77730
C	-2.16567	8.72791	0.63644
C	-1.61981	9.66450	-0.30053
H	-1.87177	9.62349	-1.35802
C	-0.77630	10.65747	0.11954
H	-0.36581	11.38883	-0.57904
C	1.92290	8.47575	7.76293
H	2.52570	9.39410	7.83391
H	2.55546	7.63141	8.05526
H	1.07944	8.53916	8.46899
C	1.75893	6.99327	5.72422
H	0.83938	6.47112	5.41730
H	2.29898	6.34589	6.42268
H	2.39782	7.15220	4.84080
C	-3.62965	6.89306	1.28413

H	-2.85430	6.28720	1.77912
H	-4.32804	6.21001	0.78961
H	-4.18670	7.46465	2.04430
C	-3.49266	7.67254	-1.11472
H	-3.99896	8.59346	-1.44597
H	-4.20246	6.84305	-1.19565
H	-2.64392	7.46296	-1.78347

7

O	-4.11850	6.39611	-5.22825
C	-5.22939	6.05786	-4.50876
C	-3.00761	6.73436	-4.50876
H	-6.06454	5.79811	-5.15962
H	-2.17246	6.99411	-5.15962
C	-5.27622	6.04403	-3.16279
C	-2.96078	6.74818	-3.16279
H	-6.21911	5.74946	-2.70210
H	-2.01789	7.04275	-2.70210
C	-4.11850	6.39610	-2.34660
C	-4.11850	6.39610	-0.96669
C	-5.27622	6.04403	-0.15051
C	-2.96078	6.74818	-0.15051
H	-6.21911	5.74945	-0.61119
H	-2.01789	7.04275	-0.61119
C	-5.22939	6.05786	1.19547
C	-3.00761	6.73436	1.19547
H	-6.06454	5.79810	1.84633
H	-2.17247	6.99412	1.84633
O	-4.11850	6.39611	1.91496

7^{rad}

O	-4.11850	6.39611	-5.18669
C	-5.22718	6.05821	-4.50750
C	-3.00983	6.73401	-4.50750
H	-6.05650	5.80082	-5.16691
H	-2.18050	6.99139	-5.16691
C	-5.27294	6.04471	-3.14680
C	-2.96407	6.74750	-3.14681
H	-6.21352	5.75130	-2.68336
H	-2.02349	7.04092	-2.68336
C	-4.11850	6.39611	-2.37231
C	-4.11850	6.39611	-0.94098
C	-5.27293	6.04471	-0.16648
C	-2.96407	6.74750	-0.16648
H	-6.21351	5.75130	-0.62993
H	-2.02349	7.04092	-0.62993
C	-5.22718	6.05820	1.19421
C	-3.00983	6.73401	1.19421
H	-6.05650	5.80082	1.85362
H	-2.18051	6.99140	1.85362
O	-4.11850	6.39611	1.87340

7^{biscat}

O	-4.11850	6.39612	-5.14428
C	-5.27839	6.43520	-4.50846
C	-2.95862	6.35701	-4.50847

H	-6.14000	6.47070	-5.18132
H	-2.09701	6.32153	-5.18134
C	-5.32744	6.43232	-3.12692
C	-2.90956	6.35988	-3.12693
H	-6.30421	6.48614	-2.64186
H	-1.93279	6.30606	-2.64187
C	-4.11850	6.39610	-2.40212
C	-4.11850	6.39610	-0.91042
C	-5.09923	5.68572	-0.18669
C	-3.13777	7.10648	-0.18669
H	-5.87782	5.09405	-0.67228
H	-2.35918	7.69815	-0.67227
C	-5.05778	5.71248	1.19487
C	-3.17923	7.07974	1.19487
H	-5.75094	5.20322	1.87063
H	-2.48608	7.58901	1.87063
O	-4.11851	6.39611	1.82800

8

C	-6.23739	1.85265	-1.08435
C	-5.74086	1.59644	0.13903
N	-5.71308	3.06979	-1.57479
H	-6.91914	1.26012	-1.69038
C	-4.82664	3.54482	-0.56300
N	-4.82648	2.60891	0.51498
H	-5.97267	0.77948	0.81895
C	-4.12355	4.70843	-0.61443
N	-4.41453	5.81204	-1.47342
C	-3.42213	6.78047	-1.19112
C	-2.57391	6.31691	-0.25680
N	-2.96893	5.02553	0.16568
H	-1.67798	6.77961	0.15102
H	-3.43744	7.74862	-1.68710
C	-5.79966	6.25585	-1.54586
H	-5.87855	7.10513	-2.24080
H	-6.43777	5.44054	-1.91528
H	-6.18757	6.56722	-0.55413
C	-1.93677	4.00569	0.28047
H	-2.33898	3.10927	0.77406
H	-1.54728	3.69823	-0.71200
H	-1.10434	4.39516	0.88544
C	-4.89669	3.13061	1.87008
H	-4.92115	2.29151	2.58160
H	-4.01605	3.75117	2.08782
H	-5.79469	3.76226	2.02658
C	-5.26783	3.12872	-2.95779
H	-4.37341	2.49750	-3.13342
H	-6.07854	2.78638	-3.61878
H	-5.00574	4.16265	-3.22520

8^{rad}

C	-6.23650	1.88661	-1.25664
C	-5.95134	1.67066	0.05296
N	-5.56443	3.03502	-1.66663
H	-6.85418	1.31340	-1.94257
C	-4.84840	3.53118	-0.58320

N	-5.10363	2.68241	0.48516	H	-5.33054	2.68430	-3.75767
H	-6.30283	0.89546	0.72839				
C	-4.12196	4.74285	-0.57293	Et-tethg			
N	-4.50849	5.91573	-1.20796	C	8.29249	4.84507	3.13147
C	-3.48684	6.84919	-1.06644	C	8.40436	4.91119	4.47862
C	-2.47799	6.27165	-0.36479	N	9.61616	5.53694	4.82860
N	-2.85088	4.96869	-0.06332	N	9.45195	5.39525	2.51438
H	-1.50946	6.66850	-0.07317	C	10.16335	4.62820	1.48344
H	-3.57127	7.85299	-1.47408	C	10.45454	5.26809	5.99706
C	-5.89286	6.28848	-1.47306	C	10.31129	5.68674	3.60794
H	-6.45364	5.43312	-1.86765	C	11.50146	5.31163	1.12302
H	-6.38693	6.63941	-0.55140	N	12.34241	5.54611	2.29665
H	-5.91237	7.09448	-2.21829	C	13.54761	4.90182	2.63450
C	-1.94309	3.95076	0.43483	C	13.65888	4.80948	3.98019
H	-1.91376	3.93045	1.53492	N	12.50483	5.35952	4.60787
H	-2.26318	2.96746	0.06155	C	11.78452	4.57756	5.62120
H	-0.93032	4.15077	0.05746	C	11.64892	5.68116	3.51990
C	-4.76312	2.94602	1.87112	H	12.41246	4.47460	6.51940
H	-5.53840	2.52159	2.52249	H	11.55707	3.56341	5.22823
H	-3.79524	2.50253	2.14889	H	9.90021	4.62753	6.69980
H	-4.72274	4.03324	2.03720	H	10.68139	6.21806	6.51091
C	-5.19918	3.26999	-3.05915	H	12.04869	4.68046	0.40634
H	-4.92505	4.32050	-3.21412	H	11.28481	6.27488	0.62984
H	-4.34288	2.63788	-3.34840	H	9.53453	4.55437	0.58293
H	-6.05528	3.02782	-3.70283	H	10.37827	3.60252	1.85274
				H	7.43670	4.53635	2.53353
g biscat				H	7.65839	4.67497	5.23600
C	-5.81231	1.60839	-1.26286	H	14.29115	4.67185	1.87280
C	-6.07978	1.78448	0.07280	H	14.51172	4.48153	4.57209
N	-5.05011	2.67579	-1.67109				
H	-6.10934	0.81245	-1.94393	Et-tethgrad (isomer 1)			
C	-4.84919	3.49902	-0.61377	C	8.17460	4.88796	3.12289
N	-5.47238	2.95461	0.45928	C	8.29561	4.91128	4.48749
H	-6.65052	1.16703	0.76446	N	9.64636	5.10513	4.80239
C	-4.10951	4.76066	-0.61369	N	9.44381	5.11063	2.55915
N	-4.65315	6.00095	-0.65637	C	10.04762	4.71871	1.27326
C	-3.64402	6.93002	-0.59372	C	10.45747	5.23740	6.01728
C	-2.45886	6.24035	-0.51513	C	10.29952	5.21491	3.61518
N	-2.76533	4.90144	-0.52524	C	11.49810	5.28620	1.10226
H	-1.43406	6.60239	-0.45008	N	12.30770	5.12052	2.31413
H	-3.84003	8.00115	-0.60936	C	13.65578	4.90211	2.62431
C	-6.08427	6.33197	-0.72352	C	13.77628	4.84585	3.98797
H	-6.23140	7.13201	-1.46056	N	12.50985	5.07053	4.55663
H	-6.65242	5.44826	-1.03742	C	11.90188	4.65871	5.83423
H	-6.43327	6.67535	0.26120	C	11.65545	5.20937	3.50359
C	-1.77613	3.81602	-0.45884	H	12.52004	5.01802	6.66920
H	-1.06762	4.02516	0.35370	H	11.87093	3.55602	5.87955
H	-2.28952	2.86856	-0.25405	H	9.97433	4.69790	6.84323
H	-1.23162	3.75016	-1.41160	H	10.51650	6.30319	6.29529
C	-5.50713	3.51317	1.81930	H	11.97595	4.75904	0.26537
H	-6.50790	3.91603	2.03285	H	11.45061	6.35807	0.84620
H	-5.26888	2.71800	2.53847	H	9.43323	5.10086	0.44577
H	-4.75867	4.30971	1.90780	H	10.06709	3.61689	1.20588
C	-4.52207	2.85044	-3.03324	H	7.28208	4.76762	2.51456
H	-4.13280	3.86986	-3.14732	H	7.52378	4.83143	5.24881
H	-3.71691	2.12401	-3.21332	H	14.42671	4.83067	1.86125

H	14.66688	4.70027	4.59358
Et-tethg^{grad} (isomer 2)			
C	8.14288	4.87560	3.05275
C	8.23626	4.92808	4.41868
N	9.58818	5.09090	4.76387
N	9.43435	5.00247	2.51600
C	10.05568		4.63555
1.23332			
C	10.38092		4.81037
5.97175			
C	10.27224		5.06810
3.58678			
C	11.51426		5.18599
1.11437			
N	12.30724		4.90429
2.32195			
C	13.65917		5.06693
2.66722			
C	13.75249		5.11894
4.03319			
N	12.46102		4.99156
4.56983			
C	11.83988		5.35996
5.85231			
C	11.62307		4.92699
3.49900			
H	11.83350		6.45996
5.94785			
H	12.42921		4.94747
6.68292			
H	10.40542		3.71987
6.14199			
H	9.90833	5.28238	6.84428
H	11.98746		4.71594
0.24120			
H	11.48847		6.27683
0.94651			
H	9.46617	5.04842	0.40297
H	10.06194		3.53567
1.13643			
H	7.25671	4.80663	2.42697
H	7.44277	4.91280	5.16167
H	14.45250		5.08199
1.92402			
H	14.63853		5.18787
4.65917			
Et-tethg^{biscat} (isomer 1)			
C	8.16211	4.93604	3.11585
C	8.28620	4.99022	4.49418
N	9.64423	5.00208	4.78616
N	9.44575	4.93508	2.58510
C	10.02858	4.71764	1.22894
C	10.46155	5.20348	6.01752
C	10.27980	4.97189	3.61938

C	11.49369	5.25171	1.10139
N	12.30841	5.01427	2.32795
C	13.66613	4.97876	2.61928
C	13.78952	4.89199	3.99600
N	12.50598	4.89442	4.52678
C	11.92085	4.65618	5.87858
C	11.67241	4.96481	3.49390
H	12.54578	5.15323	6.63266
H	11.96020	3.57105	6.06258
H	9.97835	4.68413	6.85615
H	10.45920	6.28280	6.23566
H	11.97113	4.74538	0.25156
H	11.50798	6.33545	0.90681
H	9.40932	5.23628	0.48486
H	9.97734	3.63690	1.02337
H	7.26441	4.89680	2.50047
H	7.51276	5.02276	5.26047
H	14.43991	5.01881	1.85368
H	14.68657	4.82714	4.61016
Et-tethg^{biscat} (isomer 2)			
C	8.14558	4.85971	3.04743
C	8.24079	4.90982	4.42766
N	9.58983	5.00098	4.74584
N	9.43763	4.92037	2.54148
C	10.04550	4.65587	1.20420
C	10.37721	4.83058	6.00162
C	10.24978	5.00119	3.59131
C	11.51800	5.16559	1.08445
N	12.30542	4.99376	2.34007
C	13.65453	5.08508	2.65815
C	13.74988	5.13510	4.03832
N	12.45785	5.07454	4.54449
C	11.84982	5.34004	5.88145
C	11.64562	4.99405	3.49468
H	11.90833	6.42731	6.04755
H	12.44882	4.84361	6.65665
H	10.34841	3.75834	6.25138
H	9.88665	5.38379	6.81379
H	12.00858	4.61329	0.27170
H	11.54658	6.23815	0.83614
H	9.44623	5.15284	0.42958
H	9.98685	3.56871	1.03765
H	7.26256	4.78696	2.41399
H	7.45304	4.88772	5.17971
H	14.44218	5.10683	1.90598
H	14.63297		5.20738
4.67172			
Pr-tethg			
N	-3.83475	0.84152	10.81962
N	-1.03398	1.98562	11.16448
C	-3.32164	1.47224	11.99405
C	-2.06766	1.97289	12.15145
N	-4.40960	1.62984	12.90696
N	-1.60281	2.73139	13.26860

H	-6.36360	0.60153	12.98005	C	-4.87657	3.59152	-0.59609
H	0.56509	2.88154	14.04873	N	-4.72143	2.58402	0.39605
H	-5.51020	-0.73776	10.69736	H	-5.95704	0.90245	0.80747
H	1.11142	2.43878	11.35833	C	-4.21353	4.77071	-0.62202
H	-4.75640	1.37373	15.01814	N	-4.51543	5.84314	-1.50985
H	-5.38816	2.72782	14.05883	C	-3.42480	6.81225	-1.37024
H	-3.59297	3.37435	15.63511	C	-2.88222	6.54148	0.04588
H	-3.17781	3.81240	13.98247	N	-3.12057	5.10740	0.22893
H	-1.31978	2.68286	15.45333	H	-1.81628	6.78331	0.16752
H	-2.18075	1.15791	15.19485	H	-2.64006	6.61786	-2.12418
H	-0.12280	0.57836	9.81662	H	-3.44638	7.12510	0.79521
H	-0.52687	2.25152	9.38732	H	-3.79136	7.83899	-1.51631
H	-1.96019	0.55266	8.29196	H	-7.41923	2.37877	-0.44243
H	-2.92306	1.71159	9.20499	H	-4.85339	0.70007	-0.58004
H	-3.52948	-0.82920	9.42645	C	-5.87460	6.36304	-1.46390
H	-2.09426	-0.98561	10.45489	H	-6.00392	7.13777	-2.23493

Pr-teth^gbiscat (isomer 2)

C	8.09911	4.74799	3.27911
C	8.27758	4.89769	4.62104
N	9.63003	4.97151	4.85469
N	9.34310	4.72344	2.69490
C	9.41808	4.58676	1.21460
C	10.77293	4.23381	0.64357
C	10.09025	5.05580	6.26699
C	10.29707	4.86397	3.66540
H	8.68465	3.81260	0.95088
H	9.05887	5.54039	0.79603
H	11.11304	3.23613	0.96670
H	10.64183	4.17716	-0.44826
H	9.40438	5.75620	6.76199
H	9.92047	4.05961	6.70592
C	11.83593	5.27637	0.94120
N	12.40374	5.10027	2.29059
C	13.75794	5.08275	2.51365
C	13.94702	4.88651	3.85284
N	12.70577	4.77431	4.42846
C	12.53745	4.54456	5.87477
C	11.52172	5.49127	6.48536
C	11.74696	4.90797	3.46918
H	11.67570	5.49525	7.57587
H	11.69983	6.52385	6.14316
H	12.26441	3.48830	6.03404
H	13.52807	4.70342	6.31854
H	11.44440	6.30321	0.85092
H	12.68002	5.18004	0.24735
H	14.86386	4.81236	4.43422
H	14.47921	5.21590	1.70988
H	7.18643	4.65358	2.69419
H	7.55082	4.95186	5.42909

9

C	-6.53178	2.03698	-1.00645
C	-5.49906	1.42291	-0.04677
N	-5.82789	3.18903	-1.57653
H	-6.87234	1.35034	-1.79481

C	-4.87657	3.59152	-0.59609
N	-4.72143	2.58402	0.39605
H	-5.95704	0.90245	0.80747
C	-4.21353	4.77071	-0.62202
N	-4.51543	5.84314	-1.50985
C	-3.42480	6.81225	-1.37024
C	-2.88222	6.54148	0.04588
N	-3.12057	5.10740	0.22893
H	-1.81628	6.78331	0.16752
H	-2.64006	6.61786	-2.12418
H	-3.44638	7.12510	0.79521
H	-3.79136	7.83899	-1.51631
H	-7.41923	2.37877	-0.44243
H	-4.85339	0.70007	-0.58004
C	-5.87460	6.36304	-1.46390
H	-6.00392	7.13777	-2.23493
H	-6.57639	5.54431	-1.67933
H	-6.14591	6.79963	-0.47855
C	-1.95637	4.23547	0.16156
H	-2.27063	3.20241	0.37440
H	-1.45802	4.24482	-0.83127
H	-1.22167	4.53675	0.92417
C	-4.83184	2.98208	1.78921
H	-5.85367	3.31659	2.07127
H	-4.54191	2.14207	2.43961
H	-4.14390	3.81803	1.98005
C	-5.33861	3.05812	-2.94267
H	-4.89539	4.01516	-3.25617
H	-4.56776	2.26817	-3.06401
H	-6.17819	2.82748	-3.61719

grad

C	-6.02259	1.68931	-1.34616
C	-5.87959	1.63131	0.17339
N	-5.60904	3.06394	-1.66686
H	-5.34094	0.97794	-1.84826
C	-4.88346	3.56011	-0.61003
N	-4.91562	2.70290	0.46325
H	-6.83711	1.86187	0.67719
C	-4.18792	4.79799	-0.61535
N	-4.61373	5.92958	-1.26864
C	-3.74555	7.04842	-0.87044
C	-2.49881	6.34644	-0.33923
N	-3.00322	5.02053	0.04721
H	-1.73215	6.22993	-1.12796
H	-3.53997	7.71849	-1.71708
H	-2.03617	6.86219	0.51403
H	-4.24835	7.63488	-0.07884
H	-7.04509	1.48446	-1.69624
H	-5.51909	0.65959	0.54091
C	-6.02451	6.24191	-1.46421
H	-6.11896	7.00285	-2.25124
H	-6.58416	5.35126	-1.77056
H	-6.47507	6.64135	-0.53616
C	-1.99928	3.97983	0.23199
H	-1.28274	4.30728	0.99756

H	-2.46250	3.04303	0.56286	C	4.17091	-0.91212	16.74808
H	-1.44765	3.79037	-0.70786	C	5.04212	-0.21856	17.53180
C	-4.86008	3.16671	1.84478	H	2.15839	-0.89964	14.66831
H	-5.83965	3.56605	2.16918	H	2.97881	-3.46267	16.15461
H	-4.59085	2.32277	2.49537	H	7.53218	1.16952	17.87330
H	-4.10755	3.95353	1.96358	H	5.51852	0.79037	20.16951
C	-5.26746	3.32789	-3.05921	H	7.70599	0.13634	19.32570
H	-4.95032	4.36844	-3.19308	H	5.95649	2.31298	19.33210
H	-4.45022	2.66454	-3.39718	H	3.31790	-3.02438	14.45307
H	-6.14879	3.14054	-3.68912	H	1.20839	-1.83895	15.86153
gbiscat				C	1.99974	-0.30528	17.80425
C	-5.77055	1.52833	-1.34488	C	0.79745	0.38904	17.58209
C	-6.04911	1.69599	0.16737	C	2.40964	-0.54572	19.12783
N	-5.03861	2.77115	-1.69335	C	0.04181	0.85211	18.65762
H	-5.13962	0.65748	-1.57901	C	1.64707	-0.07975	20.19768
C	-4.93045	3.54209	-0.62388	C	0.46437	0.63173	19.97288
N	-5.48385	3.03693	0.46664	H	0.48841	0.61145	16.55890
H	-7.12051	1.67828	0.41892	H	3.33328	-1.09261	19.31185
C	-4.19938	4.84614	-0.62676	H	-0.87288	1.41802	18.46289
N	-4.79808	6.02507	-0.61570	H	1.98647	-0.28164	21.21791
C	-3.77660	7.10402	-0.64273	H	-0.12141	1.01557	20.81116
C	-2.44452	6.32682	-0.54860	C	5.68934	-2.17744	15.20581
N	-2.87762	4.90932	-0.61620	C	6.60298	-1.13033	14.97800
H	-1.75422	6.54649	-1.37603	C	6.02043	-3.47260	14.76001
H	-3.88054	7.67657	-1.57781	C	7.81895	-1.38647	14.34479
H	-1.91005	6.49506	0.39957	C	7.23735	-3.71393	14.12472
H	-3.93990	7.79102	0.20079	C	8.15188	-2.67626	13.92020
H	-6.68704	1.46045	-1.95107	H	6.35114	-0.12002	15.29657
H	-5.53860	0.94425	0.78836	H	5.33370	-4.29910	14.95166
C	-6.22494	6.32682	-0.66114	H	8.51357	-0.55997	14.17201
H	-6.47651	6.82268	-1.61199	H	7.48259	-4.72847	13.79870
H	-6.81560	5.40740	-0.56139	H	9.10865	-2.87202	13.43071
H	-6.47989	7.00664	0.16561	C	3.88772	1.99548	17.74140
C	-1.91719	3.81341	-0.55455	C	3.55660	2.14701	16.38067
H	-1.35080	3.86398	0.38863	C	3.28898	2.85337	18.68308
H	-2.43480	2.84793	-0.61284	C	2.63513	3.11850	15.98780
H	-1.21059	3.89521	-1.39447	C	2.37615	3.82509	18.27723
C	-5.53403	3.61110	1.80685	C	2.03232	3.95991	16.92794
H	-6.58079	3.78999	2.09915	H	4.02237	1.49661	15.64061
H	-5.08280	2.91070	2.52588	H	3.50635	2.71526	19.74365
H	-4.98334	4.55971	1.83908	H	2.38331	3.22234	14.92842
C	-4.55029	3.00815	-3.04816	H	1.90838	4.46627	19.02838
H	-4.13071	4.01901	-3.13510	H	1.30392	4.71013	16.61169
H	-3.77402	2.27014	-3.30318	C	6.75953	-1.93359	18.11553
H	-5.38262	2.89996	-3.76043	C	5.84050	-2.97762	18.33023
Phg				C	8.13514	-2.23716	18.12553
N	2.77751	-0.70306	16.70349	C	6.29120	-4.28362	18.52315
N	4.47697	-1.96866	15.87001	C	8.57413	-3.54342	18.33357
N	6.35252	-0.61005	17.88255	C	7.65626	-4.58131	18.52177
N	4.76325	0.99845	18.18606	H	4.77407	-2.76103	18.35091
C	2.21592	-1.48623	15.60355	H	8.86023	-1.44298	17.93796
C	3.23586	-2.62916	15.47456	H	5.55959	-5.07912	18.68791
C	6.99498	0.50837	18.57721	H	9.64659	-3.75591	18.33178
C	5.79043	1.23634	19.19405	H	8.00363	-5.60624	18.67170
				Phgrad			

N	2.77901	-1.15269	17.07828	C	7.86927	-4.39889	18.54235
N	4.56894	-2.09422	16.11352	H	4.95910	-2.68255	19.02528
N	6.25924	-0.53041	18.09543	H	8.76422	-1.25298	17.56858
N	4.70958	1.08404	17.95814	H	5.90313	-4.96820	19.24379
C	2.23379	-2.06696	16.06464	H	9.71832	-3.52762	17.83884
C	3.43838	-2.97540	15.78079	H	8.28926	-5.40098	18.65352
C	6.94964	0.69971	18.50636				
C	5.77196	1.63269	18.81594				
C	4.14356	-1.11928	16.97780	Phg b iscat			
C	4.99730	-0.22217	17.66136	N	2.84557	-1.23926	17.23378
H	1.91518	-1.50808	15.16657	N	4.53851	-1.88603	15.94362
H	3.43980	-3.86858	16.42870	N	6.16455	-0.54365	18.24187
H	7.57646	1.08803	17.68511	N	4.82251	1.15440	17.71828
H	5.47551	1.58072	19.87823	C	2.21858	-2.12298	16.21990
H	7.58717	0.50347	19.37779	C	3.43759	-2.82339	15.60607
H	5.96747	2.67816	18.54518	C	6.91862	0.65501	18.68304
H	3.50353	-3.29673	14.73390	C	5.86275	1.77158	18.58031
H	1.37077	-2.60949	16.47127	C	4.13553	-1.09807	16.93871
C	1.98795	-0.49892	18.05078	C	5.04170	-0.15546	17.64411
C	0.79574	0.12418	17.65755	H	1.67854	-1.49835	15.48942
C	2.39743	-0.44981	19.39146	H	3.64486	-3.79624	16.08072
C	0.03814	0.82466	18.59472	H	7.76827	0.81603	18.00139
C	1.63817	0.26311	20.31897	H	5.42084	2.02878	19.55596
C	0.46169	0.90772	19.92459	H	7.30212	0.50245	19.70013
H	0.48471	0.09800	16.61215	H	6.24039	2.68705	18.10725
H	3.30454	-0.96875	19.70518	H	3.37075	-2.95624	14.51952
H	-0.87878	1.32593	18.27711	H	1.51149	-2.80884	16.70256
H	1.96374	0.30373	21.36134	C	2.10556	-0.54078	18.23261
H	-0.12899	1.46531	20.65407	C	0.86894	0.01815	17.88935
C	5.80971	-2.13939	15.43787	C	2.61876	-0.41328	19.53055
C	6.36731	-3.38551	15.11765	C	0.16033	0.74263	18.84676
C	6.48073	-0.96042	15.07265	C	1.90345	0.32234	20.47680
C	7.59298	-3.44940	14.45443	C	0.67739	0.90312	20.13660
C	7.71349	-1.03612	14.42617	H	0.47002	-0.08432	16.87972
C	8.27664	-2.27824	14.11713	H	3.54966	-0.90781	19.81402
H	5.85473	-4.30241	15.41218	H	-0.80009	1.18863	18.58013
H	6.03503	0.01283	15.28076	H	2.29312	0.41934	21.49266
H	8.02399	-4.42222	14.20702	H	0.11487	1.46603	20.88414
H	8.22953	-0.11623	14.14066	C	5.83689	-1.95531	15.35958
H	9.23896	-2.33212	13.60400	C	6.37759	-3.20956	15.05086
C	3.69618	1.88450	17.38208	C	6.55092	-0.77875	15.08950
C	3.32337	1.72460	16.03813	C	7.65932	-3.28307	14.50533
C	3.06192	2.85505	18.17072	C	7.83797	-0.86721	14.55906
C	2.29576	2.50333	15.50707	C	8.39518	-2.11759	14.27102
C	2.04927	3.64286	17.62337	H	5.81833	-4.12394	15.25040
C	1.65344	3.46389	16.29457	H	6.09668	0.20002	15.25314
H	3.83800	0.99805	15.40835	H	8.08698	-4.25741	14.25937
H	3.33973	2.97234	19.21941	H	8.39456	0.04494	14.33348
H	2.00172	2.36480	14.46378	H	9.39500	-2.18182	13.83664
H	1.55369	4.38863	18.24848	C	3.72321	1.87104	17.15499
H	0.85520	4.07687	15.87117	C	3.32154	1.60850	15.83780
C	6.79723	-1.82702	18.26634	C	3.05254	2.82015	17.93514
C	5.99483	-2.87580	18.74093	C	2.20915	2.27084	15.31670
C	8.14260	-2.06309	17.95232	C	1.95509	3.49148	17.39428
C	6.53057	-4.15722	18.86723	C	1.52569	3.21333	16.09233
C	8.67221	-3.34616	18.09483	H	3.88679	0.91720	15.20975
				H	3.36333	3.02131	18.96110

H	1.88910	2.06671	14.29236	C	-2.36811	9.03559	-1.04477
H	1.42574	4.22946	18.00030	H	-2.22400	10.05654	-1.40688
H	0.66790	3.74459	15.67455				
C	6.65755	-1.87954	18.34622	10^{rad}			
C	5.79151	-2.91108	18.73491	C	-5.68956	1.59496	-1.28322
C	8.00041	-2.14062	18.04996	C	-6.35386	1.98556	-0.10292
C	6.26876	-4.22190	18.78406	N	-4.80636	2.61965	-1.62327
C	8.46796	-3.45378	18.11749	C	-4.90079	3.62369	-0.66887
C	7.60494	-4.49495	18.47382	N	-5.84201	3.22752	0.27100
H	4.76574	-2.69095	19.03737	C	-4.21648	4.85575	-0.67070
H	8.67337	-1.33723	17.74875	N	-4.75815	6.08207	-0.31398
H	5.60379	-5.02813	19.10026	C	-3.75397	7.04750	-0.35733
H	9.51351	-3.66582	17.88505	C	-2.56857	6.40254	-0.76555
H	7.98151	-5.51861	18.53310	N	-2.87358	5.05506	-0.95588
				C	-6.17210	6.40979	-0.24142
10				H	-6.39418	7.23324	-0.93704
C	-6.29044	1.96238	-1.27930	H	-6.77136	5.53859	-0.52907
C	-5.75598	1.63507	-0.01485	H	-6.45514	6.72152	0.77560
N	-5.80140	3.22224	-1.66279	C	-1.86691	4.01196	-1.05571
C	-4.94105	3.67316	-0.61910	H	-1.01576	4.26794	-0.40789
N	-4.91286	2.67860	0.40133	H	-2.29047	3.05870	-0.71517
C	-4.26508	4.85187	-0.59561	H	-1.50087	3.89662	-2.08732
N	-4.57758	6.00993	-1.36725	C	-5.97598	3.76336	1.61695
C	-3.61206	6.98315	-1.05494	H	-6.99648	4.13406	1.79545
C	-2.71198	6.44296	-0.11192	H	-5.75097	2.97476	2.35230
N	-3.10618	5.12686	0.19208	H	-5.26760	4.58708	1.76132
C	-5.96908	6.41292	-1.51110	C	-4.20586	2.75089	-2.93974
H	-6.05149	7.20356	-2.26978	H	-3.93430	3.79895	-3.11845
H	-6.57745	5.55945	-1.83663	H	-3.30659	2.12407	-3.03816
H	-6.38605	6.79064	-0.55704	H	-4.93456	2.44245	-3.70431
C	-2.07338	4.10397	0.28771	C	-7.31710	1.17509	0.49608
H	-2.49348	3.16798	0.67806	H	-7.82928	1.47432	1.41143
H	-1.62167	3.89218	-0.70112	C	-5.97712	0.38365	-1.91181
H	-1.28482	4.44167	0.97291	C	-7.60780	-0.04011	-0.13567
C	-4.91471	3.08240	1.79882	H	-5.46214	0.07173	-2.82156
H	-5.89928	3.48590	2.10650	H	-8.35803	-0.70212	0.30093
H	-4.66714	2.22048	2.43456	C	-6.95423	-0.42503	-1.31790
H	-4.16172	3.86204	1.96794	H	-7.21287	-1.37755	-1.78469
C	-5.41659	3.43150	-3.05113	C	-1.36539	7.09853	-0.88127
H	-5.05496	4.45835	-3.18989	H	-0.44362	6.60371	-1.18928
H	-4.61070	2.73747	-3.35702	C	-1.39125	8.46882	-0.59401
H	-6.28424	3.27408	-3.70791	C	-3.78528	8.41616	-0.09258
C	-6.09909	0.44605	0.61916	H	-0.46791	9.04657	-0.66828
H	-5.68874	0.19031	1.59800	H	-4.70223	8.92151	0.21398
C	-7.13640	1.08566	-1.94891	C	-2.57954	9.11617	-0.21966
C	-6.97427	-0.43282	-0.04764	H	-2.56238	10.18765	-0.01080
H	-7.54138	1.33130	-2.93246				
H	-7.26069	-1.37072	0.43419	10^{biscat}			
C	-7.47709	-0.12304	-1.31201	C	-5.82207	1.68561	-1.36231
H	-8.14560	-0.82403	-1.81727	C	-6.18896	1.88730	-0.01286
C	-1.62789	7.17968	0.35119	N	-5.04169	2.77785	-1.73111
H	-0.92685	6.75934	1.07453	C	-4.92704	3.60473	-0.66609
C	-1.46409	8.49191	-0.13084	N	-5.60206	3.08518	0.38519
C	-3.46204	8.28623	-1.51854	C	-4.20175	4.87660	-0.64287
H	-0.62105	9.09037	0.22188	N	-4.77981	6.09829	-0.58297
H	-4.16001	8.71421	-2.24063	C	-3.77672	7.06189	-0.53541

C	-2.54662	6.36817	-0.57214
N	-2.85623	5.01283	-0.63700
C	-6.21232	6.39777	-0.58336
H	-6.42562	7.13800	-1.36665
H	-6.78407	5.48574	-0.79142
H	-6.50886	6.80947	0.39257
C	-1.86550	3.93653	-0.66108
H	-1.18132	4.05553	0.19079
H	-2.37125	2.96658	-0.58341
H	-1.28981	3.98119	-1.59699
C	-5.69137	3.64864	1.73333
H	-6.72907	3.94215	1.94959
H	-5.36825	2.89256	2.46265
H	-5.03559	4.52366	1.81503
C	-4.49887	2.99042	-3.07427
H	-4.01517	3.97330	-3.12816
H	-3.76540	2.20563	-3.30843
H	-5.31743	2.94979	-3.80687
C	-7.00294	0.97726	0.67507
H	-7.29817	1.12870	1.71425
C	-6.24581	0.55945	-2.08190
C	-7.42899	-0.13391	-0.04446
H	-5.95763	0.38906	-3.12034
H	-8.06972	-0.87120	0.44383
C	-7.05554	-0.33972	-1.39676
H	-7.41792	-1.23004	-1.91517
C	-1.31792	7.04158	-0.53481
H	-0.36305	6.51538	-0.55929
C	-1.37916	8.42869	-0.46517
C	-3.83418	8.46026	-0.46736
H	-0.45037	9.00208	-0.43230
H	-4.77865	9.00492	-0.43757
C	-2.61347	9.12442	-0.43405
H	-2.60227	10.21503	-0.37820

Et-teth10

C	8.27613	5.28919	3.14236
C	7.15073	4.72472	2.55918
C	6.13741	4.22266	3.40317
C	6.26408	4.29227	4.78943
C	7.40825	4.85768	5.39006
C	8.41318	5.34215	4.56090
N	9.64739	5.93113	4.84968
N	9.43132	5.85001	2.54874
C	10.09125	5.23470	1.39399
C	10.49406	5.83608	6.02832
C	10.31766	6.07888	3.62543
H	7.05471	4.65416	1.47362
H	5.24876	3.76963	2.95747
H	5.46946	3.89857	5.42755
H	7.50789	4.89692	6.47690
C	11.47068	5.88640	1.10724
N	12.31620	5.94217	2.28899
C	13.54805	5.34246	2.56450
C	13.68391	5.25638	3.98159
C	14.80727	4.67579	4.55271

C	15.81957	4.18983	3.69816
C	15.69404	4.29143	2.31378
C	14.55228	4.87416	1.72518
H	14.45432	4.94037	0.63951
H	16.48794	3.90968	1.66758
H	16.70651	3.72411	4.13409
H	14.90231	4.58019	5.63646
N	12.53075	5.80842	4.58685
C	11.86296	5.17088	5.72456
C	11.64754	6.07023	3.51562
H	12.49823	5.25848	6.61885
H	11.70233	4.09441	5.51174
H	9.97862	5.24510	6.79952
H	10.67279	6.84512	6.43959
H	11.97830	5.30443	0.32405
H	11.30848	6.90689	0.71783
H	9.45761	5.35636	0.50241
H	10.23526	4.15038	1.57605

Et-teth10^{rad} (isomer 1)

C	8.14636	5.07003	3.14910
C	6.88615	5.03071	2.56334
C	5.77582	5.03041	3.41886
C	5.92585	5.06749	4.81242
C	7.19255	5.09887	5.41242
C	8.30029	5.09299	4.57188
N	9.68028	5.08776	4.84087
N	9.43456	5.11476	2.58891
C	9.98946	4.83878	1.25861
C	10.51045	5.33884	6.02435
C	10.30461	5.11046	3.63368
H	6.76289	5.00374	1.47933
H	4.77390	5.00197	2.98604
H	5.03796	5.07000	5.44736
H	7.30363	5.12387	6.49790
C	11.45014	5.38268	1.09969
N	12.27907	5.10786	2.27871
C	13.65901	5.09983	2.54733
C	13.81307	5.04910	3.96937
C	15.07327	4.99340	4.55389
C	16.18338	5.00326	3.69813
C	16.03322	5.06578	2.30551
C	14.76654	5.11457	1.70663
H	14.65527	5.16008	0.62184
H	16.92095	5.07510	1.67043
H	17.18523	4.96204	4.13007
H	15.19669	4.94561	5.63715
N	12.52517	5.08887	4.53055
C	11.96904	4.79226	5.85594
C	11.65494	5.10926	3.48615
H	12.59531	5.25838	6.62922
H	11.98598	3.70050	6.01916
H	10.06243	4.84518	6.89788
H	10.53654	6.42407	6.22412
H	11.89646	4.90242	0.21782
H	11.42840	6.47130	0.91871

H	9.36490	5.32018	0.49341
H	9.96846	3.75002	1.07684

Et-teth10^{rad} (isomer 2)

C	7.45370	5.16960	3.56169
C	6.16277	4.83317	3.16866
C	5.30054	4.32803	4.15123
C	5.71758	4.17172	5.48095
C	7.01478	4.51538	5.88548
C	7.87776	5.00973	4.91360
N	9.22423	5.41714	4.98922
N	8.54683	5.67337	2.82899
C	8.88415	5.50155	1.40707
C	10.29222	4.96210	5.89156
C	9.59403	5.72421	3.70831
H	5.83288	4.94765	2.13482
H	4.28520	4.04177	3.86991
H	5.02038	3.76896	6.21782
H	7.33897	4.38168	6.91894
C	10.24125	6.16742	1.03085
N	11.28604	5.86339	2.01049
C	12.68993	5.90084	2.01244
C	13.11169	5.75449	3.37049
C	14.46016	5.75383	3.71108
C	15.38636	5.88725	2.66908
C	14.97350	6.01945	1.33487
C	13.61694	6.03057	0.98377
H	13.30182	6.14423	-0.05485
H	15.72484	6.12345	0.55000
H	16.45247	5.89168	2.90487
H	14.78607	5.65520	4.74780
N	11.95289	5.62437	4.15014
C	11.66374	5.63132	5.58404
C	10.89658	5.73978	3.30498
H	11.67594	6.67114	5.95366
H	12.44183	5.07201	6.12184
H	10.38607	3.86497	5.80326
H	10.02321	5.20320	6.92999
H	10.54302	5.79322	0.04262
H	10.11880	7.26212	0.96143
H	8.10189	5.95774	0.78412
H	8.91569	4.42179	1.17741

Et-teth10^{biscat} (isomer 1)

C	8.14823	5.05591	3.14845
C	6.88657	5.00995	2.55236
C	5.79099	5.02256	3.41236
C	5.94273	5.07696	4.81809
C	7.19625	5.11951	5.42425
C	8.30239	5.10538	4.57217
N	9.68251	5.12118	4.82389
N	9.44091	5.07391	2.60514
C	9.98886	4.84801	1.24637
C	10.51140	5.33280	6.03457
C	10.28454	5.10644	3.63572
H	6.75819	4.96550	1.46964

H	4.78492	4.98927	2.98869
H	5.04938	5.08504	5.44593
H	7.30298	5.16170	6.50952
C	11.44917	5.37571	1.08925
N	12.27704	5.13893	2.29592
C	13.65703	5.11068	2.54708
C	13.81108	5.03451	3.96963
C	15.07262	4.97237	4.56459
C	16.16814	4.99467	3.70474
C	16.01651	5.07368	2.30020
C	14.76313	5.13326	1.69516
H	14.65648	5.19505	0.61082
H	16.90980	5.08783	1.67240
H	17.17406	4.94916	4.12763
H	15.20088	4.90800	5.64632
N	12.51855	5.04843	4.51333
C	11.96965	4.80202	5.86827
C	11.67500	5.10457	3.48372
H	12.60387	5.30845	6.60801
H	12.02424	3.71807	6.05864
H	10.04897	4.80568	6.87979
H	10.50488	6.41101	6.26070
H	11.90938	4.86178	0.23473
H	11.46019	6.45776	0.88241
H	9.35676	5.36912	0.51510
H	9.92995	3.76759	1.03805

Et-teth10^{biscat} (isomer 2)

C	7.45752	5.05303	3.54596
C	6.11936	4.90688	3.17562
C	5.21998	4.61366	4.19728
C	5.63650	4.46939	5.54191
C	6.96964	4.60724	5.92187
C	7.88104	4.89800	4.90496
N	9.27092	5.08856	4.91463
N	8.60846	5.33617	2.79821
C	8.89487	5.33875	1.34483
C	10.32796	4.79408	5.91115
C	9.63025	5.32716	3.65377
H	5.78925	5.01374	2.14117
H	4.16301	4.48708	3.95335
H	4.88973	4.23751	6.30378
H	7.28126	4.48519	6.96048
C	10.26684	5.99001	0.99489
N	11.32400	5.69507	1.99115
C	12.71397	5.88512	2.00072
C	13.13752	5.73000	3.35969
C	14.47576	5.87552	3.72993
C	15.37521	6.16823	2.70817
C	14.95866	6.31257	1.36357
C	13.62541	6.17535	0.98372
H	13.31377	6.29745	-0.05488
H	15.70550	6.54400	0.60163
H	16.43226	6.29430	2.95199
H	14.80587	5.76857	4.76438
N	11.98651	5.44725	4.10756

C	11.70022	5.44474	5.56094
C	10.96468	5.45669	3.25206
H	11.74543	6.48985	5.90632
H	12.48528	4.88058	6.08236
H	10.41874	3.69807	5.97775
H	10.01138	5.17131	6.89319
H	10.58341	5.61357	0.01254
H	10.17575	7.08603	0.92910
H	8.10960	5.90256	0.82331
H	8.85017	4.29361	0.99950

Pr-teth10

C	8.05397	4.74728	3.21961
C	6.78137	4.71701	2.65619
C	5.66961	4.66787	3.51857
C	5.83923	4.66146	4.90162
C	7.12660	4.70288	5.47067
C	8.22632	4.73666	4.61767
N	9.59460	4.79921	4.89012
N	9.31412	4.82261	2.62601
C	9.43510	5.33066	1.27751
C	10.60124	4.76386	0.48998
C	10.03136	5.29609	6.17685
C	10.30856	4.90998	3.65184
H	6.63357	4.74176	1.57539
H	4.66514	4.64347	3.08949
H	4.96733	4.63268	5.55891
H	7.24575	4.71626	6.55516
H	8.50189	5.07009	0.76204
H	9.50924	6.44092	1.28017
H	10.59052	3.66216	0.53233
H	10.47128	5.06563	-0.56338
H	10.06330	6.40840	6.17987
H	9.26605	4.99615	6.90413
C	11.94365	5.29617	0.95389
N	12.38041	4.79921	2.24059
C	13.74869	4.73664	2.51303
C	13.92104	4.74729	3.91110
C	15.19365	4.71701	4.47452
C	16.30540	4.66785	3.61214
C	16.13578	4.66142	2.22909
C	14.84840	4.70283	1.66004
H	14.72925	4.71618	0.57554
H	17.00768	4.63262	1.57179
H	17.30987	4.64346	4.04121
H	15.34145	4.74178	5.55532
N	12.66090	4.82263	4.50470
C	12.53990	5.33070	5.85319
C	11.37380	4.76382	6.64072
C	11.66646	4.90998	3.47887
H	11.38458	3.66212	6.59834
H	11.50375	5.06557	7.69409
H	13.47313	5.07019	6.36866
H	12.46568	6.44095	5.85052
H	11.91164	6.40848	0.95096
H	12.70897	4.99633	0.22659

Pr-teth10^{rad} (isomer 1)

N	-3.73123	0.38448	11.03958
N	-0.93783	1.68834	11.27682
C	-3.27905	1.17947	12.08730
C	-1.95856	1.65686	12.23219
N	-4.36690	1.35322	12.94680
N	-1.40707	2.15399	13.40949
C	-5.45453	0.63043	12.45801
C	-0.05994	2.43742	13.21858
C	-5.05716	0.02570	11.25418
C	0.23531	2.13897	11.87848
C	-4.54106	2.12347	14.17710
C	-3.40282	3.05000	14.54511
C	-2.07792	2.31399	14.68719
C	-0.89473	1.35767	9.85311
C	-2.21692	1.01029	9.20378
C	-2.94448	-0.11488	9.92755
H	-4.70458	1.40423	14.99994
H	-5.47340	2.70067	14.07056
H	-3.66775	3.51309	15.50779
H	-3.29244	3.87125	13.81874
H	-1.39636	2.88576	15.32698
H	-2.22438	1.33004	15.17007
H	-0.20106	0.50586	9.73363
H	-0.43539	2.21410	9.33400
H	-1.98768	0.69262	8.17486
H	-2.87883	1.88786	9.12915
H	-3.64567	-0.61335	9.24833
H	-2.23328	-0.88508	10.27930
C	-6.74174	0.45673	12.97109
C	-7.61799	-0.34980	12.23597
C	-7.22013	-0.95556	11.03373
C	-5.93129	-0.77728	10.52015
H	-7.06063	0.91611	13.90679
H	-8.62892	-0.51838	12.61269
H	-7.92812	-1.58199	10.48789
H	-5.63219	-1.25800	9.58824
C	0.92305	2.90676	14.09046
C	2.21133	3.07564	13.57127
C	2.50451	2.78296	12.23008
C	1.51937	2.30761	11.35728
H	3.52070	2.92679	11.85752
H	1.75972	2.07001	10.32093
H	0.71069	3.13185	15.13611
H	3.00421	3.43954	14.22711

Pr-teth10^{rad} (isomer 2)

C	8.08002	5.05135	3.22769
C	6.81424	5.07528	2.63918
C	5.71284	5.14789	3.49831
C	5.87854	5.19046	4.89129
C	7.14960	5.17395	5.47593
C	8.24987	5.12163	4.61709
N	9.62064	5.09059	4.87179
N	9.34197	4.92573	2.65649

C	9.41368	4.66801	1.22053	H	11.18769	3.18277	1.13910
C	10.73919	4.15334	0.71290	H	10.69935	3.95587	-0.36688
C	10.06766	4.91381	6.24957	H	10.65427	6.24623	6.30090
C	10.31667	4.96690	3.66046	H	9.35304	5.18517	6.86194
H	6.67594	5.03810	1.55859	C	11.78045	5.25313	0.96607
H	4.70728	5.16805	3.07348	N	12.36249	5.16055	2.31032
H	4.99872	5.23575	5.53580	C	13.73073	5.21342	2.53825
H	7.25868	5.19637	6.56029	C	13.91441	5.00469	3.91694
H	8.62101	3.93826	0.99357	C	15.18883	4.99573	4.50159
H	9.15288	5.59879	0.68543	C	16.26197	5.19723	3.64234
H	11.00689	3.18801	1.17321	C	16.07837	5.39829	2.25165
H	10.62080	3.97035	-0.36601	C	14.81592	5.41161	1.67269
H	9.33383	5.43511	6.87619	H	14.69176	5.58333	0.60313
H	10.01034	3.84002	6.51175	H	16.95472	5.55408	1.61940
C	11.85774	5.15682	0.92336	H	17.27532	5.20405	4.04978
N	12.40286	5.09972	2.26817	H	15.34581	4.83981	5.56890
C	13.77360	5.15307	2.50277	N	12.65362	4.81438	4.47325
C	13.96110	5.06535	3.89147	C	12.56750	4.43682	5.90071
C	15.24046	5.06456	4.45139	C	11.18112	4.12178	6.41371
C	16.32536	5.16484	3.57554	C	11.71400	4.92922	3.48746
C	16.13658	5.26205	2.18777	H	10.78735	3.18276	5.99159
C	14.85609	5.25972	1.62719	H	11.27567	3.95585	7.49759
H	14.72233	5.34690	0.54854	H	13.23283	3.57057	6.03378
H	17.00470	5.34527	1.53143	H	13.00186	5.27444	6.46843
H	17.33787	5.16820	3.98393	H	11.32071	6.24625	0.82983
H	15.40632	4.98365	5.52606	H	12.62196	5.18522	0.26878
N	12.69797	4.97649	4.47487				
C	12.54964	4.66137	5.88598				
C	11.44847	5.44102	6.57156				
C	11.72017	4.99854	3.48008				
H	11.58422	5.33119	7.65900				
H	11.53484	6.51466	6.33699				
H	12.38625	3.57438	6.01408				
H	13.51055	4.90303	6.35441				
H	11.51326	6.18104	0.68766				
H	12.68904	4.93179	0.24526				

Pr-teth10^{biscat} (isomer 1)

C	8.06061	5.00470	3.21377
C	6.78618	4.99574	2.62912
C	5.71304	5.19724	3.48835
C	5.89664	5.39830	4.87904
C	7.15908	5.41162	5.45801
C	8.24427	5.21343	4.59246
N	9.61251	5.16055	4.82040
N	9.32139	4.81438	2.65747
C	9.40752	4.43680	1.23002
C	10.79390	4.12178	0.71700
C	10.19455	5.25311	6.16466
C	10.26101	4.92922	3.64326
H	6.62922	4.83982	1.56180
H	4.69969	5.20406	3.08090
H	5.02028	5.55409	5.51129
H	7.28323	5.58334	6.52757
H	8.74220	3.57052	1.09697
H	8.97312	5.27439	0.66229

Pr-teth10^{biscat} (isomer 2)

C	8.08714	4.87922	3.24025
C	6.81243	4.78377	2.66381
C	5.73367	4.87215	3.53543
C	5.91311	5.04523	4.92988
C	7.17672	5.14975	5.49972
C	8.26522	5.06970	4.61955
N	9.63596	5.14673	4.84588
N	9.35444	4.81446	2.67259
C	9.44843	4.55374	1.21754
C	10.83406	4.34296	0.64693
C	10.09212	5.41590	6.23142
C	10.28989	4.98170	3.65563
H	6.65799	4.64557	1.59373
H	4.72001	4.80401	3.13462
H	5.03278	5.09992	5.57344
H	7.29804	5.28651	6.57419
H	8.82169	3.67117	1.02273
H	8.96580	5.41359	0.72640
H	11.26878	3.38028	0.96114
H	10.71368	4.28649	-0.44562
H	9.54914	6.31222	6.56556
H	9.72596	4.56868	6.83216
C	11.79548	5.47314	0.98632
N	12.39243	5.25551	2.30813
C	13.76204	5.18454	2.52912
C	13.93580	4.86266	3.89183
C	15.21180	4.73406	4.46066
C	16.29169	4.92778	3.60955

C	16.11650	5.23768	2.23750
C	14.85540	5.37199	1.67189
H	14.73805	5.62838	0.61848
H	16.99875	5.38280	1.61088
H	17.30457	4.83814	4.00819
H	15.36570	4.48574	5.51133
N	12.66272	4.73106	4.43144
C	12.39954	4.46017	5.84686
C	11.58036	5.59323	6.44952
C	11.73696	4.98436	3.46842
H	11.73536	5.61792	7.53890
H	11.94549	6.55827	6.06273
H	11.89654	3.48401	5.94350
H	13.37561	4.37146	6.33511
H	11.30675	6.46112	0.95999
H	12.62614	5.50364	0.27370

11

C	-2.02948	-4.26742	-0.53168
C	-3.08575	-3.92442	0.22581
N	-1.27907	-3.20225	-1.05902
C	-1.69088	-1.97326	-0.46533
S	-3.29873	-2.16214	0.33957
C	-0.82883	-0.93150	-0.36452
N	-1.07781	0.37930	0.05909
C	0.05880	1.17284	0.09982
C	1.18975	0.58095	-0.33006
S	0.89719	-1.09546	-0.81474
C	-2.41304	0.89379	0.27970
H	-2.40619	1.98703	0.15700
H	-3.10084	0.46907	-0.46775
H	-2.80334	0.65074	1.28195
C	-1.04079	-3.22173	-2.50295
H	-1.96060	-3.00319	-3.07867
H	-0.27471	-2.48052	-2.77095
H	-0.66374	-4.21453	-2.79378
H	-0.03668	2.19875	0.45541
H	2.18026	1.02168	-0.40647
H	-1.72932	-5.28614	-0.78573
H	-3.77820	-4.59483	0.73169

11^{rad}

C	-2.35060	-4.20939	-0.74728
C	-3.15698	-3.90270	0.29557
N	-1.51290	-3.18317	-1.14391
C	-1.63143	-2.04106	-0.37598
S	-2.86494	-2.28154	0.86050
C	-0.80494	-0.90800	-0.45939
N	-1.11541	0.35214	0.01486
C	-0.05832	1.24241	-0.03766
C	1.07454	0.73271	-0.57344
S	0.86611	-0.93810	-1.01808
C	-2.45985	0.78485	0.39833
H	-2.52294	1.87360	0.27773
H	-3.20116	0.31615	-0.26147
H	-2.68664	0.52853	1.44463

C	-0.72193	-3.27745	-2.37138
H	-0.80419	-2.33970	-2.93794
H	0.33683	-3.48690	-2.15588
H	-1.12687	-4.09160	-2.98492
H	2.01849	1.24381	-0.75208
H	-0.20591	2.26122	0.31857
H	-2.32730	-5.15094	-1.29397
H	-3.91563	-4.52807	0.76158

11^{biscat}

C	-2.22797	-4.26434	-0.69360
C	-2.82720	-4.09887	0.52421
N	-1.39894	-3.21484	-1.02846
C	-1.35837	-2.24203	-0.09741
S	-2.34985	-2.61555	1.24887
C	-0.55891	-1.01411	-0.16730
N	-0.78759	0.02217	-0.99671
C	0.07644	1.07961	-0.80947
C	0.98045	0.85532	0.19203
S	0.74913	-0.69676	0.89265
C	-1.85420	0.06020	-2.01780
H	-1.42531	-0.18255	-3.00135
H	-2.64212	-0.65413	-1.75302
H	-2.28322	1.07033	-2.04433
C	-0.63496	-3.20491	-2.29323
H	0.16246	-2.45557	-2.23550
H	-0.18399	-4.19544	-2.44068
H	-1.31634	-2.98238	-3.12716
H	-3.52309	-4.77608	1.02481
H	-2.34082	-5.11007	-1.37410
H	1.76298	1.52799	0.55005
H	-0.01834	1.97608	-1.42430

12

S	4.98156	5.03104	11.62484
S	2.14754	6.16659	8.36422
N	2.37987	5.39360	11.70449
N	4.73290	5.81078	8.78169
C	3.44723	5.45912	10.80408
C	3.49938	5.80914	9.49409
C	2.81508	5.53124	13.08709
C	4.53171	5.48537	7.36343
C	4.11484	4.75084	13.21761
C	3.05046	5.15700	7.12642
C	1.08998	5.98072	11.40167
C	5.58720	6.97471	8.98437
H	0.36154	5.64368	12.15424
H	0.73770	5.65062	10.41865
H	1.11283	7.09171	11.41474
H	5.13406	7.90558	8.58199
H	6.55462	6.81046	8.48248
H	5.78970	7.11385	10.05558
H	4.74196	5.11781	14.04182
H	3.92853	3.67442	13.35323
H	2.03892	5.13038	13.75921
H	2.97731	6.59814	13.35709

H	5.16380	4.63407	7.05284
H	4.81627	6.35141	6.73824
H	2.72019	5.43429	6.11515
H	2.83212	4.09205	7.29870

H	5.05234	6.38222	6.93912
H	3.26997	6.47231	6.97394
H	3.44041	4.08761	6.62033
H	5.06945	3.98921	7.36196

12^{rad}

S	5.04616	5.10317	11.75708
S	2.14924	4.91097	8.57484
N	2.48181	5.56143	11.70827
N	4.52933	5.96009	8.65997
C	3.55968	5.49664	10.88805
C	3.52138	5.56388	9.47417
C	2.73225	5.07569	13.07241
C	4.36138	5.56111	7.25637
C	4.20234	5.35243	13.36971
C	2.86145	5.51507	6.99431
C	1.15830	6.06414	11.35713
C	5.74612	6.66118	9.04698
H	0.75078	6.61131	12.21962
H	0.46336	5.24811	11.09907
H	1.22683	6.74935	10.50487
H	5.96930	7.42760	8.29018
H	6.60435	5.97098	9.10828
H	5.61451	7.15171	10.01752
H	4.37931	6.38364	13.70874
H	4.62672	4.65090	14.09873
H	2.50563	3.99527	13.13192
H	2.07219	5.60274	13.77548
H	4.82848	4.57262	7.09348
H	4.86487	6.29061	6.60662
H	2.44059	6.50590	6.76753
H	2.59090	4.81208	6.19661

13

C	-2.17157	-4.20374	-0.70319
C	-3.11894	-3.84231	0.28213
N	-1.56950	-3.11194	-1.32198
C	-1.83562	-1.89444	-0.66243
S	-3.26530	-2.07889	0.42196
C	-1.01540	-0.81974	-0.69634
N	-1.25405	0.44811	-0.14152
C	-0.09716	1.18494	0.07987
C	1.05267	0.60716	-0.50381
S	0.65543	-0.89359	-1.35590
C	-2.57098	1.02047	0.04118
H	-2.57304	2.06734	-0.30823
H	-3.29734	0.45703	-0.55864
H	-2.90242	1.00209	1.09369
C	-1.12220	-3.18659	-2.70137
H	-1.25573	-2.20381	-3.17520
H	-0.06079	-3.47446	-2.79407
H	-1.73099	-3.92384	-3.25150
C	-3.84272	-4.80971	0.97025
H	-4.57812	-4.51997	1.72423
C	-1.94725	-5.55203	-0.99342
C	-3.61033	-6.16393	0.67809
H	-1.20227	-5.84132	-1.73691
H	-4.16563	-6.93278	1.21943
C	-2.67396	-6.52619	-0.29341
H	-2.49124	-7.58143	-0.51174
C	2.29797	1.21326	-0.39274
H	3.17665	0.75656	-0.85391
C	2.40623	2.41313	0.32903
C	0.01283	2.38768	0.78405
H	3.38169	2.89125	0.44308
H	-0.86184	2.83892	1.25460
C	1.27369	2.99043	0.90578
H	1.36645	3.92195	1.46917

12^{biscat}

S	2.20097	6.94153	11.53689
S	3.33406	3.99155	9.04953
N	3.97772	5.15558	12.13581
N	4.16842	6.43740	8.86577
C	3.43044	5.80620	11.13996
C	3.72549	5.53281	9.70223
C	3.33542	5.42616	13.45310
C	4.15210	6.00206	7.44215
C	2.61811	6.76973	13.33804
C	4.08424	4.47391	7.42169
C	5.03319	4.13788	12.08253
C	4.57703	7.81818	9.15575
H	4.61660	3.17831	12.42840
H	5.84505	4.43893	12.76086
H	5.42352	4.02890	11.06577
H	5.60081	7.96808	8.78090
H	4.54075	8.02073	10.23077
H	3.90168	8.50731	8.62505
H	4.10401	5.42960	14.23912
H	2.64168	4.58966	13.64936
H	1.68410	6.80857	13.91460
H	3.24987	7.62881	13.60670

13^{rad}

C	-2.23994	-4.26009	-0.69844
C	-3.08229	-3.92578	0.38027
N	-1.50440	-3.16940	-1.16820
C	-1.66224	-2.02224	-0.42582
S	-2.88080	-2.24244	0.83211
C	-0.84255	-0.88540	-0.50567
N	-1.14566	0.35736	0.00247
C	-0.05409	1.22583	0.07601
C	1.11740	0.67607	-0.48149
S	0.83226	-0.95634	-1.05789
C	-2.49865	0.82210	0.30111
H	-2.60071	1.85782	-0.05120
H	-3.22765	0.20405	-0.23401
H	-2.71165	0.78623	1.38083

C	-0.79822	-3.23990	-2.44483
H	-0.71464	-2.23653	-2.87740
H	0.20678	-3.67487	-2.33015
H	-1.38291	-3.86460	-3.13403
C	-3.93787	-4.86456	0.95912
H	-4.59405	-4.59183	1.78752
C	-2.22184	-5.56816	-1.19908
C	-3.91762	-6.16517	0.45303
H	-1.56000	-5.85323	-2.01740
H	-4.56786	-6.92309	0.89365
C	-3.06303	-6.51060	-0.60736
H	-3.05387	-7.53672	-0.98049
C	2.31429	1.39213	-0.52074
H	3.21423	0.95658	-0.95837
C	2.32799	2.67375	0.03111
C	-0.03596	2.51760	0.61735
H	3.25539	3.24949	0.03296
H	-0.92581	2.95773	1.06814
C	1.16516	3.22630	0.59163
H	1.20000	4.22754	1.02551
13 biscat			
C	-2.29161	-4.24485	-0.67556
C	-2.80092	-4.11939	0.64004
N	-1.51222	-3.14398	-1.03840
C	-1.40724	-2.21525	-0.07659
S	-2.25114	-2.63170	1.36332
C	-0.57031	-1.01384	-0.14423
N	-1.01834	0.24282	-0.00645
C	-0.00623	1.20317	0.02922
C	1.27920	0.61979	-0.08597
S	1.14592	-1.11410	-0.22769
C	-2.43568	0.63670	0.07179
H	-2.62353	1.42028	-0.67403
H	-3.07680	-0.22400	-0.14042
H	-2.65067	1.02679	1.07717
C	-0.93597	-3.03130	-2.38957
H	-0.45291	-2.05647	-2.51062
H	-0.19809	-3.83186	-2.54053
H	-1.74530	-3.13384	-3.12571
C	-3.61946	-5.10234	1.20735
H	-4.01268	-5.00246	2.22066
C	-2.59808	-5.37004	-1.45853
C	-3.91565	-6.21311	0.42396
H	-2.21376	-5.48733	-2.47236
H	-4.55178	-7.00068	0.83398
C	-3.41025	-6.34386	-0.89035
H	-3.66647	-7.23062	-1.47376
C	2.44181	1.39899	-0.06540
H	3.43269	0.94864	-0.14694
C	2.28193	2.77463	0.06727
C	-0.15628	2.59356	0.15631
H	3.16656	3.41476	0.09226
H	-1.13627	3.06233	0.24940
C	1.00057	3.36204	0.17309
H	0.91817	4.44614	0.27755

14

C	-7.83965	1.80649	1.55149
C	-6.61494	1.28571	1.97839
C	-7.89104	2.82595	0.58210
C	-5.45837	2.80091	0.51963
C	-5.40297	1.77444	1.45953
H	-4.44623	1.36320	1.78895
H	-8.76875	1.41604	1.97448
H	-6.59498	0.49130	2.72873
C	-6.69461	3.32073	0.07823
H	-8.84836	3.21426	0.22737
N	-6.47166	4.27583	-0.95736
C	-5.04637	4.56098	-0.85114
N	-4.43255	3.44723	-0.17476
C	-7.03826	3.83383	-2.23990
H	-8.10561	3.61206	-2.09823
H	-6.54793	2.91479	-2.61758
H	-6.95279	4.62075	-2.99280
C	-3.30200	2.69237	-0.68289
H	-3.56428	1.62318	-0.77923
H	-2.41257	2.76342	-0.02981
H	-3.02247	3.07057	-1.67650
C	-4.44827	5.78088	-0.92618
N	-4.97237	6.92728	-1.54917
C	-4.15093	8.15190	-1.30369
C	-3.26770	7.68316	-0.14056
C	-3.11108	6.14856	-0.25181
H	-3.78227	7.91470	0.80490
H	-2.29554	8.19755	-0.11843
C	-4.99013	9.36289	-0.88296
H	-5.57930	9.15997	0.02001
H	-5.67051	9.67360	-1.68788
H	-4.31807	10.20801	-0.66766
C	-3.33536	8.58284	-2.53700
H	-2.77301	9.49983	-2.30336
H	-4.00430	8.80340	-3.38166
H	-2.61426	7.82294	-2.85649
C	-1.86244	5.78362	-1.08171
H	-1.93985	6.10537	-2.12895
H	-1.68507	4.70137	-1.07753
H	-0.97170	6.26721	-0.64713
C	-2.94458	5.57981	1.16967
H	-2.16266	6.15374	1.69433
H	-3.88061	5.66859	1.74061
H	-2.64477	4.52560	1.17829
C	-5.98645	6.91279	-2.55998
C	-7.31257	7.31573	-2.24870
C	-8.26887	7.35091	-3.27326
C	-7.95403	6.97528	-4.57522
C	-6.66379	6.54257	-4.86761
C	-5.66594	6.50114	-3.88394
H	-9.28608	7.67253	-3.03785
H	-8.71576	7.00995	-5.35827
H	-6.42440	6.21953	-5.88310
C	-7.78010	7.65983	-0.83963
C	-8.38443	9.07172	-0.75426

H	-7.71180	9.84142	-1.15670	C	-1.95601	6.12222	0.27082
H	-8.61468	9.33024	0.29235	H	-1.52122	6.16525	-0.73650
H	-9.32946	9.13316	-1.31749	H	-1.87122	5.09861	0.65786
C	-8.79821	6.62930	-0.32374	H	-1.33382	6.75351	0.92219
H	-6.90311	7.60125	-0.18273	C	-3.90163	6.45762	1.77994
H	-9.69293	6.59349	-0.96624	H	-3.26286	7.02279	2.47712
H	-9.13167	6.89685	0.69293	H	-4.93495	6.81818	1.90079
H	-8.34078	5.63266	-0.29340	H	-3.86418	5.39777	2.07782
C	-4.30215	5.94818	-4.28538	C	-6.15137	6.86276	-2.30635
C	-4.35276	4.42680	-4.50936	C	-7.35813	7.59485	-2.08614
H	-4.59250	3.89691	-3.57809	C	-8.40025	7.45447	-3.01226
H	-3.37966	4.05792	-4.87320	C	-8.29491	6.61700	-4.11771
H	-5.11424	4.15680	-5.25900	C	-7.12456	5.89356	-4.31044
C	-3.73291	6.64684	-5.53101	C	-6.03855	5.99445	-3.42802
H	-3.61407	6.12305	-3.45296	H	-9.32367	8.01449	-2.85664
H	-4.33022	6.41746	-6.42776	H	-9.12331	6.52574	-4.82400
H	-2.70518	6.30088	-5.72824	H	-7.04271	5.23559	-5.17715
H	-3.71057	7.74099	-5.41832	C	-7.63206	8.52687	-0.90238
				C	-7.89471	9.97662	-1.36599
14^{rad}				H	-7.15239	10.34046	-2.08441
C	-6.91595	0.58432	-0.12218	H	-7.90243	10.65783	-0.50047
C	-5.58206	0.15569	-0.26050	H	-8.87965	10.05264	-1.85207
C	-7.25251	1.93984	-0.12422	C	-8.85550	8.09782	-0.06515
C	-4.87133	2.42135	-0.40276	H	-6.74819	8.51421	-0.24680
C	-4.53364	1.06722	-0.40192	H	-9.77342	8.12147	-0.67141
H	-3.50179	0.73018	-0.50837	H	-9.00216	8.80207	0.76812
H	-7.70697	-0.16005	-0.01331	H	-8.77096	7.09310	0.36699
H	-5.36056	-0.91357	-0.25639	C	-4.81964	5.13560	-3.75835
C	-6.20274	2.84852	-0.27064	C	-5.18300	3.63876	-3.75644
H	-8.28823	2.26793	-0.02747	H	-5.67821	3.32393	-2.82891
N	-6.18434	4.23862	-0.33557	H	-4.28366	3.01987	-3.90229
C	-4.90129	4.67893	-0.53656	H	-5.87232	3.39940	-4.57988
N	-4.09165	3.56287	-0.58292	C	-4.19765	5.50449	-5.11618
C	-7.32444	5.06343	0.00869	H	-4.05617	5.30303	-2.98960
H	-7.86388	4.59523	0.84426	H	-4.89585	5.29652	-5.94154
H	-8.00021	5.18296	-0.84840	H	-3.29063	4.90549	-5.29408
H	-6.96575	6.04682	0.32392	H	-3.91884	6.56624	-5.17376
C	-2.75651	3.46694	-1.15772				
H	-2.76290	2.68507	-1.93038	14^{biscat}			
H	-2.00941	3.20921	-0.39548	C	-6.67520	0.48816	-0.12096
H	-2.48611	4.41806	-1.62272	C	-5.34220	0.15980	-0.46633
C	-4.45297	6.03407	-0.62592	C	-7.10036	1.80718	0.00097
N	-5.04967	7.02488	-1.38405	C	-4.81032	2.46576	-0.58165
C	-4.06199	8.17857	-1.49037	C	-4.38356	1.13847	-0.70731
C	-3.45698	8.13688	-0.08547	H	-3.35982	0.87569	-0.97575
C	-3.40261	6.64500	0.33084	H	-7.38889	-0.31860	0.05696
H	-4.11558	8.69163	0.59988	H	-5.05789	-0.89203	-0.54321
H	-2.46827	8.61385	-0.05040	C	-6.13439	2.79219	-0.23781
C	-4.68459	9.52895	-1.81067	H	-8.12957	2.05102	0.26685
H	-5.30909	9.90454	-0.99430	N	-6.20887	4.18368	-0.22214
H	-5.27540	9.49358	-2.73611	C	-5.00199	4.69103	-0.54246
H	-3.87300	10.25417	-1.96837	N	-4.13499	3.67155	-0.76295
C	-3.03337	7.85754	-2.58572	C	-7.42739	4.91896	0.09200
H	-2.21745	8.59420	-2.55682	H	-7.93210	4.42610	0.93310
H	-3.50215	7.91197	-3.57746	H	-8.08941	4.94411	-0.78458
H	-2.59276	6.85951	-2.46790	H	-7.17152	5.93772	0.38376

C	-2.76751	3.71851	-1.28078				
H	-2.71552	3.09498	-2.18314	18			
H	-2.06638	3.33411	-0.52858	C	-2.70985	1.50856	0.36447
H	-2.49566	4.74122	-1.54739	N	-4.16746	2.88353	-0.64281
C	-4.58142	6.11916	-0.58752	C	-3.24637	3.71133	0.04732
N	-4.95541	6.95909	-1.50329	N	-2.35821	2.82647	0.73285
C	-3.93345	8.15082	-1.55051	C	-4.69262	3.26624	-1.94089
C	-3.51261	8.19020	-0.07438	H	-4.34427	2.56452	-2.71788
C	-3.70433	6.75140	0.48488	H	-4.30270	4.25721	-2.18699
H	-4.14410	8.89998	0.47825	H	-5.79113	3.30955	-1.95573
H	-2.47422	8.53121	0.02870	C	-2.08850	3.02429	2.15559
C	-4.49729	9.44729	-2.10336	H	-2.69421	2.33343	2.76800
H	-5.14613	9.97007	-1.39624	H	-2.36048	4.04893	2.43055
H	-5.03878	9.28310	-3.04560	H	-1.02568	2.86654	2.39804
H	-3.65297	10.11446	-2.32777	C	-3.14458	5.07953	0.05287
C	-2.79565	7.66502	-2.46039	N	-4.18723	6.04553	-0.20922
H	-2.00279	8.42630	-2.45835	C	-3.71916	7.35292	0.35042
H	-3.13259	7.53212	-3.49681	C	-2.25323	7.32508	-0.09573
H	-2.35502	6.72248	-2.10859	C	-1.79883	5.84042	-0.03079
C	-2.38348	6.05070	0.83432	H	-1.62535	7.98121	0.52478
H	-1.67170	6.04904	-0.00090	H	-2.18623	7.69322	-1.13117
H	-2.54054	5.02064	1.18473	C	-4.45959	8.57244	-0.19493
H	-1.91470	6.60294	1.66133	H	-4.28646	8.72448	-1.26684
C	-4.61058	6.76404	1.74998	H	-4.09949	9.46954	0.33224
H	-4.08639	7.32909	2.53584	H	-5.54305	8.49615	-0.01929
H	-5.56991	7.26943	1.56255	C	-3.80763	7.41030	1.88901
H	-4.80246	5.75061	2.13467	H	-3.35602	6.52527	2.35503
C	-6.11465	6.79383	-2.37728	H	-4.85087	7.48080	2.22174
C	-7.28277	7.52918	-2.03040	H	-3.27565	8.29782	2.26527
C	-8.42961	7.29417	-2.79932	C	-1.11832	5.44822	-1.36029
C	-8.42768	6.39611	-3.86443	H	-1.81976	5.57646	-2.19936
C	-7.25925	5.71737	-4.19589	H	-0.79695	4.39511	-1.33604
C	-6.07500	5.88969	-3.46413	H	-0.23063	6.07611	-1.55282
H	-9.34544	7.83715	-2.55911	C	-0.77682	5.64986	1.09969
H	-9.33750	6.23177	-4.44604	H	-1.20358	5.87318	2.08828
H	-7.26286	5.03675	-5.04837	H	0.07476	6.33125	0.93838
C	-7.37640	8.58853	-0.92790	H	-0.37630	4.62802	1.11399
C	-7.72253	9.96181	-1.54500	C	-3.79458	1.54841	-0.42997
H	-7.11580	10.19591	-2.42871	H	-2.16650	0.65346	0.75860
H	-7.57733	10.75989	-0.80083	H	-4.33577	0.73869	-0.91359
H	-8.77750	9.99230	-1.85738	C	-5.57217	5.70401	-0.32304
C	-8.40831	8.27388	0.17200	C	-6.25490	6.04390	-1.52939
H	-6.39825	8.66938	-0.43349	C	-7.58196	5.63440	-1.70717
H	-9.39012	8.01446	-0.25187	C	-8.24082	4.87064	-0.74727
H	-8.55157	9.15943	0.80868	C	-7.57903	4.54496	0.43243
H	-8.10201	7.45704	0.83938	C	-6.26268	4.96316	0.67753
C	-4.84102	5.11578	-3.91114	H	-8.10147	5.89406	-2.63254
C	-5.11808	3.60334	-3.98004	H	-9.26570	4.53048	-0.91839
H	-5.55514	3.21005	-3.05044	H	-8.09871	3.95836	1.19388
H	-4.19335	3.04800	-4.20105	C	-5.66790	4.62951	2.04152
H	-5.82434	3.36429	-4.78808	C	-6.38137	5.40752	3.16104
C	-4.33250	5.62466	-5.27265	H	-6.43389	6.48493	2.94837
H	-4.03821	5.28464	-3.17871	H	-5.85108	5.27382	4.11902
H	-5.09162	5.47281	-6.05496	H	-7.41445	5.04742	3.29718
H	-3.42872	5.07487	-5.57672	C	-5.69419	3.12787	2.36537
H	-4.09132	6.69830	-5.25301	H	-4.61841	4.93637	2.02414

H	-5.14934	2.93542	3.30423	C	-7.16226	5.27108	-3.05619
H	-5.23068	2.53190	1.57044	C	-7.43046	5.41015	-1.69833
H	-6.72367	2.76070	2.50925	C	-6.41667	5.68244	-0.77012
C	-5.59480	6.80802	-2.67411	H	-5.65100	5.32125	-4.58050
C	-6.33294	8.12781	-2.96582	H	-7.97137	5.05718	-3.75774
H	-7.30620	7.93748	-3.44763	H	-8.45797	5.30251	-1.34613
H	-5.74444	8.75803	-3.65268	C	-6.84061	5.84011	0.68971
H	-6.52623	8.70571	-2.05210	C	-7.79799	7.04112	0.83664
C	-5.49381	5.99331	-3.97735	H	-7.43597	7.93277	0.30886
H	-4.56955	7.03374	-2.35501	H	-7.93813	7.29778	1.89833
H	-5.04492	6.61288	-4.77088	H	-8.78934	6.79644	0.42453
H	-6.48446	5.66369	-4.33129	C	-7.53808	4.59673	1.27377
H	-4.86640	5.09952	-3.86687	H	-5.93819	6.03010	1.28812

18^{rad}

C	-1.88786	2.11005	-1.74018
N	-3.76212	2.83203	-0.82635
C	-2.85410	3.84204	-0.66996
N	-1.69523	3.38694	-1.24710
C	-5.08710	2.79542	-0.23181
H	-5.25627	1.80799	0.21989
H	-5.86143	3.00856	-0.97947
H	-5.12681	3.55801	0.54789
C	-0.50475	4.17233	-1.54806
H	-0.19139	3.95510	-2.57762
H	0.31499	3.93316	-0.85896
H	-0.75206	5.23529	-1.46434
C	-3.03264	5.10321	0.00183
N	-4.01450	6.03170	-0.30502
C	-3.57568	7.36593	0.25898
C	-2.92784	6.90846	1.57511
C	-2.32993	5.49569	1.31487
H	-3.69861	6.85213	2.35819
H	-2.16573	7.62148	1.91840
C	-2.52920	8.00894	-0.66873
H	-1.70369	7.31818	-0.88723
H	-2.10362	8.89927	-0.18211
H	-2.97504	8.32532	-1.62058
C	-4.71365	8.35120	0.47197
H	-5.41155	8.01961	1.24686
H	-5.26907	8.52999	-0.46045
H	-4.28878	9.31113	0.80045
C	-0.79518	5.53461	1.29879
H	-0.43376	5.89806	2.27288
H	-0.39846	6.21138	0.53078
H	-0.36284	4.53448	1.15003
C	-2.77606	4.51013	2.41636
H	-3.87372	4.46762	2.48998
H	-2.38419	4.82930	3.39593
H	-2.39924	3.49309	2.21898
C	-3.18309	1.77122	-1.49343
H	-1.09686	1.56282	-2.24520
H	-3.73612	0.86574	-1.72766
C	-5.08284	5.82543	-1.24860
C	-4.80357	5.70254	-2.63466
C	-5.85753	5.41673	-3.51301

C	-7.16226	5.27108	-3.05619
C	-7.43046	5.41015	-1.69833
C	-6.41667	5.68244	-0.77012
H	-5.65100	5.32125	-4.58050
H	-7.97137	5.05718	-3.75774
H	-8.45797	5.30251	-1.34613
C	-6.84061	5.84011	0.68971
C	-7.79799	7.04112	0.83664
H	-7.43597	7.93277	0.30886
H	-7.93813	7.29778	1.89833
H	-8.78934	6.79644	0.42453
C	-7.53808	4.59673	1.27377
H	-5.93819	6.03010	1.28812
H	-7.93751	4.82717	2.27365
H	-6.86990	3.73349	1.38626
H	-8.38846	4.28214	0.64969
C	-3.42475	5.90701	-3.24665
C	-3.39761	7.18027	-4.11161
H	-4.03406	7.06398	-5.00242
H	-2.37515	7.39506	-4.46150
H	-3.76679	8.05691	-3.55907
C	-2.97864	4.69337	-4.07689
H	-2.70676	6.04347	-2.42964
H	-1.94040	4.82096	-4.42371
H	-3.60201	4.57118	-4.97545
H	-3.04487	3.75544	-3.50860

18^{biscat}

C	-3.49882	1.58261	1.15594
N	-3.78827	2.77992	-0.67473
C	-3.46905	3.64326	0.31344
N	-3.28715	2.91352	1.44311
C	-4.09304	3.10413	-2.06778
H	-3.60233	2.37227	-2.72152
H	-3.71251	4.09947	-2.29395
H	-5.17987	3.08807	-2.22396
C	-3.06883	3.38300	2.81815
H	-3.86760	2.97794	3.45124
H	-3.10729	4.47281	2.85477
H	-2.09399	3.03339	3.18105
C	-3.23740	5.11245	0.22559
N	-4.16867	5.98420	-0.01625
C	-3.66575	7.40737	0.41946
C	-2.16489	7.24028	0.15949
C	-1.84429	5.72952	0.31812
H	-1.57826	7.85436	0.85435
H	-1.92005	7.57503	-0.85896
C	-4.31364	8.56619	-0.31267
H	-3.97905	8.66156	-1.34906
H	-4.02318	9.48824	0.21193
H	-5.41009	8.50310	-0.28394
C	-3.99080	7.51828	1.91670
H	-3.56005	6.69640	2.50404
H	-5.07181	7.55083	2.09856
H	-3.56227	8.45882	2.29183
C	-1.09924	5.18494	-0.93116

H	-1.66801	5.36015	-1.85708	H	-2.90092	0.90622	-0.00572
H	-0.87120	4.11165	-0.84217	H	-2.92944	1.34178	1.72779
H	-0.14394	5.72456	-1.02077	H	-2.27036	2.46872	0.50730
C	-1.00299	5.42460	1.56722	N	-5.36685	5.85130	1.32889
H	-1.45925	5.81026	2.48837	C	-4.64291	7.15038	1.29058
H	-0.03204	5.92712	1.45026	C	-3.52822	6.86072	0.25734
H	-0.79442	4.35178	1.68054	C	-3.23120	5.34283	0.31853
C	-3.80717	1.49837	-0.17238	H	-2.62686	7.46471	0.43796
H	-3.42859	0.81142	1.92027	H	-3.89940	7.12730	-0.74416
H	-4.03900	0.63830	-0.79680	C	-5.52936	8.30116	0.81069
C	-5.50752	5.66831	-0.51067	H	-4.92651	9.22100	0.75305
C	-5.78289	5.92170	-1.88371	H	-6.36748	8.48452	1.49564
C	-7.03413	5.51200	-2.36335	H	-5.95132	8.10057	-0.18370
C	-7.97054	4.89260	-1.53946	C	-4.05684	7.50143	2.67580
C	-7.67881	4.68080	-0.19521	H	-3.60326	6.61880	3.14685
C	-6.44737	5.06128	0.35653	H	-4.83402	7.87570	3.35308
H	-7.28366	5.69097	-3.41067	H	-3.28529	8.28331	2.59052
H	-8.93659	4.58426	-1.94549	C	-2.93014	4.79529	-1.09018
H	-8.42953	4.21797	0.44709	H	-3.75471	5.00304	-1.78495
C	-6.23097	4.84625	1.84731	H	-2.77452	3.70910	-1.09089
C	-7.10687	5.80955	2.66913	H	-2.02221	5.27664	-1.49017
H	-6.98975	6.85367	2.34311	C	-2.01064	5.09960	1.23320
H	-6.84886	5.75053	3.73806	H	-2.14220	5.57340	2.21494
H	-8.17294	5.55644	2.56550	H	-1.10613	5.52761	0.76986
C	-6.50194	3.39040	2.26344	H	-1.82940	4.03269	1.40851
H	-5.18438	5.07988	2.08766	C	-6.79056	5.74185	1.18533
H	-6.22958	3.23223	3.31875	C	-7.63207	5.85702	2.31999
H	-5.95407	2.66744	1.64082	C	-9.01504	5.70118	2.16623
H	-7.56991	3.14193	2.17738	C	-9.57697	5.41610	0.92469
C	-4.85414	6.64517	-2.86261	C	-8.75044	5.31860	-0.19037
C	-5.51157	7.96863	-3.32038	C	-7.36348	5.49762	-0.09237
H	-6.30325	7.76784	-4.05791	H	-9.66311	5.78682	3.04147
H	-4.76726	8.61438	-3.81106	H	-10.65650	5.27622	0.82361
H	-5.97078	8.52899	-2.49641	H	-9.19511	5.11483	-1.16729
C	-4.48234	5.83843	-4.12531	C	-6.55159	5.47122	-1.38212
H	-3.91378	6.87854	-2.34058	C	-6.37315	4.05864	-1.96323
H	-3.98115	6.50315	-4.84455	H	-5.78258	3.41867	-1.29676
H	-5.37268	5.43062	-4.62726	H	-5.84226	4.10529	-2.92929
H	-3.78926	5.00657	-3.93892	H	-7.34980	3.58030	-2.14580
				C	-7.14513	6.41032	-2.44716
22				H	-5.55340	5.85068	-1.14185
C	-6.63194	2.07843	1.17324	H	-8.09091	6.01840	-2.85494
C	-5.45557	1.30885	0.53713	H	-6.44811	6.51767	-3.29424
N	-5.98796	3.12658	1.96097	H	-7.35053	7.41292	-2.03951
H	-7.27999	1.44139	1.79220	C	-7.08024	6.13125	3.70965
H	-7.25440	2.55463	0.40045	C	-7.32920	7.58724	4.14173
C	-4.84795	3.48400	1.16738	H	-6.95233	8.31168	3.40712
N	-4.37787	2.30710	0.46626	H	-6.84235	7.79826	5.10869
H	-5.70749	0.90715	-0.46019	H	-8.40899	7.77572	4.26076
H	-5.15413	0.45188	1.17132	C	-7.64724	5.18600	4.77922
C	-4.52663	4.78633	0.93842	H	-5.99639	5.96277	3.65174
C	-5.60269	2.70413	3.30567	H	-8.70342	5.41094	5.00087
H	-6.49611	2.38490	3.86475	H	-7.08624	5.29709	5.72170
H	-5.15240	3.55313	3.83891	H	-7.58677	4.13745	4.46131
H	-4.87315	1.86724	3.32636				
C	-3.06394	1.73889	0.69733				

22^{rad}

C	-6.68562	2.56477	0.72024	H	-4.21052	3.98577	-5.78307
C	-5.52715	1.56351	0.59024	H	-2.69913	3.55008	-4.97145
N	-6.04239	3.87597	0.51276	H	-3.23490	5.24768	-4.99562
H	-7.17739	2.52685	1.70063	C	-7.24268	7.16357	-0.69206
H	-7.45061	2.39981	-0.05449	C	-7.61898	8.64805	-0.82535
C	-4.81785	3.67644	-0.08187	H	-6.81038	9.25455	-1.25336
N	-4.51113	2.36104	-0.10777	H	-7.87317	9.06542	0.16198
H	-5.79717	0.68813	-0.01818	H	-8.50478	8.78073	-1.46470
H	-5.13739	1.19839	1.55735	C	-8.44606	6.39500	-0.10667
C	-4.00429	4.75206	-0.55572	H	-6.40577	7.07984	0.01205
C	-6.11864	4.83292	1.61924	H	-9.34054	6.54859	-0.72943
H	-7.16354	5.09360	1.81863	H	-8.68509	6.75583	0.90688
H	-5.57914	5.74797	1.35503	H	-8.25568	5.31331	-0.06779
H	-5.67187	4.40736	2.53631				
C	-3.38527	1.71769	-0.74887	22 biscat			
H	-3.72406	0.80408	-1.25804	C	-6.10979	1.79019	0.27788
H	-2.61286	1.43981	-0.01212	C	-4.80228	1.21407	-0.28569
H	-2.94939	2.38819	-1.49393	N	-5.80895	3.23347	0.38953
N	-4.55868	5.81869	-1.21893	H	-6.38107	1.38331	1.26205
C	-3.57274	6.96971	-1.31597	H	-6.96796	1.65913	-0.40125
C	-2.58310	6.59166	-0.20370	C	-4.67655	3.51491	-0.23585
C	-2.57029	5.04719	-0.08687	N	-4.05593	2.42858	-0.68957
H	-2.94390	7.01796	0.74533	H	-4.95292	0.55958	-1.15569
H	-1.58164	7.00200	-0.39118	H	-4.21029	0.66402	0.46413
C	-2.93786	7.02361	-2.71316	C	-4.07662	4.88663	-0.39191
H	-2.17752	7.81771	-2.73746	C	-6.78753	4.14545	0.94877
H	-3.69629	7.25991	-3.47285	H	-7.64867	4.24401	0.27112
H	-2.45015	6.08519	-2.99700	H	-6.33544	5.12729	1.09799
C	-4.21068	8.32804	-1.03699	H	-7.12882	3.75923	1.92055
H	-4.67308	8.37427	-0.04203	C	-2.77581	2.28295	-1.36822
H	-4.96127	8.58269	-1.79488	H	-2.91641	1.65816	-2.26003
H	-3.42218	9.09468	-1.08213	H	-2.04721	1.79639	-0.70287
C	-1.43109	4.45376	-0.94798	H	-2.38712	3.25398	-1.68349
H	-1.60088	4.57075	-2.02600	N	-4.44432	5.70906	-1.32140
H	-1.27049	3.38903	-0.73777	C	-3.34271	6.81729	-1.49869
H	-0.49335	4.97388	-0.69912	C	-2.78075	6.84624	-0.06975
C	-2.34893	4.61120	1.37244	C	-3.00325	5.43054	0.53549
H	-3.11014	5.03601	2.04336	H	-3.32098	7.59601	0.52563
H	-1.36336	4.95603	1.72231	H	-1.71991	7.12880	-0.06654
H	-2.36954	3.51569	1.47911	C	-2.33107	6.26015	-2.50841
C	-5.64769	5.72415	-2.17538	H	-1.48376	6.95836	-2.56163
C	-6.82499	6.50181	-2.00157	H	-2.76295	6.18436	-3.51326
C	-7.74944	6.56068	-3.05387	H	-1.93545	5.27912	-2.21438
C	-7.56441	5.84759	-4.23227	C	-3.88022	8.14130	-2.00779
C	-6.45373	5.02040	-4.35552	H	-4.43952	8.69589	-1.24937
C	-5.48121	4.93413	-3.34979	H	-4.50643	8.00270	-2.90018
H	-8.65073	7.16305	-2.93205	H	-3.02392	8.76261	-2.30719
H	-8.29564	5.91718	-5.04084	C	-1.71847	4.58701	0.63138
H	-6.32753	4.42991	-5.26463	H	-1.18268	4.51664	-0.32336
C	-4.33932	3.95195	-3.59502	H	-1.92169	3.57395	1.00780
C	-4.87484	2.50826	-3.58575	H	-1.04414	5.07089	1.35198
H	-5.39679	2.27049	-2.64756	C	-3.64243	5.52135	1.94662
H	-4.05525	1.78674	-3.72931	H	-4.55832	6.13013	1.94861
H	-5.59306	2.35248	-4.40468	H	-2.91916	6.01336	2.61458
C	-3.58046	4.20783	-4.90806	H	-3.86502	4.52869	2.36704
H	-3.61995	4.04834	-2.77220	C	-5.70866	5.57325	-2.05919

C	-6.82422	6.30778	-1.56667	H	-4.27117	10.32111	-0.98975
C	-8.07042	6.02055	-2.14031	C	-1.85891	5.90936	-0.82251
C	-8.21237	5.07708	-3.15527	H	-1.87217	6.07658	-1.90778
C	-7.08934	4.42937	-3.66107	H	-1.60013	4.85836	-0.64839
C	-5.80947	4.66211	-3.13673	H	-1.04307	6.51704	-0.39859
H	-8.94964	6.56232	-1.78774	C	-3.16039	5.75150	1.30530
H	-9.19820	4.86603	-3.57616	H	-2.35043	6.24990	1.86298
H	-7.20552	3.73472	-4.49404	H	-4.11112	5.95377	1.82092
C	-4.62122	3.99468	-3.81485	H	-2.98536	4.66802	1.33996
C	-4.84197	2.49308	-4.05476	C	-5.98888	6.89984	-2.60033
H	-5.18304	1.97286	-3.14666	C	-7.30251	7.40879	-2.39009
H	-3.91553	2.01788	-4.41107	C	-8.21584	7.38369	-3.45166
H	-5.59898	2.31295	-4.83160	C	-7.87834	6.85167	-4.69203
C	-4.31360	4.70444	-5.14946	C	-6.61381	6.30251	-4.87424
H	-3.74281	4.11222	-3.16653	C	-5.65613	6.30639	-3.85128
H	-5.15712	4.59625	-5.84813	H	-9.22204	7.77826	-3.29464
H	-3.42382	4.26586	-5.62684	H	-8.60558	6.84845	-5.50799
H	-4.14006	5.78298	-5.01652	H	-6.35930	5.85145	-5.83583
C	-6.75311	7.46263	-0.56335	C	-7.80399	7.93134	-1.04639
C	-7.01081	8.79228	-1.31136	C	-8.35159	9.36588	-1.14729
H	-6.45850	8.86846	-2.25544	H	-7.63956	10.05705	-1.61790
H	-6.73658	9.64706	-0.67378	H	-8.60000	9.75656	-0.14680
H	-8.08052	8.88875	-1.55190	H	-9.27830	9.39392	-1.74285
C	-7.74800	7.38985	0.60951	C	-8.88889	7.02137	-0.44419
H	-5.74101	7.49200	-0.13080	H	-6.95317	7.91491	-0.35383
H	-8.78498	7.29167	0.25562	H	-9.75247	6.92532	-1.12217
H	-7.69406	8.32456	1.18702	H	-9.25714	7.45010	0.50282
H	-7.55556	6.57212	1.31437	H	-8.49580	6.01586	-0.24391
25				C	-4.32796	5.61182	-4.14152
C	-7.56867	0.91721	0.85950	C	-4.53236	4.09679	-4.32096
C	-6.27331	0.60979	1.28353	H	-5.00461	3.64719	-3.43802
C	-7.80351	2.04548	0.05892	H	-3.56825	3.59448	-4.50559
C	-5.42118	2.56594	0.15332	H	-5.18556	3.88687	-5.18322
C	-5.19049	1.42849	0.92895	C	-3.61615	6.18974	-5.37562
H	-4.18077	1.18674	1.26787	H	-3.67372	5.75424	-3.27428
H	-8.40462	0.27528	1.14718	H	-4.20048	6.01305	-6.29247
C	-6.72949	2.86119	-0.28748	H	-2.63749	5.70181	-5.51540
H	-8.80938	2.28022	-0.29778	H	-3.44758	7.27315	-5.28994
S	-6.75424	4.28126	-1.34474	H	-6.09603	-0.27292	1.90262
C	-5.03974	4.63512	-0.86215	C	-3.27833	8.46050	-2.60412
N	-4.44937	3.45947	-0.32410	H	-3.90461	8.66166	-3.48587
C	-3.24399	2.88125	-0.91421	H	-2.62536	7.61351	-2.83810
H	-3.44583	1.86155	-1.28691	H	-2.64184	9.34244	-2.43399
H	-2.41097	2.82378	-0.19229	25^{rad}			
H	-2.92556	3.50175	-1.76015	C	-7.59214	0.69721	0.08551
C	-4.46545	5.86231	-0.89619	C	-6.29757	0.33139	0.49315
N	-5.01628	6.98417	-1.54825	C	-7.84090	1.96399	-0.44153
C	-4.16978	8.20333	-1.37524	C	-5.47319	2.49532	-0.13406
C	-3.37828	7.82020	-0.11766	C	-5.22578	1.21685	0.38508
C	-3.19326	6.28401	-0.13665	H	-4.23182	0.92002	0.72152
H	-3.97892	8.09434	0.76371	H	-8.41306	-0.01510	0.18795
H	-2.42022	8.35482	-0.04197	C	-6.76956	2.85547	-0.54099
C	-4.97249	9.48429	-1.13142	H	-8.84027	2.25484	-0.77143
H	-5.59979	9.41624	-0.23394	S	-6.79548	4.47293	-1.19792
H	-5.60979	9.72549	-1.99291	C	-5.08077	4.69776	-0.80946

N	-4.53837	3.51115	-0.35467	H	-2.47056	7.33939	-2.74354
C	-3.12499	3.15686	-0.43222	H	-2.36431	9.09730	-2.52241
H	-3.04438	2.13314	-0.82230				
H	-2.63334	3.20224	0.55028	25 biscat			
H	-2.61935	3.82713	-1.12862	C	-7.19706	0.62415	-0.18244
C	-4.43532	5.95450	-0.87410	C	-5.92175	0.03650	-0.34351
N	-4.92954	6.99009	-1.60786	C	-7.36521	2.00311	-0.16144
C	-4.06817	8.23178	-1.50359	C	-4.94688	2.20447	-0.49500
C	-3.43824	7.97751	-0.13373	C	-4.78036	0.81469	-0.50261
C	-3.24940	6.44241	-0.00436	H	-3.79700	0.35802	-0.62734
H	-4.14055	8.32194	0.64079	H	-8.07072	-0.02088	-0.06959
H	-2.49632	8.52248	0.00816	C	-6.21773	2.79602	-0.32055
C	-4.85067	9.54272	-1.55309	H	-8.35515	2.44187	-0.03618
H	-5.49158	9.69393	-0.67809	N	-6.14564	4.19008	-0.34567
H	-5.46275	9.61024	-2.46327	C	-4.91984	4.67868	-0.56021
H	-4.12666	10.36988	-1.58096	S	-3.73162	3.43296	-0.68528
C	-1.82773	6.04257	-0.49561	C	-4.50977	6.09679	-0.64920
H	-1.77527	5.86550	-1.57816	N	-5.05883	7.00321	-1.41169
H	-1.45352	5.14898	0.01625	C	-4.14539	8.28470	-1.44583
H	-1.11916	6.85032	-0.26530	C	-3.42277	8.12617	-0.10821
C	-3.42526	6.02767	1.46690	C	-3.33197	6.61202	0.18217
H	-2.68018	6.55480	2.08263	H	-4.01069	8.62123	0.67938
H	-4.42464	6.29719	1.83996	H	-2.43338	8.60034	-0.12743
H	-3.28113	4.95053	1.62622	C	-4.88661	9.60097	-1.55650
C	-5.99704	6.86424	-2.56759	H	-5.50686	9.82138	-0.68196
C	-7.28260	7.37216	-2.24092	H	-5.48981	9.65280	-2.47022
C	-8.31719	7.17133	-3.16301	H	-4.12282	10.38996	-1.62712
C	-8.10183	6.49968	-4.36294	C	-1.95130	6.04173	-0.22699
C	-6.83530	6.00482	-4.66282	H	-1.73810	6.14389	-1.29845
C	-5.76160	6.16008	-3.77835	H	-1.82019	4.99254	0.06934
H	-9.31681	7.53913	-2.92527	H	-1.18694	6.61332	0.31968
H	-8.92593	6.35149	-5.06449	C	-3.57789	6.29629	1.67261
H	-6.67867	5.46863	-5.60060	H	-2.83626	6.84481	2.27256
C	-7.62166	8.07518	-0.92823	H	-4.57606	6.61917	2.00682
C	-8.22133	9.47027	-1.18374	H	-3.45272	5.22590	1.89360
H	-7.60040	10.07318	-1.86024	C	-6.13869	6.82254	-2.37638
H	-8.33380	10.01914	-0.23582	C	-7.36678	7.53431	-2.20869
H	-9.22158	9.39575	-1.63851	C	-8.32260	7.40163	-3.22361
C	-8.57252	7.25281	-0.04162	C	-8.10238	6.61830	-4.35224
H	-6.69231	8.19380	-0.35799	C	-6.90981	5.91581	-4.47734
H	-9.49012	6.97213	-0.58252	C	-5.90213	5.98597	-3.50557
H	-8.87272	7.84800	0.83491	H	-9.27168	7.92911	-3.12387
H	-8.09691	6.33127	0.32166	H	-8.86507	6.55065	-5.13113
C	-4.43303	5.50602	-4.14956	H	-6.74700	5.29700	-5.36064
C	-4.56920	3.97440	-4.22817	C	-7.77639	8.39498	-1.00719
H	-4.92279	3.54329	-3.28084	C	-8.09155	9.85093	-1.42175
H	-3.60171	3.51417	-4.48451	H	-7.34075	10.29261	-2.08471
H	-5.28834	3.67771	-5.00636	H	-8.18038	10.48586	-0.52726
C	-3.87227	6.05413	-5.47251	H	-9.05575	9.89898	-1.94925
H	-3.70302	5.72834	-3.36114	C	-9.03708	7.86611	-0.28685
H	-4.54200	5.81924	-6.31417	H	-6.94845	8.39926	-0.27949
H	-2.89499	5.59649	-5.69283	H	-9.89982	7.84922	-0.96819
H	-3.73983	7.14566	-5.44798	H	-9.29458	8.54243	0.54147
H	-6.12480	-0.66150	0.91349	H	-8.93379	6.86020	0.13924
C	-3.06045	8.25826	-2.66430	C	-4.65555	5.14190	-3.76543
H	-3.58716	8.41481	-3.61617	C	-5.02763	3.64612	-3.80216

H	-5.63629	3.33633	-2.94116	H	-2.21459	6.91333	1.98806
H	-4.12261	3.02133	-3.83927	H	-3.98110	6.68780	2.09410
H	-5.61944	3.41489	-4.70003	H	-2.91227	5.28641	1.86347
C	-3.93882	5.51762	-5.07440	C	-6.14049	6.83507	-2.26263
H	-3.93234	5.29346	-2.95089	C	-7.40873	7.49125	-2.17012
H	-4.57925	5.32252	-5.94715	C	-8.36114	7.27716	-3.17646
H	-3.03150	4.90597	-5.19216	C	-8.12287	6.41785	-4.24241
H	-3.64111	6.57454	-5.10555	C	-6.90261	5.75845	-4.31406
C	-7.32548	5.01050	-0.07567	C	-5.89642	5.95137	-3.35589
H	-7.00683	6.01392	0.21179	H	-9.32657	7.78243	-3.10895
H	-7.88025	4.56002	0.75690	H	-8.88579	6.25902	-5.00884
H	-7.95575	5.05897	-0.97284	H	-6.71286	5.07826	-5.14644
H	-5.82995	-1.05188	-0.34258	C	-7.85273	8.40027	-1.01873
C	-3.25568	8.12266	-2.68410	C	-8.16802	9.83378	-1.49562
H	-3.85063	8.23184	-3.60076	H	-7.36771	10.27307	-2.10120
H	-2.72923	7.16260	-2.72023	H	-8.34704	10.49561	-0.63249
H	-2.50193	8.92305	-2.67486	H	-9.08276	9.84365	-2.10971
25 [(E) isomer]				C	-9.11715	7.89350	-0.29255
C	-7.30554	0.67471	-0.76656	H	-7.03357	8.43100	-0.28783
C	-6.13984	0.07246	-0.28709	H	-9.98033	7.86731	-0.97573
C	-7.39368	2.06855	-0.89674	H	-9.37525	8.58282	0.52737
C	-5.12029	2.23998	-0.05934	H	-9.00401	6.89340	0.14172
C	-5.03509	0.85746	0.07545	C	-4.59186	5.19113	-3.60664
H	-4.12758	0.39346	0.46863	C	-4.80167	3.66742	-3.61838
H	-8.16069	0.05604	-1.04872	H	-5.19331	3.29555	-2.66689
C	-6.29333	2.85454	-0.54351	H	-3.84797	3.15576	-3.82612
H	-8.29963	2.53669	-1.28546	H	-5.51049	3.36785	-4.40621
N	-6.23595	4.24710	-0.56264	C	-3.93961	5.60368	-4.94044
C	-4.95387	4.77661	-0.28023	H	-3.89487	5.41536	-2.79272
S	-3.90447	3.43959	0.37471	H	-4.55349	5.27719	-5.79498
C	-4.49119	6.03122	-0.52594	H	-2.95377	5.12155	-5.04337
N	-5.13634	7.07650	-1.25400	H	-3.79778	6.68911	-5.02812
C	-4.20228	8.24694	-1.41625	C	-7.42831	4.97602	-0.16303
C	-3.26658	8.06251	-0.21890	H	-7.12737	5.96419	0.19467
C	-3.16695	6.55268	0.06686	H	-7.94731	4.44680	0.65699
H	-3.71243	8.56699	0.65249	H	-8.12588	5.10605	-1.00183
H	-2.28173	8.51929	-0.39668	H	-6.08299	-1.01374	-0.18585
C	-4.88402	9.61083	-1.32929	C	-3.45541	8.21377	-2.76001
H	-5.44632	9.73749	-0.39494	H	-4.16557	8.32378	-3.59225
H	-5.55442	9.77678	-2.18011	H	-2.89737	7.28490	-2.90880
H	-4.10878	10.39220	-1.36889	H	-2.73983	9.04858	-2.81387
C	-1.91476	5.94501	-0.60131				
H	-1.86661	6.17065	-1.67456				
H	-1.88342	4.85273	-0.48552				
H	-1.01016	6.36302	-0.12924				
C	-3.06740	6.33941	1.58925				

5. References

- 1 D. L. Lichtenberger, R. L. Johnston, K. Hinkelmann, T. Suzuki and F. Wudl, *J. Am. Chem. Soc.*, 1990, **112**, 3302.
- 2 T. Murata, Y. Morita and K. Nakasuji, *Tetrahedron*, 2005, **61**, 6056.
- 3 J. Broggi, T. Terme and P. Vanelle, *Angew. Chem. Int. Ed.*, 2014, **53**, 384.
- 4 Y. Morita, E. Miyazaki, K. Fukui, S. Maki and K. Nakasuji, *Bull. Chem. Soc. Jpn.*, 2005, **78**, 2014.
- 5 J. Pak, R. Ali and J. S. Park, *Bull. Korean Chem. Soc.*, 2016, **37**, 732.
- 6 L. Boudiba, L. Kaboub, A. Gouasmia and J. M. Fabre, *Synthesis*, 2005, **2005**, 1291.
- 7 T. M. Bockman and J. K. Kochi, *J. Org. Chem.*, 1990, **55**, 4127.
- 8 J. R. Ames, M. A. Houghtaling, D. L. Terrian and T. P. Mitchell, *Can. J. Chem.*, 1997, **75**, 28.
- 9 J. A. Murphy, J. Garnier, S. R. Park, F. Schoenebeck, S. Z. Zhou and A. T. Turner, *Org. Lett.*, 2008, **10**, 1227.
- 10 S. Hünig, H. Schlaf, G. Kießlich and D. Scheutzow, *Tetrahedron Lett.*, 1969, **10**, 2271.
- 11 L. Krause, R. Herbst-Irmer, G. M. Sheldrick and D. Stalke, *J. Appl. Crystallogr.*, 2015, **48**, 3.
- 12 G. M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3.
- 13 G. M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3.
- 14 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339.
- 15 V. Khodorkovsky, A. Edzifna and O. Neilands, *J. Mol. Electron.*, 1989, **5**, 33.
- 16 S. Hünig, J. Groß and W. Schenk, *Liebigs Ann.*, 1973, 324.
- 17 J. Garnier, A. R. Kennedy, L. E. A. Berlouis, A. T. Turner and J. A. Murphy, *Beilstein J. Org. Chem.*, 2010, **6**, 73.
- 18 D. J. Sandman, T. J. Holmes and D. E. Warner, *J. Org. Chem.*, 1979, **44**, 880.
- 19 Z. Shi, V. Gouille and R. P. Thummel, *Tetrahedron Lett.*, 1996, **37**, 2357.
- 20 V. Gouille, S. Chirayil and R. P. Thummel, *Tetrahedron Lett.*, 1990, **31**, 1539.
- 21 D. Munz, J. Chu, M. Melaimi and G. Bertrand, *Angew. Chem. Int. Ed.*, 2016, **55**, 12886.
- 22 S. Hünig, D. Scheutzow, H. Schlaf and H. Pütter, *Liebigs Ann.*, 1974, 1436.
- 23 A. Stanger, *J. Org. Chem.*, 2010, **75**, 2281.