Supplementary Information (SI) for New Journal of Chemistry.

Supporting information

Structures, Aromaticity, AIM, and NBO analyses of hydroxy and mercapto azaazulene: A DFT Study

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Computational Methods

$$\text{percentage contents } (T\%) = (e^{-\frac{\Delta G_i}{RT}} / \sum_i e^{-\frac{\Delta G_i}{RT}}) \times 100 \quad (1)$$

where R represents the gas constant and T represents the temperature in Kelvin.

$$HOMA = 1 - \frac{1}{n}\sum_{j=1}^{n} \alpha_i (R_{opt,i} - R_j)^2 \quad (2)$$

Where n is the number of bonds forming the ring, α_i is the normalization constant (α_{CC}= 257.7 and α_{CN} = 93.52). R_{opt} denotes the optimized bond length; for the C−C bond, R_{opt} = 1.388 Å and the C−N bond, R_{opt} = 1.334 Å.

$$I_{ring}(A) = \sum_{i_1, i_2, \ldots, i_N} n_{i_1} \ldots n_{i_N} S_{i_1 i_2}(A_1) S_{i_2 i_3}(A_2) \ldots S_{i_N i_1}(A_N) \quad (3)$$

Where $n_i \in [0.1]$ is the occupancy of MO, i and S_{ij} is the overlap between MOs i and j within the molecular space allocated to atom A. MCI is calculated by adding up all the possible I_{ring} values derived from permutations of the atoms in A. MCI is defined as:

$$MCI(A) = \frac{1}{2N}\sum_{P(A)} I_{ring}(A) \quad (4)$$

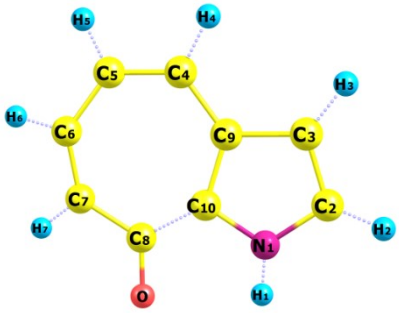
Where P(A) is an operator that acts on A that generates all the N permutations of its atoms.

$$FLU = \frac{1}{n}\sum_{A-B}^{ring} \left[\left(\frac{FLU(B)}{FLU(A)} \right)^{\alpha} \left(\frac{\delta(A,B) - \delta_{ref}(A,B)}{\delta_{ref}(A,B)} \right) \right]^2 \quad (5)$$

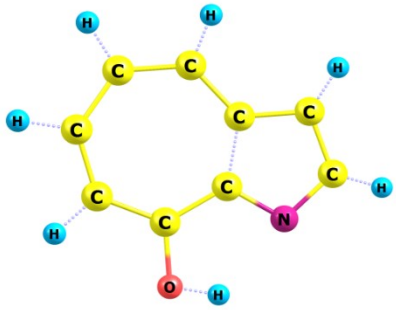
Where the summation is applied to all neighbouring pairs of atoms around the ring, n equals the number of atoms in the ring, δ_{ref} is the reference delocalization index value [δ_{ref}(C-C) = 1.468 and δ_{ref}(C-N) = 1.566], α is a basic function to make sure that the atomic valence ratio is higher than one. While FLU-π is determined by considering only the fluctuation of π electrons.

$$\alpha = \begin{cases} 1 & FLU(B) > FLU(A) \\ -1 & FLU(B) \leq FLU(A) \end{cases} \quad (6)$$

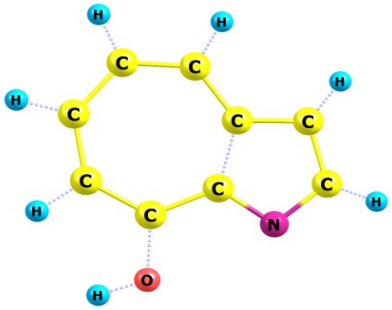
FLU in aromatic species is close to zero, while it is higher than zero in non-aromatic or antiaromatic species.



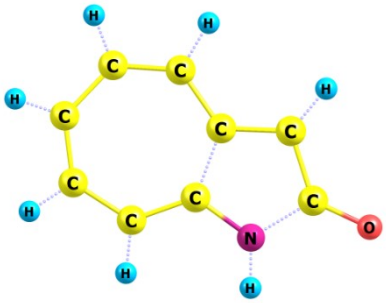
8O-AZ



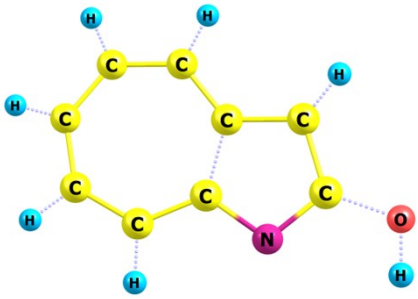
8OH-AZ



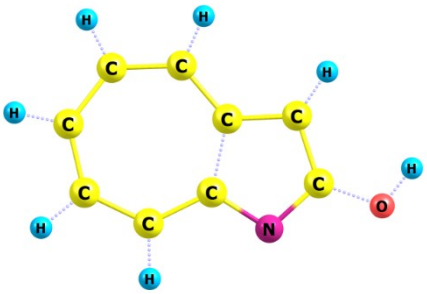
8OH-AZ-R



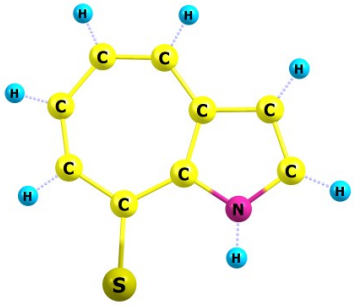
2O-AZ



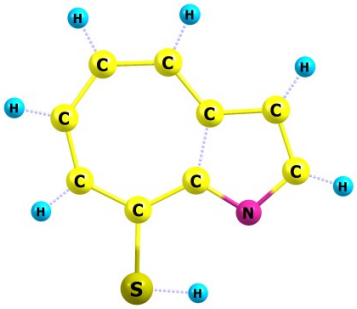
2OH-AZ



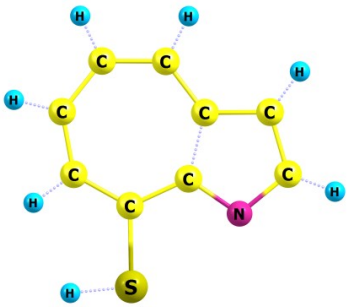
2OH-AZ-R



8S-AZ



8SH-AZ



8SH-AZ-R

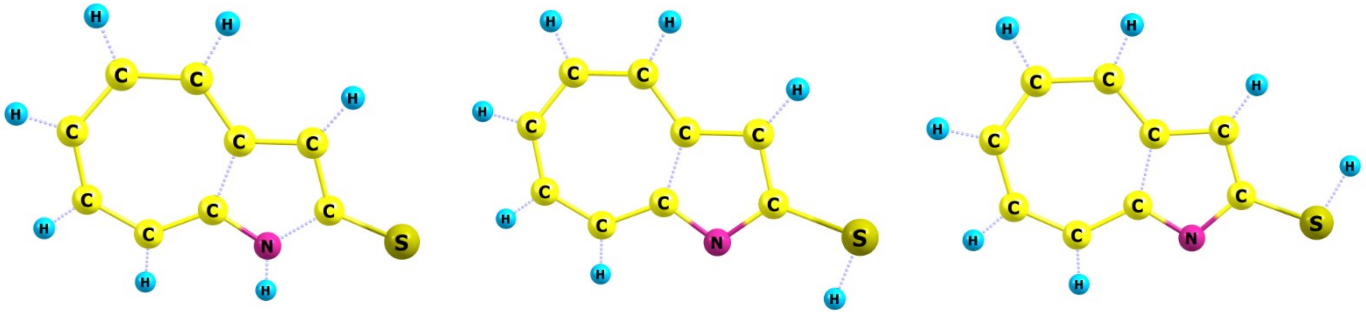


Fig. S1 Optimized structures for the investigated tautomers and rotamers at B3LYP/6-311+G(d,p).

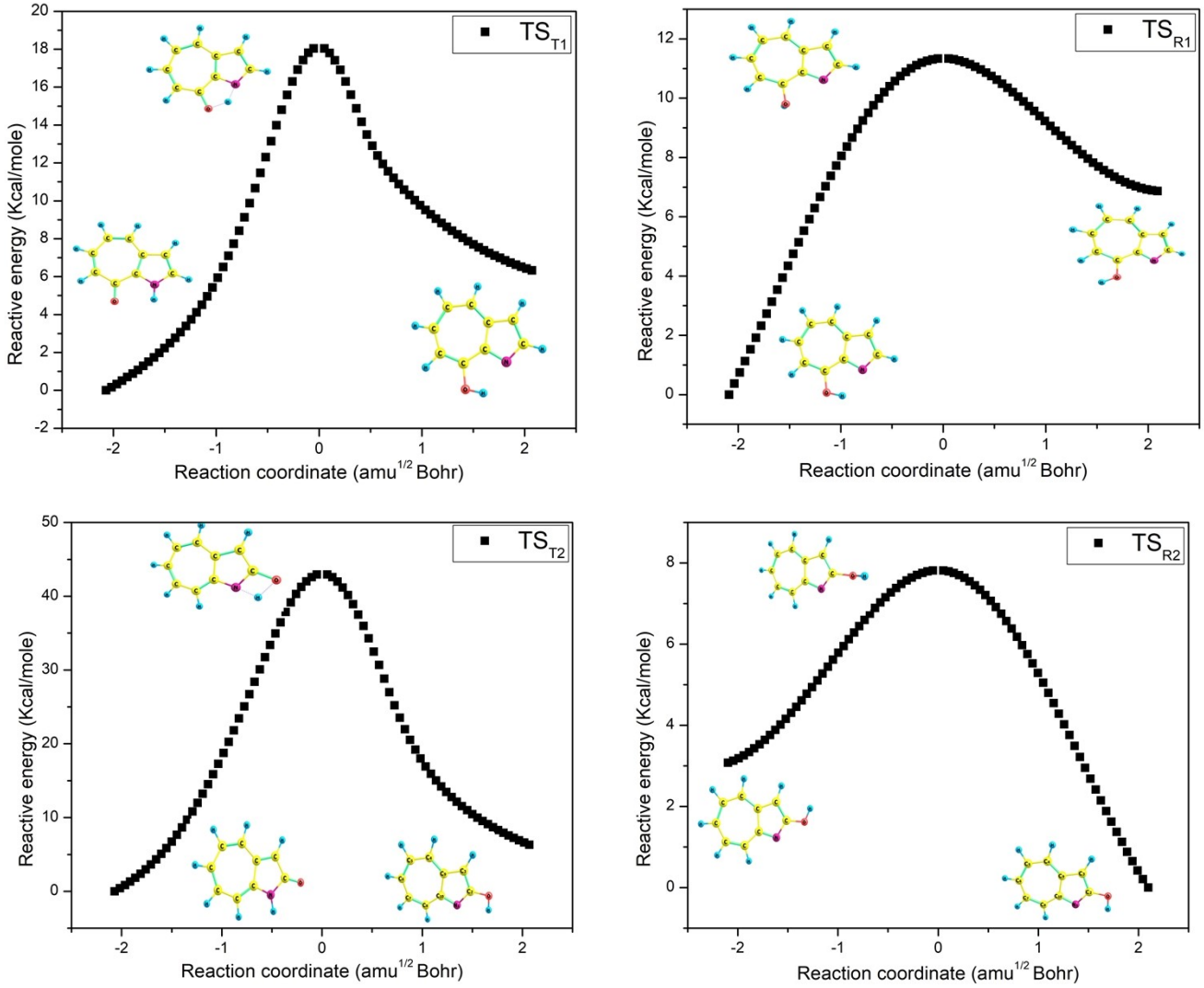


Fig. S2 Relative energy profiles from the IRC calculation for tautomerization and rotamerization of **8OH-AZ and 2OH-AZ** at the B3LYP/6-311+G(d,p) level.

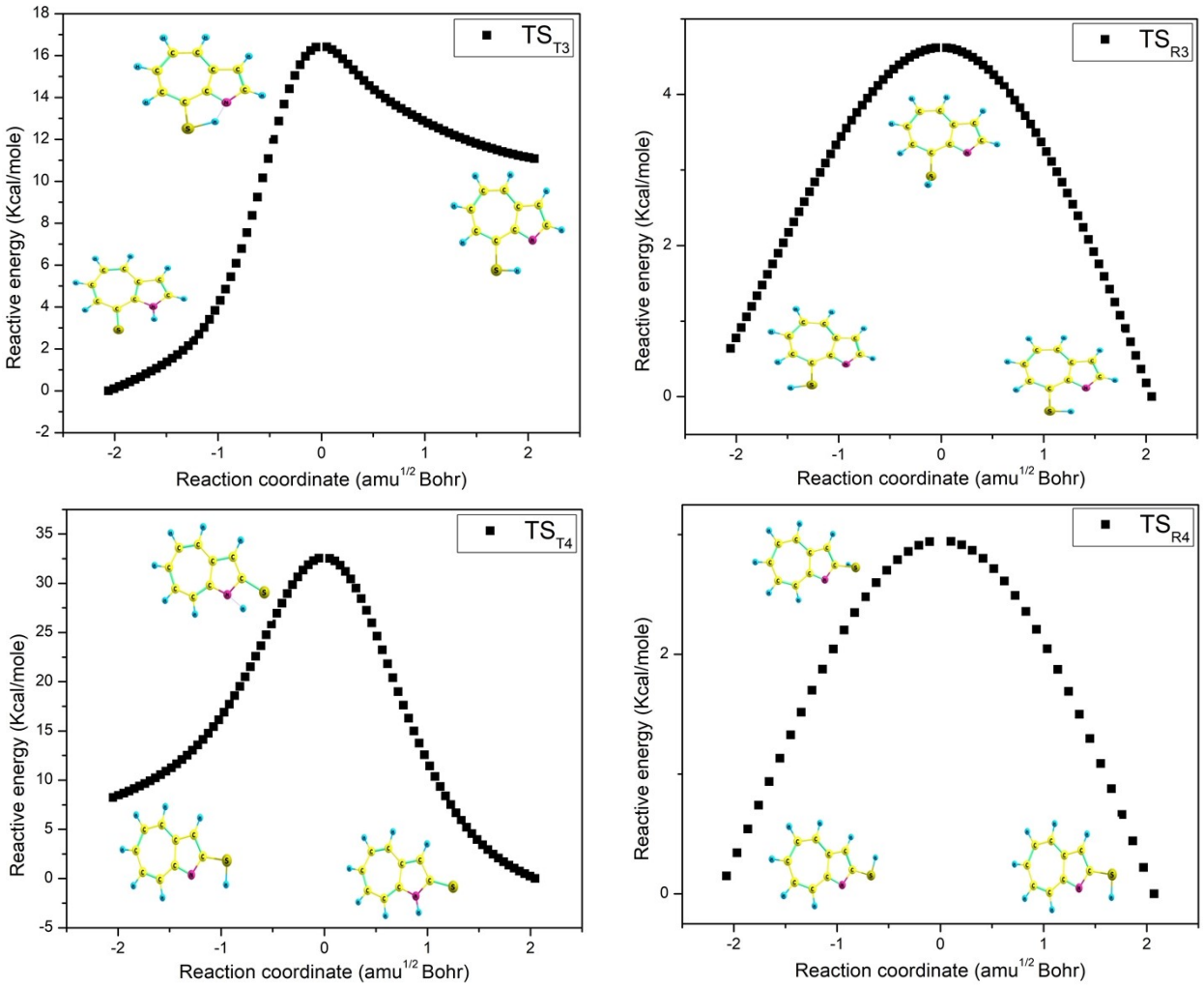


Fig. S3 Relative energy profiles from the IRC calculation for tautomerization and rotamerization of **8SH-AZ and 2SH-AZ** at the B3LYP/6-311+G(d,p) level.

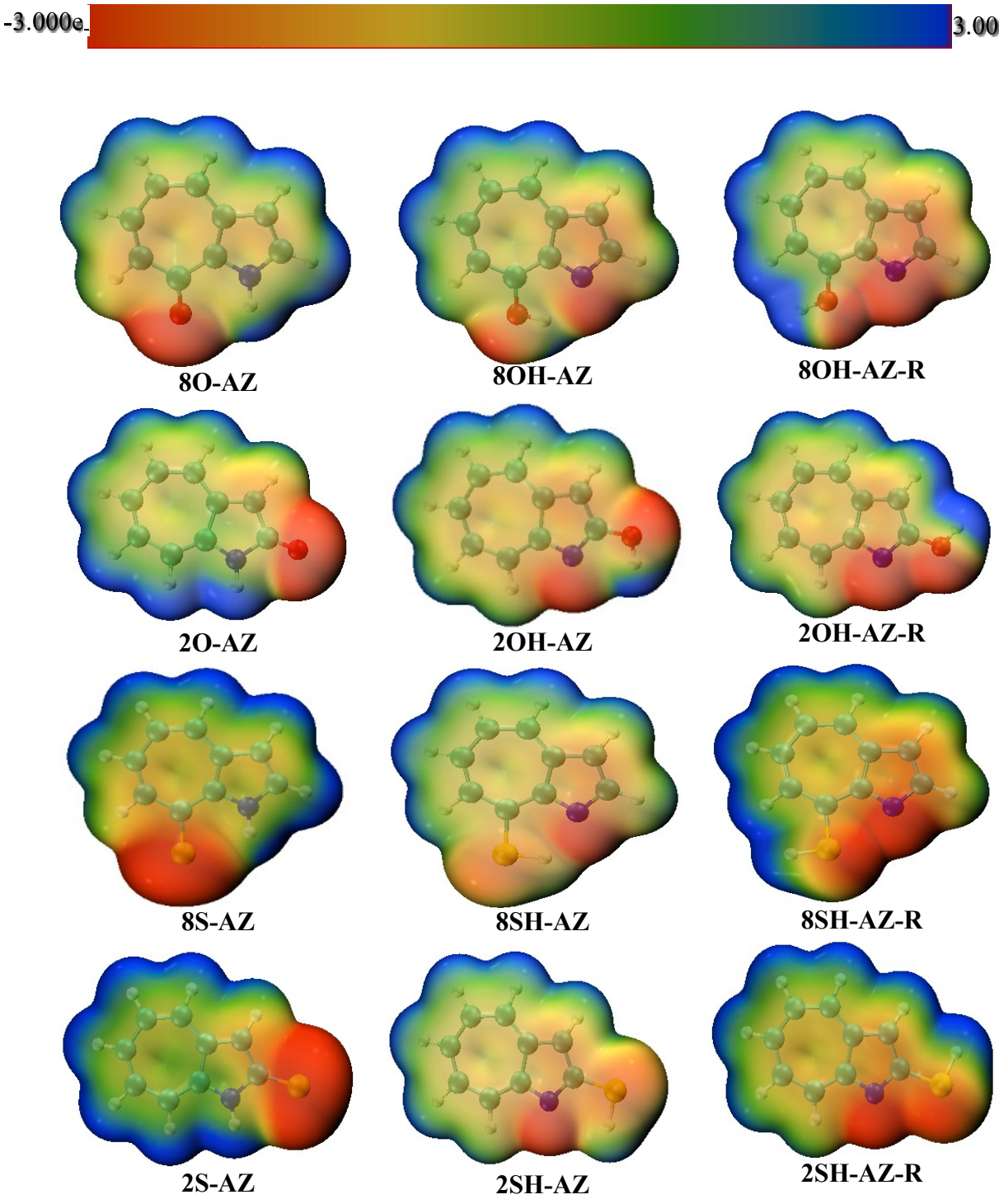

-3.000e-
3.000e-
8O-AZ
8OH-AZ
8OH-AZ-R
2O-AZ
2OH-AZ
2OH-AZ-R
8S-AZ
8SH-AZ
8SH-AZ-R
2S-AZ
2SH-AZ
2SH-AZ-R

Fig. S4 Electrostatic potential surface of the studied structures at B3LYP/6-311+G(d,p) in the gas phase.

Table S1 Geometrical parameters for the investigated tautomers and rotamers were calculated at B3LYP/6-311+G(d,p) in the gas phase, bond lengths R in Å and bond angles < in degrees.

Parameters	**8O-AZ**	**8OH-AZ**	**8OH-AZ-R**	**2O-AZ**	**2OH-AZ**	**2OH-AZ-R**
R(N1-C2)	1.369	1.357	1.355	1.426	1.340	1.337
R(N1-C10)	1.363	1.347	1.343	1.363	1.354	1.350
R(C2-C3)	1.373	1.395	1.394	1.450	1.407	1.412
R(C8-C10)	1.457	1.404	1.406	1.373	1.387	1.389
R(C8/C2-O)	1.240	1.341	1.351	1.217	1.340	1.345
R(N/O-H)	1.011	0.980	0.964	1.009	0.967	0.963
R(N/O…H)	2.393	2.041		2.634	2.324	
R(N…O)	2.702	2.651	2.696	2.330	2.331	2.303
<(C2-N1-C10)	110.54	105.68	105.85	112.58	105.49	105.50
<(N1-C2-C3)	108.21	112.81	113.38	104.02	114.61	114.41
<(N1-C2-O)	-	-	-	123.37	120.81	118.32
<(C8/C2-O-H)	-	105.75	109.94	-	107.21	109.56
<(C10-C8-O)	118.92	116.47	115.20	-	-	-
<(C9-C10-N1)	107.29	111.32	110.77	105.68	109.96	110.45
	8S-AZ	**8SH-AZ**	**8SH-AZ-R**	**2S-AZ**	**2SH-AZ**	**2SH-AZ-R**
R(N1-C2)	1.367	1.355	1.354	1.399	1.348	1.347
R(N1-C10)	1.363	1.347	1.344	1.363	1.351	1.350
R(C2-C3)	1.373	1.393	1.395	1.429	1.408	1.409
R(C8-C10)	1.439	1.408	1.404	1.377	1.390	1.390
R(C8/C2-S)	1.692	1.765	1.774	1.665	1.759	1.761
R(N/S-H)	1.016	1.358	1.350	1.010	1.348	1.349
R(N/S…H)	2.530	2.107	-	2.895	2.574	-
R(N…S)	2.979	2.976	2.851	2.702	2.717	2.668
<(C2-N1-C10)	111.04	106.44	106.19	112.83	105.71	105.77
<(N1-C2-C3)	108.31	112.94	113.13	104.73	113.79	113.81
<(N1-C2-S)	-	-	-	123.49	121.40	117.72
<(C8/C2-S-H)	-	93.19	95.20	-	94.48	96.02
<(C10-C8-S)	119.90	118.11	113.88	-	-	-
<(C9-C10-N1)	106.50	110.12	110.44	105.39	110.29	110.30

Table S2 Absolute Gibbs free energy G (au) and relative Gibbs free energy ΔG (kcal/mol), at T = 298.15 K, for the investigated tautomers and rotamers, in the gas-phase calculated at the B3LYP / 6-311+G(d,p), M06-2X/6-311++G(2d,2p), G3MP2 levels of theory.

Tautomers	B3LYP / 6-311+G(d,p)		M062X/6-311++G(2d,2p)		G3MP2	
	G (au)	ΔG (Kcal/mol)	G (au)	ΔG (Kcal/mol)	G (au)	ΔG (Kcal/mol)
8O-AZ	-477.156708	0.00	-476.973536	0.00	-476.416906	0.00
8OH-AZ	-477.144592	7.60	-476.961723	7.41	-476.406403	6.59
8OH-AZ-R	-477.128116	17.94	-476.945852	17.37	-476.39084	16.36
2O-AZ	-477.155904	0.51	-476.967998	3.48	-476.413101	2.38
2OH-AZ	-477.144714	7.53	-476.960378	8.26	-476.405402	7.22
2OH-AZ-R	-477.137948	11.77	-476.954220	12.12	-476.399611	10.85
8S-AZ	-800.124671	0.00	-799.936286	0.00	-799.023033	0.00
8SH-AZ	-800.109956	9.23	-799.920064	10.18	-799.010344	7.96
8SH-AZ-R	-800.104483	12.67	-799.915887	12.80	-799.006285	10.51
2S-AZ	-800.121035	2.28	-799.927737	5.37	-799.015041	5.02
2SH-AZ	-800.111753	8.11	-799.920380	9.98	-799.00979	8.31
2SH-AZ-R	-800.109957	9.23	-799.918950	10.88	-799.008805	8.93

Table S3 Absolute zero-point corrected energy E_0 (au) and relative zero-point corrected energy ΔE (kcal/mol) for the investigated tautomers and rotamers, in the gas-phase calculated at the B3LYP / 6-311+G(d,p) and M06-2X/6-311++G(2d,2p) levels of theory, and in water calculated at M06-2X/6-311++G(2d,2p).

Tautomers	B3LYP / 6-311+G(d,p)		M062X/6-311++G(2d,2p)		G3MP2	
	E_0 (au)	Δ E_0 (Kcal/mol)	E_0 (au)	Δ E_0 (Kcal/mol)	E_0 (au)	Δ E_0 (Kcal/mol)
8O-AZ	-477.123841	0.00	-476.940669	0.00	-476.383805	0.00
8OH-AZ	-477.111986	7.44	-476.929117	7.25	-476.37364	6.38
8OH-AZ-R	-477.095210	17.97	-476.912946	17.40	-476.357766	16.34
2O-AZ	-477.122933	0.57	-476.935027	3.54	-476.379797	2.52
2OH-AZ	-477.111947	7.46	-476.927611	8.19	-476.372456	7.12
2OH-AZ-R	-477.105109	11.75	-476.921381	12.10	-476.366584	10.81
8S-AZ	-800.091003	0.00	-799.902618	0.00	-798.989145	0.00
8SH-AZ	-800.076299	9.23	-799.886407	10.17	-798.976379	8.01
8SH-AZ-R	-800.070555	12.83	-799.88196	12.96	-798.972187	10.64
2S-AZ	-800.087182	2.40	-799.893885	5.48	-798.980936	5.15
2SH-AZ	-800.077730	8.33	-799.886357	10.20	-798.975543	8.54
2SH-AZ-R	-800.075898	9.48	-799.884891	11.12	-798.974495	9.19

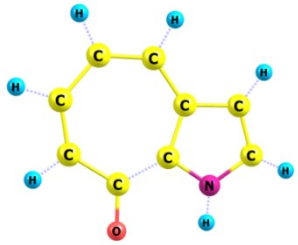
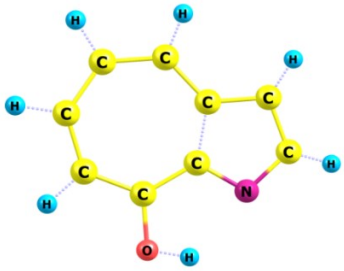
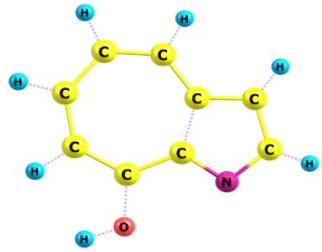
Table S4 Four NICS parameters (in ppm) for the five-/four-membered ring transition states of the investigated structures calculated at B3LYP/6–311+G(d, p) level in the gas phase.

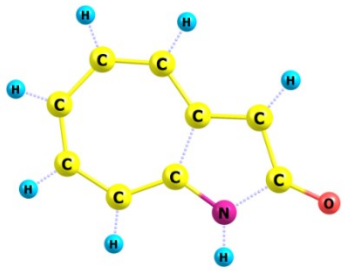
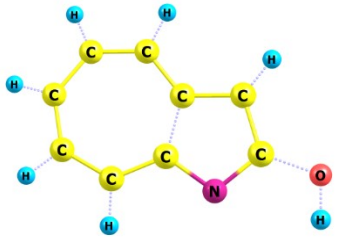
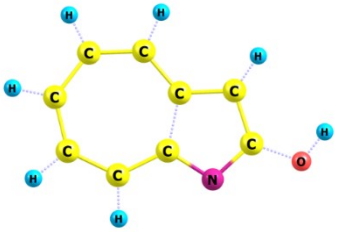
	NICS (0)	**$NICS_{zz}$ (0)**	**NICS (1)**	**$NICS_{zz}$ (1)**
TS_{T1} (five-member ring)	-0.13	23.53	-1.43	0.34
TS_{T2} (four-member ring)	1.33	41.56	0.43	6.05
TS_{T3} (five-member ring)	-1.53	22.42	-1.64	1.27
TS_{T4} (four-member ring)	-0.59	41.57	0.27	8.64

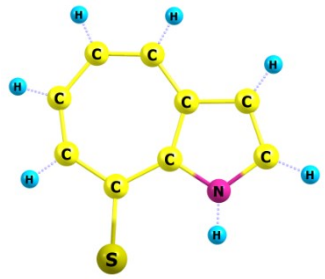
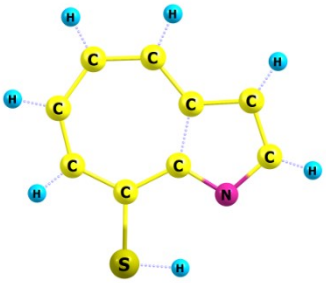
Table S5 Global chemical descriptor (eV) of the investigated tautomers and rotamers estimated at B3LYP/6-311+G(d,p) level in the gas phase.

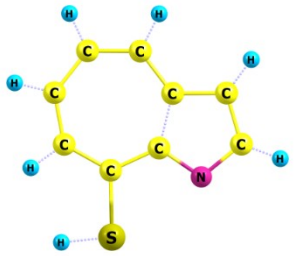
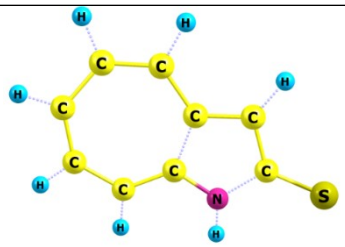
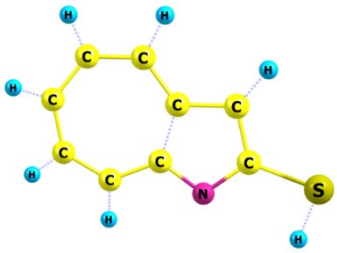
	E_{HOMO}	E_{LUMO}	Eg	IP	EA	χ	η	S	μ	ω
8O-AZ	-6.29	-2.05	4.24	6.29	2.05	4.17	2.12	0.24	-4.17	4.11
8OH-AZ	-6.33	-2.41	3.92	6.33	2.41	4.37	1.96	0.26	-4.37	4.87
8OH-AZ-R	-6.18	-2.35	3.82	6.18	2.35	4.26	1.91	0.26	-4.26	4.75
2O-AZ	-5.87	-2.34	3.53	5.87	2.34	4.11	1.76	0.28	-4.11	4.78
2OH-AZ	-6.13	-2.30	3.83	6.13	2.30	4.21	1.92	0.26	-4.21	4.63
2OH-AZ-R	-6.17	-2.30	3.87	6.17	2.30	4.23	1.94	0.26	-4.23	4.63
8S-AZ	-5.88	-2.49	3.39	5.88	2.49	4.18	1.70	0.29	-4.18	5.15
8SH-AZ	-6.33	-2.54	3.79	6.33	2.54	4.44	1.90	0.26	-4.44	5.19
8SH-AZ-R	-6.28	-2.52	3.76	6.28	2.52	4.40	1.88	0.27	-4.40	5.15
2S-AZ	-5.59	-2.71	2.87	5.59	2.71	4.15	1.44	0.35	-4.15	6.00
2SH-AZ	-6.07	-2.49	3.58	6.07	2.49	4.28	1.79	0.28	-4.28	5.11
2SH-AZ-R	-6.10	-2.49	3.60	6.10	2.49	4.30	1.80	0.28	-4.30	5.12

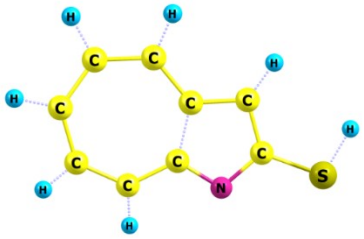
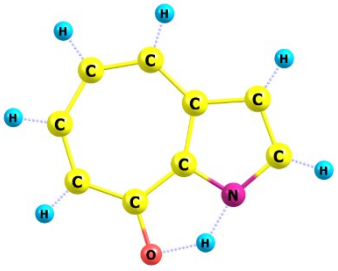
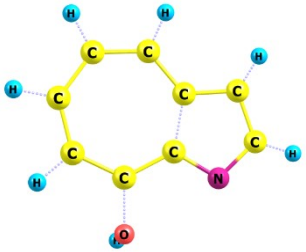
Table S6 The coordinates of optimized geometry of the investigated structures at B3LYP / 6-311+G(d,p) in the gas phase.

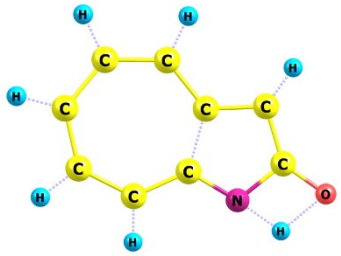
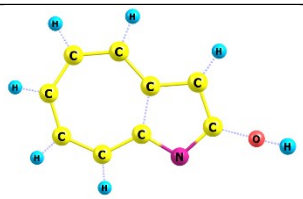
Structure	Coordinate
 **8O-AZ** Zero-point correction= 0.139652 (Hartree/Particle) Thermal correction to Energy= 0.147619 Thermal correction to Enthalpy= 0.148563 Thermal correction to Gibbs Free Energy= 0.106785 Sum of electronic and zero-point Energies= -477.123841 Sum of electronic and thermal Energies= -477.115874 Sum of electronic and thermal Enthalpies= -477.114930 Sum of electronic and thermal Free Energies= -477.156708	6 -2.461523000 -0.370851000 0.000129000 6 -1.818722000 -1.649185000 -0.000119000 6 -0.483337000 -1.928778000 -0.000229000 6 -1.960588000 0.898769000 0.000086000 6 0.592231000 -0.996973000 -0.000141000 6 -0.583971000 1.372987000 -0.000511000 6 0.510919000 0.411984000 -0.000175000 1 -3.547308000 -0.427560000 0.000363000 1 -2.491644000 -2.500553000 -0.000129000 1 -0.197129000 -2.976764000 -0.000333000 1 -2.674154000 1.716938000 0.000447000 6 1.987246000 -1.321321000 -0.000181000 1 2.411357000 -2.313516000 -0.000284000 6 2.687669000 -0.140022000 0.000160000 7 1.787064000 0.891389000 0.000020000 1 1.969871000 1.886028000 -0.000107000 8 -0.318741000 2.583919000 0.000682000 1 3.749944000 0.044697000 0.000332000
 **8OH-AZ** Zero-point correction= 0.139294 (Hartree/Particle) Thermal correction to Energy= 0.147128 Thermal correction to Enthalpy= 0.148073 Thermal correction to Gibbs Free Energy= 0.106688 Sum of electronic and zero-point Energies= -477.111986 Sum of electronic and thermal Energies= -477.104151 Sum of electronic and thermal Enthalpies= -477.103207 Sum of electronic and thermal Free Energies= -477.144592	6 -2.442428000 -0.370090000 0.000090000 6 -1.827869000 -1.635336000 0.000155000 6 -0.476721000 -1.942711000 0.000134000 6 -1.900986000 0.904510000 -0.000022000 6 0.604568000 -1.054092000 0.000048000 6 -0.545758000 1.270302000 -0.000086000 6 0.559308000 0.403752000 -0.000052000 1 -3.528490000 -0.395871000 0.000118000 1 -2.508629000 -2.480328000 0.000196000 1 -0.223210000 -2.999812000 0.000125000 1 -2.592741000 1.740099000 -0.000079000 6 1.984790000 -1.352532000 -0.000303000 1 2.430979000 -2.336045000 -0.000563000 6 2.648229000 -0.125879000 0.000506000 7 1.798144000 0.932158000 -0.000212000 1 0.701677000 2.653984000 -0.000271000 8 -0.275452000 2.583574000 -0.000187000 1 3.718224000 0.036734000 0.000633000
 **8OH-AZ-R** Zero-point correction= 0.138328 (Hartree/Particle) Thermal correction to Energy= 0.146479 Thermal correction to Enthalpy= 0.147423 Thermal correction to Gibbs Free Energy= 0.105422 Sum of electronic and zero-point Energies= -477.095210 Sum of electronic and thermal Energies= -477.087059	6 -2.385235000 -0.590376000 0.000015000 6 -1.674203000 -1.796099000 0.000037000 6 -0.298020000 -1.967527000 0.000039000 6 -1.934788000 0.721248000 -0.000009000 6 0.695584000 -0.986862000 0.000019000 6 -0.623988000 1.233693000 -0.000018000 6 0.566706000 0.485786000 -0.000006000 1 -3.466622000 -0.693294000 0.000018000

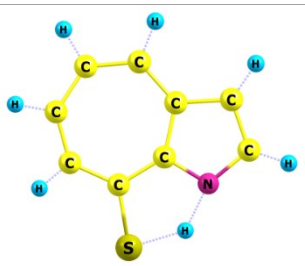
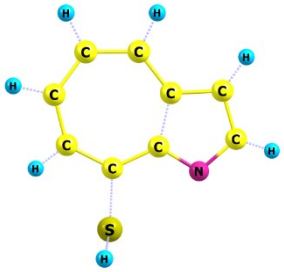
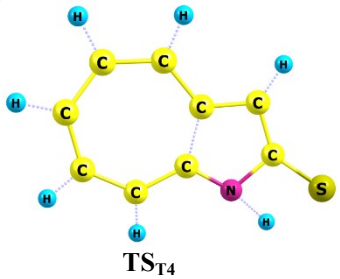
Sum of electronic and thermal Free Energies= -477.128116	1	-2.274882000	-2.699498000	0.000062000
	1	0.057928000	-2.994857000	0.000077000
	1	-2.717579000	1.477628000	-0.000027000
	6	2.086833000	-1.206492000	0.000090000
	1	2.584433000	-2.165173000	0.000166000
	6	2.676048000	0.057058000	-0.000056000
	7	1.776326000	1.069764000	-0.000038000
	1	-1.320609000	3.010211000	-0.000083000
	8	-0.460817000	2.574338000	-0.000067000
	1	3.735955000	0.279366000	-0.000074000
 **2O-AZ**	6	2.899188000	-0.064146000	0.000003000
	6	2.319869000	1.232901000	0.000037000
	6	1.000777000	1.604478000	0.000043000
	6	2.266934000	-1.283785000	-0.000031000
	6	-0.164795000	0.785805000	0.000011000
	6	0.882379000	-1.577917000	-0.000041000
	6	-0.166578000	-0.692083000	-0.000027000
	1	3.984097000	-0.089087000	0.000007000
	1	3.033219000	2.051980000	0.000065000
	1	0.801269000	2.672277000	0.000078000
Zero-point correction= 0.138920 (Hartree/Particle)	1	2.915720000	-2.154535000	-0.000050000
Thermal correction to Energy= 0.147035	6	-1.471870000	1.208674000	0.000044000
Thermal correction to Enthalpy= 0.147979	1	-1.825890000	2.227766000	0.000111000
Thermal correction to Gibbs Free Energy= 0.105949	6	-2.360766000	0.062508000	-0.000055000
Sum of electronic and zero-point Energies= -477.122933	7	-1.478867000	-1.058624000	-0.000028000
Sum of electronic and thermal Energies= -477.114818	1	0.619143000	-2.632050000	-0.000066000
Sum of electronic and thermal Enthalpies= -477.113874	1	-1.822155000	-2.007701000	-0.000030000
Sum of electronic and thermal Free Energies= -477.155904	8	-3.573020000	-0.039612000	0.000023000
 **2OH-AZ**	6	2.900812000	-0.094564000	-0.000002000
	6	2.362420000	1.201190000	0.000035000
	6	1.034212000	1.598961000	0.000045000
	6	2.246117000	-1.319919000	-0.000037000
	6	-0.116066000	0.798744000	0.000022000
	6	0.873204000	-1.591053000	-0.000045000
	6	-0.180082000	-0.689327000	-0.000020000
	1	3.985655000	-0.144855000	-0.000002000
	1	3.091061000	2.006389000	0.000058000
Zero-point correction= 0.138975 (Hartree/Particle)	1	0.857744000	2.671571000	0.000076000
Thermal correction to Energy= 0.146980	1	2.890342000	-2.194038000	-0.000061000
Thermal correction to Enthalpy= 0.147925	6	-1.447131000	1.215551000	0.000036000
Thermal correction to Gibbs Free Energy= 0.106208	1	-1.828929000	2.224362000	0.000066000
Sum of electronic and zero-point Energies= -477.111947	6	-2.200876000	0.028010000	-0.000001000
Sum of electronic and thermal Energies= -477.103941	7	-1.471046000	-1.096268000	-0.000032000
Sum of electronic and thermal Enthalpies= -477.102997	1	0.574547000	-2.634937000	-0.000075000
Sum of electronic and thermal Free Energies= -477.144714	1	-3.790714000	-0.957247000	-0.000029000
	8	-3.539755000	-0.022868000	-0.000001000
 **2OH-AZ-R**	6	2.903958000	-0.054734000	-0.000005000
	6	2.344286000	1.229877000	0.000037000

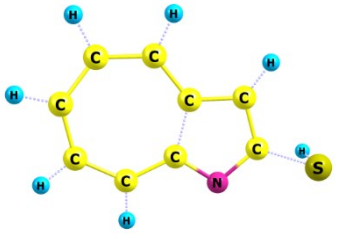
Zero-point correction=	0.138650 (Hartree/Particle)	6	1.007517000	1.604581000	0.000050000
Thermal correction to Energy=	0.146757	6	2.269763000	-1.292933000	-0.000045000
Thermal correction to Enthalpy=	0.147701	6	-0.125500000	0.783824000	0.000025000
Thermal correction to Gibbs Free Energy=	0.105811	6	0.903950000	-1.588147000	-0.000054000
Sum of electronic and zero-point Energies=	-477.105109	6	-0.167714000	-0.704494000	-0.000026000
Sum of electronic and thermal Energies=	-477.097002	1	3.989510000	-0.086883000	-0.000006000
Sum of electronic and thermal Enthalpies=	-477.096058	1	3.058411000	2.048001000	0.000061000
Sum of electronic and thermal Free Energies=	-477.137948	1	0.813336000	2.674278000	0.000079000
		1	2.929913000	-2.155103000	-0.000071000
		6	-1.466756000	1.170827000	0.000022000
		1	-1.857375000	2.178292000	0.000039000
		6	-2.199665000	-0.035773000	0.000009000
		7	-1.445756000	-1.140190000	-0.000022000
		1	0.621155000	-2.636333000	-0.000082000
		1	-3.953231000	0.692555000	0.000017000
		8	-3.537559000	-0.176455000	0.000004000
 **8S-AZ**		6	-0.011439000	2.534905000	0.000093000
		6	1.390280000	2.288101000	0.000083000
		6	2.031273000	1.081083000	0.000038000
		6	-1.085236000	1.680887000	0.000064000
		6	1.436423000	-0.206598000	-0.000008000
		6	-1.153767000	0.246180000	0.000016000
		6	0.052065000	-0.538804000	-0.000016000
		1	-0.277907000	3.588487000	0.000131000
		1	2.018723000	3.172823000	0.000115000
		1	3.117403000	1.095592000	0.000040000
Zero-point correction=	0.137515 (Hartree/Particle)	1	-2.063009000	2.150245000	0.000080000
Thermal correction to Energy=	0.145789	6	2.153992000	-1.443051000	-0.000045000
Thermal correction to Enthalpy=	0.146734	1	3.227087000	-1.555367000	-0.000043000
Thermal correction to Gibbs Free Energy=	0.103847	6	1.229161000	-2.457470000	-0.000095000
Sum of electronic and zero-point Energies=	-800.091003	7	-0.019393000	-1.900371000	-0.000075000
Sum of electronic and thermal Energies=	-800.082729	1	-0.924241000	-2.361966000	-0.000096000
Sum of electronic and thermal Enthalpies=	-800.081785	16	-2.661280000	-0.523190000	-0.000021000
Sum of electronic and thermal Free Energies=	-800.124671	1	1.361667000	-3.527567000	-0.000138000
 **8SH-AZ**		6	-0.263853000	2.516250000	-0.000066000
		6	-1.615259000	2.139960000	0.000092000
		6	-2.144755000	0.860344000	0.000183000
		6	0.889391000	1.746474000	-0.000187000
		6	-1.457927000	-0.356992000	0.000127000
		6	1.037461000	0.346958000	-0.000213000
		6	-0.003820000	-0.600595000	-0.000089000
		1	-0.087830000	3.588329000	-0.000115000
		1	-2.330201000	2.956287000	0.000101000
		1	-3.229420000	0.787395000	0.000183000
Zero-point correction=	0.133468 (Hartree/Particle)	1	1.818814000	2.308012000	-0.000263000
Thermal correction to Energy=	0.141940	6	-2.029376000	-1.645024000	-0.000181000
Thermal correction to Enthalpy=	0.142885	1	-3.083570000	-1.880140000	-0.000388000
Thermal correction to Gibbs Free Energy=	0.099811				
Sum of electronic and zero-point Energies=	-800.076299				
Sum of electronic and thermal Energies=	-800.067826				
Sum of electronic and thermal Enthalpies=	-800.066882				
Sum of electronic and thermal Free Energies=	-800.109956				

	6	-0.962221000	-2.540736000	0.000243000
	7	0.244200000	-1.924684000	0.000228000
	1	2.317012000	-1.547501000	0.000458000
	16	2.700345000	-0.244850000	-0.000084000
	1	-1.017569000	-3.621823000	0.000316000
 **8SH-AZ-R** Zero-point correction= 0.133230 (Hartree/Particle) Thermal correction to Energy= 0.141927 Thermal correction to Enthalpy= 0.142871 Thermal correction to Gibbs Free Energy= 0.099303 Sum of electronic and zero-point Energies= -800.070555 Sum of electronic and thermal Energies= -800.061859 Sum of electronic and thermal Enthalpies= -800.060915 Sum of electronic and thermal Free Energies= -800.104483	6	0.258405000	2.509864000	0.000045000
	6	1.611016000	2.144017000	0.000084000
	6	2.151051000	0.866980000	0.000078000
	6	-0.895035000	1.736327000	-0.000010000
	6	1.470198000	-0.351334000	0.000033000
	6	-1.034395000	0.336597000	-0.000050000
	6	0.013298000	-0.597743000	-0.000032000
	1	0.075728000	3.580934000	0.000064000
	1	2.319684000	2.965768000	0.000118000
	1	3.236238000	0.801936000	0.000095000
	1	-1.819933000	2.303518000	-0.000013000
	6	2.037755000	-1.639806000	-0.000023000
	1	3.091270000	-1.877787000	-0.000037000
	6	0.966234000	-2.533541000	-0.000016000
	7	-0.239640000	-1.918126000	0.000015000
	1	-3.317047000	0.778071000	0.000037000
	16	-2.650054000	-0.396176000	-0.000062000
	1	1.021250000	-3.614900000	-0.000026000
 **2S-AZ** Zero-point correction= 0.137051 (Hartree/Particle) Thermal correction to Energy= 0.145504 Thermal correction to Enthalpy= 0.146448 Thermal correction to Gibbs Free Energy= 0.103199 Sum of electronic and zero-point Energies= -800.087182 Sum of electronic and thermal Energies= -800.078730 Sum of electronic and thermal Enthalpies= -800.077786 Sum of electronic and thermal Free Energies= -800.121035	6	-3.315013000	-0.084098000	0.000021000
	6	-2.752414000	1.219535000	-0.000033000
	6	-1.436273000	1.605358000	-0.000058000
	6	-2.672019000	-1.301268000	0.000072000
	6	-0.268863000	0.792212000	-0.000063000
	6	-1.288416000	-1.583356000	0.000076000
	6	-0.252011000	-0.676708000	0.000002000
	1	-4.399561000	-0.120737000	0.000043000
	1	-3.475746000	2.029562000	-0.000034000
	1	-1.245419000	2.674616000	-0.000058000
	1	-3.315149000	-2.176062000	0.000127000
	6	1.045755000	1.216074000	0.000057000
	1	1.395670000	2.236200000	0.000228000
	6	1.919371000	0.085765000	-0.000281000
	7	1.066291000	-1.023337000	0.000071000
	1	-1.011043000	-2.633573000	0.000135000
	1	1.425877000	-1.966913000	0.000237000
	16	3.580040000	-0.032551000	0.000005000
 **2SH-AZ** Zero-point correction= 0.133171 (Hartree/Particle) Thermal correction to Energy= 0.141919 Thermal correction to Enthalpy= 0.142863 Thermal correction to Gibbs Free Energy= 0.099148	6	3.319563000	-0.112243000	-0.000001000
	6	2.795143000	1.187645000	0.000033000
	6	1.468862000	1.596871000	0.000044000
	6	2.654710000	-1.334804000	-0.000034000
	6	0.315026000	0.804302000	0.000023000
	6	1.282016000	-1.593722000	-0.000041000
	6	0.235536000	-0.678989000	-0.000017000

Sum of electronic and thermal Energies=	-800.068982	1	4.403945000	-0.172757000	-0.000003000
Sum of electronic and thermal Enthalpies=	-800.068038	1	3.531243000	1.985891000	0.000056000
Sum of electronic and thermal Free Energies=	-800.111753	1	1.301164000	2.670940000	0.000075000
		1	3.293069000	-2.213138000	-0.000058000
		6	-1.015095000	1.230202000	0.000043000
		1	-1.375400000	2.247740000	0.000079000
		6	-1.787888000	0.052765000	-0.000007000
		7	-1.055006000	-1.078916000	-0.000027000
		1	0.971331000	-2.634045000	-0.000070000
		1	-3.615247000	-1.340636000	-0.000045000
		16	-3.545768000	0.006015000	-0.000006000
 **2SH-AZ-R**		6	-3.321259000	-0.094773000	0.000008000
		6	-2.787171000	1.200753000	-0.000036000
		6	-1.457483000	1.600139000	-0.000050000
		6	-2.665750000	-1.322770000	0.000051000
		6	-0.310218000	0.798856000	-0.000024000
		6	-1.295453000	-1.592048000	0.000061000
		6	-0.241737000	-0.685210000	0.000030000
		1	-4.406081000	-0.146946000	0.000011000
		1	-3.517187000	2.004582000	-0.000059000
Zero-point correction=	0.133205 (Hartree/Particle)	1	-1.282327000	2.673073000	-0.000077000
Thermal correction to Energy=	0.141971	1	-3.310929000	-2.196073000	0.000080000
Thermal correction to Enthalpy=	0.142916	6	1.023614000	1.214077000	-0.000005000
Thermal correction to Gibbs Free Energy=	0.099146	1	1.389651000	2.229686000	-0.000006000
Sum of electronic and zero-point Energies=	-800.075898	6	1.786287000	0.029180000	-0.000031000
Sum of electronic and thermal Energies=	-800.067132	7	1.044582000	-1.094646000	0.000035000
Sum of electronic and thermal Enthalpies=	-800.066188	1	-0.991728000	-2.634404000	0.000093000
Sum of electronic and thermal Free Energies=	-800.109957	1	3.812111000	1.174798000	-0.000005000
		16	3.538090000	-0.145713000	-0.000019000
 **TS_{T1}**		6	-2.459575000	-0.187896000	0.000005000
		6	-1.921442000	-1.502583000	0.000044000
		6	-0.607036000	-1.932835000	0.000058000
		6	-1.878174000	1.066941000	-0.000033000
		6	0.536326000	-1.112699000	0.000034000
		6	-0.488880000	1.334678000	-0.000041000
		6	0.494266000	0.303230000	-0.000010000
		1	-3.546421000	-0.170000000	0.000004000
		1	-2.670053000	-2.288287000	0.000068000
Zero-point correction=	0.135162 (Hartree/Particle)	1	-0.446291000	-3.007469000	0.000090000
Thermal correction to Energy=	0.142607	1	-2.532961000	1.931486000	-0.000059000
Thermal correction to Enthalpy=	0.143551	6	1.932910000	-1.417987000	0.000045000
Thermal correction to Gibbs Free Energy=	0.102852	1	2.379757000	-2.401134000	0.000075000
Sum of electronic and zero-point Energies=	-477.096318	6	2.612346000	-0.206377000	0.000008000
Sum of electronic and thermal Energies=	-477.088873	7	1.725519000	0.835572000	-0.000025000
Sum of electronic and thermal Enthalpies=	-477.087929	1	1.263950000	2.036549000	-0.000061000
Sum of electronic and thermal Free Energies=	-477.128628	8	0.058798000	2.502227000	-0.000075000
		1	3.678562000	-0.034791000	0.000004000
		6	-2.403514000	-0.546680000	0.013146000

	6	-1.711681000	-1.762929000	0.012154000
Zero-point correction= 0.137191 (Hartree/Particle)	6	-0.338583000	-1.964855000	-0.003887000
Thermal correction to Energy= 0.145007	6	-1.924818000	0.757253000	-0.005380000
Thermal correction to Enthalpy= 0.145951	6	0.676387000	-1.007098000	-0.012961000
Thermal correction to Gibbs Free Energy= 0.104490	6	-0.606201000	1.236999000	-0.010562000
Sum of electronic and zero-point Energies= -477.089138	6	0.568852000	0.475040000	-0.006792000
Sum of electronic and thermal Energies= -477.081323	1	-3.486364000	-0.631857000	0.017502000
Sum of electronic and thermal Enthalpies= -477.080378	1	-2.327638000	-2.656330000	0.021295000
Sum of electronic and thermal Free Energies= -477.121840	1	-0.006296000	-3.000083000	-0.003874000
	1	-2.674616000	1.541651000	-0.034751000
	6	2.059671000	-1.249460000	-0.004459000
	1	2.543675000	-2.215099000	-0.005631000
	6	2.670023000	0.007426000	0.012262000
	7	1.793055000	1.035847000	0.012112000
	1	-0.609052000	3.021534000	0.750744000
	8	-0.458287000	2.600812000	-0.102328000
	1	3.734389000	0.208585000	0.027417000
	6	2.886178000	-0.147909000	-0.000002000
TS_{T2}	6	2.369526000	1.158721000	0.000034000
	6	1.054699000	1.589989000	0.000045000
	6	2.201629000	-1.354386000	-0.000037000
	6	-0.127547000	0.827490000	0.000023000
	6	0.822429000	-1.594341000	-0.000045000
	6	-0.203939000	-0.664117000	-0.000019000
	1	3.969149000	-0.220704000	-0.000003000
	1	3.114886000	1.948667000	0.000057000
Zero-point correction= 0.133660 (Hartree/Particle)	1	0.906276000	2.666363000	0.000075000
Thermal correction to Energy= 0.141500	1	2.822385000	-2.245375000	-0.000062000
Thermal correction to Enthalpy= 0.142444	6	-1.438889000	1.316720000	0.000036000
Thermal correction to Gibbs Free Energy= 0.100834	1	-1.748310000	2.349110000	0.000066000
Sum of electronic and zero-point Energies= -477.052575	6	-2.267665000	0.175832000	0.000004000
Sum of electronic and thermal Energies= -477.044735	7	-1.518006000	-0.969225000	-0.000029000
Sum of electronic and thermal Enthalpies= -477.043791	1	0.505137000	-2.632499000	-0.000075000
Sum of electronic and thermal Free Energies= -477.085401	1	-2.756084000	-1.364376000	-0.000040000
	8	-3.495740000	-0.195576000	-0.000007000
	6	-2.903198000	-0.067609000	0.010244000
TS_{R2}	6	-2.353582000	1.221805000	0.004760000
	6	-1.018661000	1.603656000	-0.001174000
	6	-2.265359000	-1.303632000	0.007974000
	6	0.117593000	0.788767000	-0.002844000
	6	-0.896821000	-1.590064000	-0.001442000
	6	0.166861000	-0.699263000	-0.006102000
Zero-point correction= 0.137435 (Hartree/Particle)	1	-3.988738000	-0.105503000	0.015836000
Thermal correction to Energy= 0.145234	1	-3.073772000	2.034341000	0.005704000
Thermal correction to Enthalpy= 0.146178	1	-0.829482000	2.674288000	-0.003931000
Thermal correction to Gibbs Free Energy= 0.104735	1	-2.921604000	-2.168526000	0.011639000
Sum of electronic and zero-point Energies= -477.098565	6	1.458124000	1.181090000	-0.010401000
Sum of electronic and thermal Energies= -477.090767	1	1.854457000	2.184925000	-0.028729000
Sum of electronic and thermal Enthalpies= -477.089822				
Sum of electronic and thermal Free Energies= -477.131266				

	6	2.198085000	-0.015711000	-0.012592000
	7	1.449956000	-1.126768000	-0.012702000
	1	-0.607320000	-2.636590000	-0.006574000
	1	3.944605000	-0.003893000	0.796993000
	8	3.556738000	-0.100738000	-0.079071000
 **TS_{T3}**	6	1.059520000	-2.322118000	0.000011000
	6	2.215349000	-1.512850000	0.000032000
	6	2.313338000	-0.133507000	0.000047000
	6	-0.288668000	-2.002625000	-0.000011000
	6	1.258543000	0.790909000	0.000041000
	6	-0.885731000	-0.726017000	-0.000024000
	6	-0.150422000	0.488749000	0.000003000
	1	1.264545000	-3.389363000	0.000013000
	1	3.155209000	-2.055510000	0.000039000
	1	3.317240000	0.282671000	0.000065000
	1	-0.977364000	-2.840902000	-0.000024000
	6	1.325510000	2.211616000	0.000052000
	1	2.222398000	2.813376000	0.000082000
	6	0.016541000	2.670597000	0.000022000
	7	-0.863801000	1.628634000	-0.000008000
	1	-2.131052000	1.029542000	-0.000047000
	16	-2.603260000	-0.482546000	-0.000070000
	1	-0.336082000	3.691960000	0.000020000
Zero-point correction= 0.131281 (Hartree/Particle) Thermal correction to Energy= 0.139188 Thermal correction to Enthalpy= 0.140133 Thermal correction to Gibbs Free Energy= 0.098104 Sum of electronic and zero-point Energies= -800.069425 Sum of electronic and thermal Energies= -800.061517 Sum of electronic and thermal Enthalpies= -800.060573 Sum of electronic and thermal Free Energies= -800.102602				
 **TS_{R3}**	6	0.172525000	2.516618000	0.001163000
	6	1.533018000	2.202971000	0.009167000
	6	2.119903000	0.943779000	0.004568000
	6	-0.944881000	1.684170000	-0.013093000
	6	1.492713000	-0.299890000	-0.003135000
	6	-1.034929000	0.284662000	-0.003325000
	6	0.030919000	-0.624431000	-0.003353000
	1	-0.057228000	3.578346000	-0.001099000
	1	2.214084000	3.048036000	0.015906000
	1	3.206872000	0.920725000	0.008884000
	1	-1.900154000	2.195672000	-0.037187000
	6	2.125280000	-1.551502000	-0.000650000
	1	3.189797000	-1.734739000	0.000339000
	6	1.099150000	-2.499685000	0.002399000
	7	-0.138800000	-1.960024000	0.002255000
	1	-2.942302000	-0.332556000	1.253576000
	16	-2.719770000	-0.394914000	-0.076536000
	1	1.214661000	-3.576841000	0.005921000
Zero-point correction= 0.132273 (Hartree/Particle) Thermal correction to Energy= 0.140578 Thermal correction to Enthalpy= 0.141522 Thermal correction to Gibbs Free Energy= 0.098555 Sum of electronic and zero-point Energies= -800.060638 Sum of electronic and thermal Energies= -800.052333 Sum of electronic and thermal Enthalpies= -800.051388 Sum of electronic and thermal Free Energies= -800.094356				
 **TS_{T4}**	6	-3.287617000	-0.235246000	0.000065000
	6	-2.831984000	1.091065000	0.000059000
	6	-1.534155000	1.578412000	0.000033000
	6	-2.551417000	-1.415873000	0.000044000
	6	-0.326414000	0.862103000	0.000009000
	6	-1.167417000	-1.595636000	0.000012000
	6	-0.181687000	-0.615155000	-0.000003000
Zero-point correction= 0.130536 (Hartree/Particle) Thermal correction to Energy= 0.138783 Thermal correction to Enthalpy= 0.139727 Thermal correction to Gibbs Free Energy= 0.096806				

Sum of electronic and thermal Energies=	-800.025601	1	-4.366341000	-0.356354000	0.000089000
Sum of electronic and thermal Enthalpies=	-800.024657	1	-3.611359000	1.847267000	0.000077000
Sum of electronic and thermal Free Energies=	-800.067578	1	-1.430346000	2.660017000	0.000033000
		1	-3.135694000	-2.331089000	0.000052000
		6	0.970263000	1.395695000	-0.000013000
		1	1.237353000	2.440281000	-0.000012000
		6	1.846084000	0.302116000	-0.000037000
		7	1.141101000	-0.878638000	-0.000033000
		1	-0.801781000	-2.617807000	-0.000003000
		1	2.384085000	-1.423978000	-0.000052000
		16	3.507652000	-0.142048000	-0.000060000
		6	3.324538000	-0.088590000	0.008806000
TS_{R4}		6	2.791374000	1.206029000	0.004239000
		6	1.458441000	1.601134000	-0.001245000
		6	2.676166000	-1.321704000	0.007192000
		6	0.317789000	0.795949000	-0.004821000
		6	1.306924000	-1.593764000	-0.000165000
		6	0.252564000	-0.688332000	-0.004967000
		1	4.409734000	-0.137912000	0.013764000
		1	3.520361000	2.010412000	0.005882000
Zero-point correction=	0.132464 (Hartree/Particle)	1	1.279175000	2.673485000	-0.003246000
Thermal correction to Energy=	0.140758	1	3.325732000	-2.191404000	0.010962000
Thermal correction to Enthalpy=	0.141702	6	-1.022168000	1.201882000	-0.012057000
Thermal correction to Gibbs Free Energy=	0.098719	1	-1.403611000	2.211272000	-0.023455000
Sum of electronic and zero-point Energies=	-800.069317	6	-1.779582000	0.019228000	-0.006585000
Sum of electronic and thermal Energies=	-800.061023	7	-1.033066000	-1.103293000	-0.010103000
Sum of electronic and thermal Enthalpies=	-800.060079	1	1.004226000	-2.636618000	-0.002479000
Sum of electronic and thermal Free Energies=	-800.103062	1	-3.760331000	0.038247000	1.261930000
		16	-3.568756000	-0.064715000	-0.070938000