

Supporting Information

for

**Enantio- and Diastereoselectivities in Chiral Sulfur Ylide
Promoted Asymmetric Aziridination Reactions**

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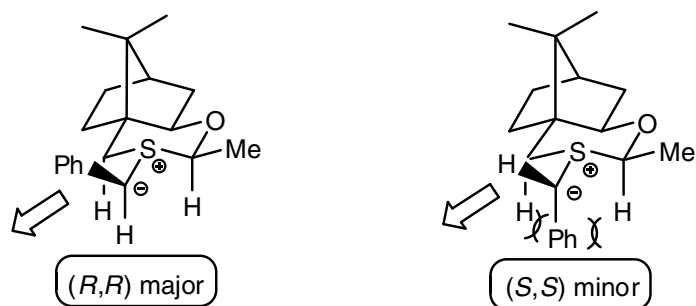


Figure S1. Ylide conformational preference as a rationalization of enantioselection (ref 14c).

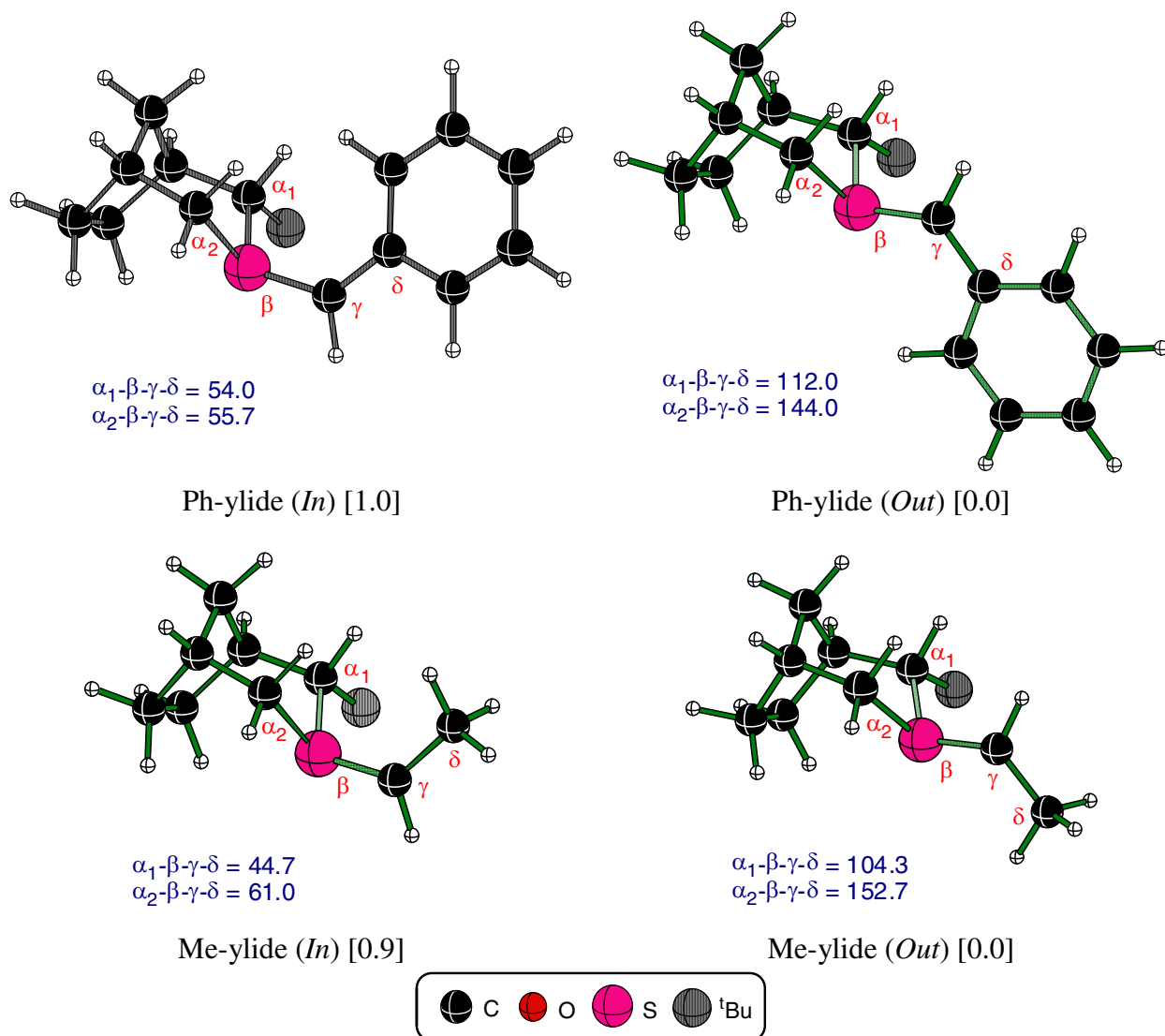


Figure S2. Optimized geometries and relative energies of *In* and *Out* conformers for semistabilized and non-stabilized ylides. The ΔE is obtained at the PCM_(MeCN)/B3LYP/6-311G**//B3LYP/6-31G* in kcal mol⁻¹ and angles in °.

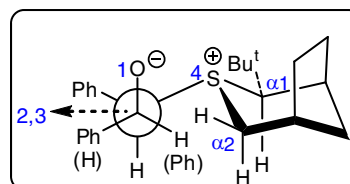
Table S1. The computed Activation Energies ($\Delta E^\ddagger$ in kcal mol⁻¹) Obtained at the PCM_(MeCN)/B3LYP/6-311G**//B3LYP/6-31G* level for the Epoxidation Reaction between Semistabilized ylide and Benzaldehyde^{g,h}

$(si, si)^i$	$(si, re)^i$	(re, si)	$(re, re)^i$	Product Configuration ^j
<i>c</i>	<i>c</i>	<i>c</i>	<i>t</i>	<i>c</i>
9.5	8.0	10.2	13.8	7.7
(2 <i>S</i> ,3 <i>S</i>)- <i>trans</i>				

^g $\Delta E^\ddagger$ relative to the sum of energies of corresponding ylide conformer and aldehyde; ^h 'c' and 't' denote cisoid and transoid addition modes; ⁱ transoid TS could not be located; ^j Product corresponding to the lowest energy TS.

Table S2. Donor-Acceptor Interaction Energies for Transition States for Epoxide Formation^g

Interaction	$E^{(2)}$ (kcal mol ⁻¹)			
Epoxide	$si, si-c^\ddagger$	$si, re-c^\ddagger$	$re, si-c^\ddagger$	$re, re-c^\ddagger$
$n_O \rightarrow \sigma_{C2-C3}^*$	48.93	53.93	52.38	56.66
$\sigma_{C2-C3} \rightarrow \sigma_{S4-C\alpha1}^*$	3.36	3.62	2.90	3.51
$n_O \rightarrow \sigma_{Heq-C\alpha2}^*$	5.99	4.37	1.50	3.10
$n_O \rightarrow \sigma_{S4-C\alpha1}^*$	1.75	0.77	4.10	2.22



^gNBO delocalization energies ($E^{(2)}$) computed at the B3LYP/6-311+G**//B3LYP/6-31G* level.

Table S3. The computed Activation Energies ($\Delta E^\ddagger$ in kcal mol⁻¹) Obtained at the PCM_(MeCN)/B3LYP/6-311G**//B3LYP/6-31G* level for the Aziridination Reaction of Stabilized (**1-4**) and Semistabilized (**5-8**) Ylides with N-substituted Benzaldimines^{g,h}

System		(si, si)		$(si, re)^i$		(re, si)		(re, re)		Product Configuration ^j
		c	t	c	c	T	c	t		
(R = COMe)										
1	X = Ph Y = SO ₂ Me	21.1	19.5	18.5	17.2	17.9	16.4	16.1	(2 <i>S</i> ,3 <i>S</i>) <i>cis</i>	
2	X = Me Y = SO ₂ Me	12.7	10.9	14.1	11.3	12.5	11.2	9.9	(2 <i>S</i> ,3 <i>S</i>) <i>cis</i>	
3	X = Ph Y = CO ₂ Me	19.8	16.0	17.2	15.4	17.1	14.8	15.5	(2 <i>S</i> ,3 <i>S</i>) <i>cis</i>	
4	X = Me Y = CO ₂ Me	13.1	9.6	12.5	9.6	11.9	11.2	9.6	-- ^k	
(R = Ph)										
5	X = Ph Y = SO ₂ Me	6.4	10.1	7.7	8.8	8.8	8.6	8.5	(2 <i>S</i> ,3 <i>R</i>) <i>cis</i>	
6	X = Me Y = SO ₂ Me	2.4	5.9	3.8	3.6	5.4	4.6	-- ⁱ	(2 <i>S</i> ,3 <i>R</i>) <i>cis</i>	
7	X = Ph Y = CO ₂ Me	5.8	8.2	6.8	8.2	8.2	7.3	8.6	(2 <i>S</i> ,3 <i>R</i>) <i>cis</i>	
8	X = Me Y = CO ₂ Me	2.5	4.2	3.3	2.9	5.5	3.3	4.7	(2 <i>S</i> ,3 <i>R</i>) <i>cis</i>	

^g $\Delta E^\ddagger$ with respect to the sum of energies of corresponding ylide conformer and imine; ^h 'c' and 't' denote cisoid and transoid addition modes; ⁱ transoid TS could not be located; ^j Product corresponding to the lowest energy TS; ^k TSs leading to diastereomeric products for system **4** are degenerate.

Table S4. The computed Relative Energies ($\Delta\Delta E^\ddagger$ in kcal mol⁻¹) Obtained at the PCM_(MeCN)/B3LYP/6-311G**//B3LYP/6-31G* level for the Aziridination Reaction between Non-stabilized Ylide and N-substituted Benzaldimines (**9-12**)^{g,h}

System		(si, si)		$(si, re)^i$		(re, si)		(re, re)		Product Configuration ^j	ee, de (%)
		c	t	c	c	t	c	t			
9	X = Ph	1.8	2.3	2.2	0.9	0.0	1.3	0.0	-- ^k	-- ^k	
	Y = SO ₂ Me										
10	X = Me	0.9	0.8	1.5	0.7	0.0	0.6	0.2	(2 <i>R</i> ,3 <i>R</i>) <i>trans</i>	85, 17	
	Y = SO ₂ Me										
11	X = Ph	2.3	3.5	2.2	2.7	0.0	0.6	0.1	(2 <i>R</i> ,3 <i>R</i>) <i>trans</i>	95, 8	
	Y = CO ₂ Me										
12	X = Me	1.7	1.8	2.2	0.1	0.0	1.0	0.2	(2 <i>R</i> ,3 <i>R</i>) <i>trans</i>	95, 17	
	Y = CO ₂ Me										

^g $\Delta\Delta E^\ddagger$ relative to the most stable TS isomer; ^h 'c' and 't' denote cisoid and transoid addition modes; ⁱ transoid TS could not be located; ^j Product corresponding to the lowest energy TS; ^k TSs leading to diastereomeric products for system **9** are found to be degenerate.

Table S5. The computed Activation Energies ($\Delta E^\ddagger$ in kcal mol⁻¹) Obtained at the PCM_(MeCN)/B3LYP/6-311G**//B3LYP/6-31G* level for the Aziridination Reaction between Non-stabilized Ylide and N-substituted Benzaldimines (**9-12**)^{g,h}

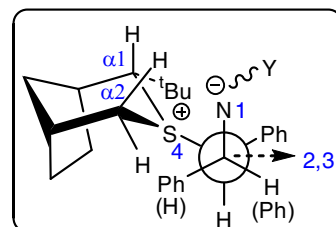
System		(si, si)		$(si, re)^i$	(re, si)		(re, re)		Product Configuration ^j
		c	t	c	c	t	c	t	
9	X = Ph	0.1	0.6	0.5	0.1	−0.8	0.5	−0.8	-- ^k
	Y = SO ₂ Me								
10	X = Me	−2.0	−2.1	−1.4	−1.2	−2.0	−1.4	−1.8	(2 <i>R</i> ,3 <i>R</i>) <i>trans</i>
	Y = SO ₂ Me								
11	X = Ph	0.4	1.5	0.2	1.7	−1.0	−0.5	−0.9	(2 <i>R</i> ,3 <i>R</i>) <i>trans</i>
	Y = CO ₂ Me								
12	X = Me	−1.4	−1.4	−1.0	−2.2	−2.3	−1.3	−2.1	(2 <i>R</i> ,3 <i>R</i>) <i>trans</i>
	Y = CO ₂ Me								

^g $\Delta E^\ddagger$ with respect to the sum of energies of corresponding ylide conformer and imine; ^h c and t denote cisoid and transoid addition modes; ⁱ transoid TS could not be located; ^j

*Product corresponding to the lowest energy TS; ^k TSs leading to diastereomeric products for system **9** are degenerate.*

Table S6. Donor-acceptor stabilizing interactions for TSs resulting from addition of semistabilized ylide to imine^g

Interaction	$E^{(2)}$ (kcal mol ⁻¹)			
Mesyl	$si, si-c^{\ddagger}$	$si, re-c^{\ddagger}$	$re, si-c^{\ddagger}$	$re, re-t^{\ddagger}$
$n_N \rightarrow \sigma^*_{C2-C3}$	63.84	78.30	64.19	56.46
$\sigma_{C2-C3} \rightarrow \sigma^*_{S4-C\alpha1}$	6.49	6.30	5.39	5.03
$n_N \rightarrow \sigma^*_{Heq-C\alpha2}$ or $n_O(SO_2Me) \rightarrow \sigma^*_{Heq-C\alpha2}$	5.47	5.15	2.97	-- ^h
Carbamate	$si, si-c^{\ddagger}$	$si, re-c^{\ddagger}$	$re, si-c^{\ddagger}$	$re, re-t^{\ddagger}$
$n_N \rightarrow \sigma^*_{C2-C3}$	69.89	3.25	75.02	0.65
$\sigma_{C2-C3} \rightarrow \sigma^*_{S4-C\alpha1}$	7.65	5.35	5.63	5.89
$n_N \rightarrow \sigma^*_{Heq-C\alpha2}$ or $n_O(CO_2Me) \rightarrow \sigma^*_{Heq-C\alpha2}$	7.36	5.03	2.19	5.10
$\pi_{N-C(CO_2Me)} \rightarrow \sigma^*_{C2-C3}$	-- ^h	38.03	-- ^h	36.95



^gNBO delocalization energies ($E^{(2)}$) computed at the B3LYP/6-311+G**//B3LYP/6-31G* level. ^h This particular interaction is absent in TS. Atom numbering scheme adopted for NBO analysis is also provided.

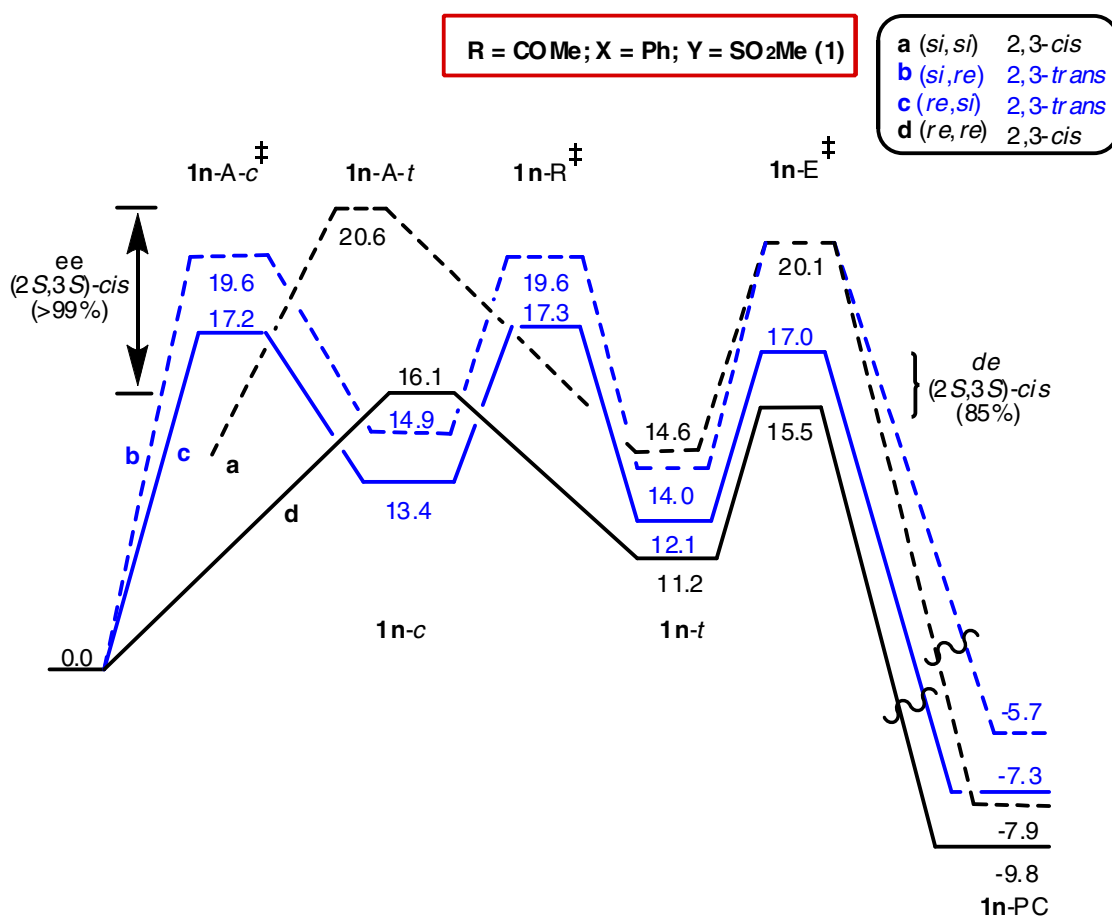


Figure S3. Reaction profiles for enantiomeric and diastereomeric pathways (**a** - **d**) for the addition of stabilized ylide to N-mesyl benzaldimine [Higher and lower energy diastereomeric pathways are respectively represented using dotted and bold lines. $\Delta E^{\ddagger}$ (kcal mol⁻¹) is computed at the PCM_(MeCN)/B3LYP/6-311G**//B3LYP/6-31G* level].

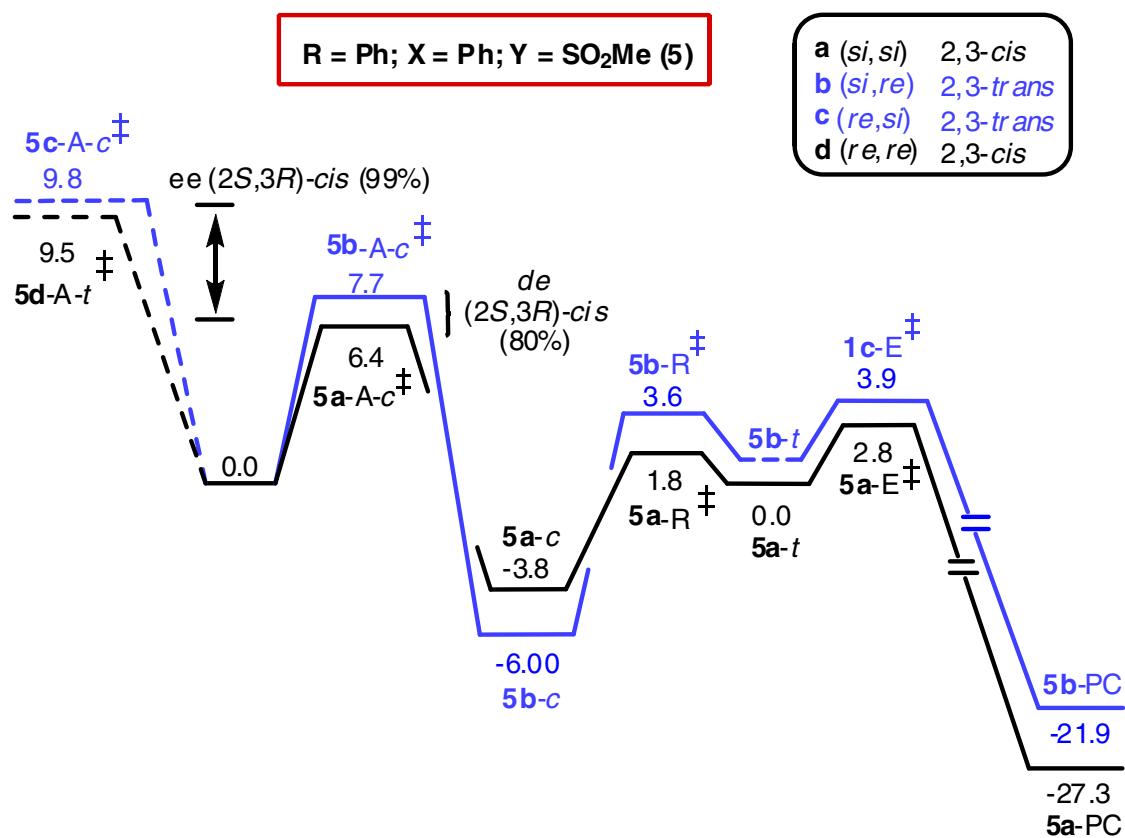


Figure S4. Reaction profiles for the lower energy diastereomeric pathways (**a** and **b**) for the addition of semistabilized ylide to N-mesyl benzaldimine [$\Delta E^\ddagger$ (kcal mol⁻¹) is computed at the PCM_(MeCN)/B3LYP/6-311G**//B3LYP/6-31G* level; We could not locate the intermediate **5b-t** due to factors that already mentioned in the text regarding optimization of *si, re* *transoid* TSs, all attempts resulted in the formation of either **5b-c** or **5b-PC**].

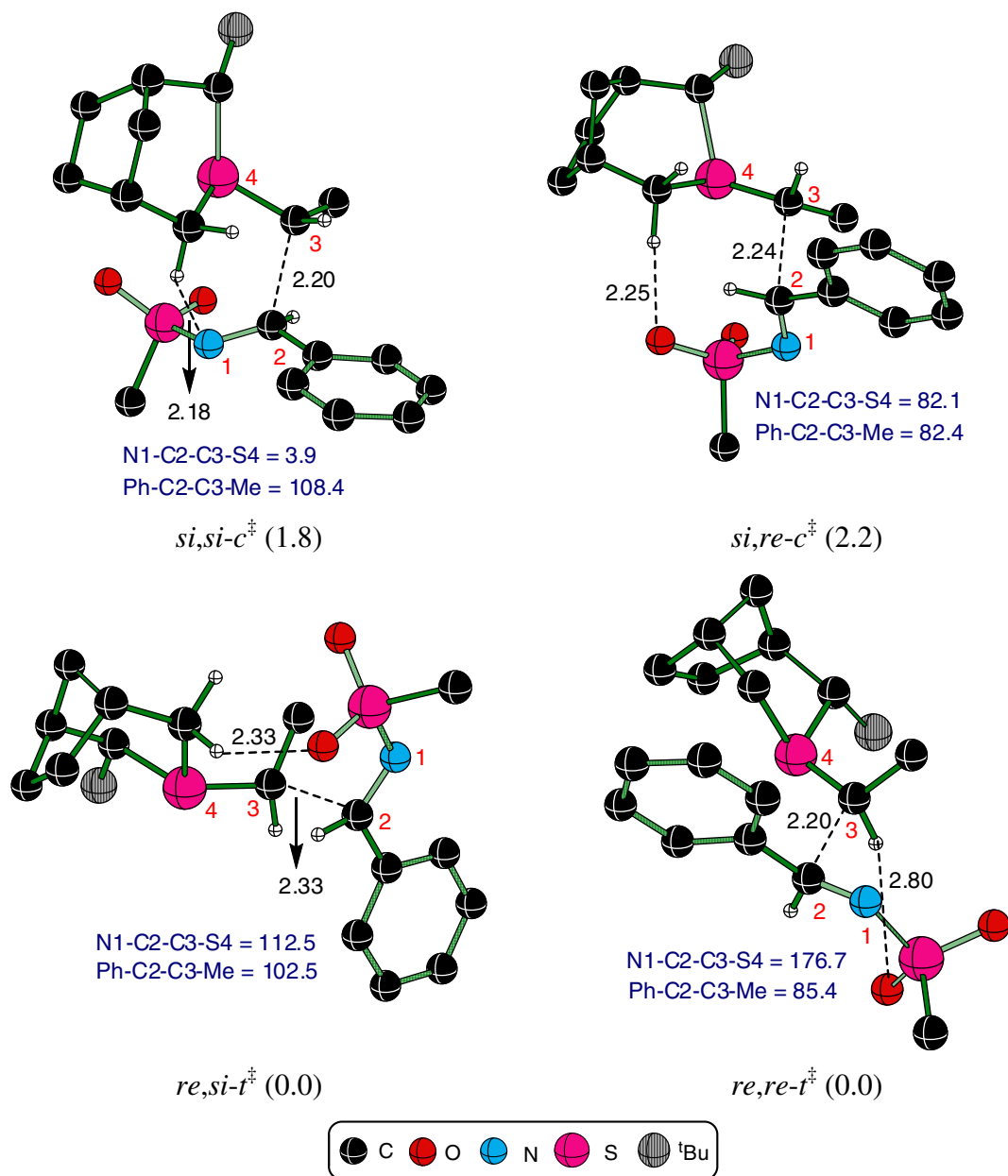


Figure S5. Optimized geometries and relative energies of lowest energy TSs for nonstabilized ylide addition to substituted imines (**9**). The $\Delta\Delta E^\ddagger$ is obtained at the PCM_(MeCN)/B3LYP/6-311G**//B3LYP/6-31G* level. Energies in kcal mol⁻¹, distances in Å and angles in °.

Table S7. Population of different TSs for addition of stabilized ylide (**1**) calculated using the Boltzmann distribution law

TS	ϵ_i	$e^{-\epsilon_i/kT}$	N_i
1a-A-c	6.0	0.00004	0.00002
1a-A-t	4.5	0.00050	0.00028
1b-A-c	3.5	0.00271	0.00150
1c-A-c	1.1	0.15606	0.08623
1c-A-t	1.8	0.04785	0.02644
1d-A-c	0.3	0.60254	0.33295
1d-A-t	0.0	1.00000	0.55258
$\Sigma_i e^{-\epsilon_i/kT} = 1.8097$			
(T= 298K, k = 1.9872 cal mol ⁻¹ K ⁻¹)			

*Since the two lower energy TSs (**1d-A-t** and **1d-A-c**) lead to a single product, the total contribution of (2S,3S) cis aziridine toward the product complex amounts to 88%. Hence, selecting the lowest energy isomer for ee calculations will not alter the final outcome.*

Table S8. Population of different TSs for addition of semistabilized ylide (**5**) calculated using the Boltzmann distribution law

TS	ϵ_i	$e^{-\epsilon_i/kT}$	N_i
5a-A-c	0.0	1.00000	0.886
5a-A-t	3.7	0.00193	0.002
5b-A-c	1.3	0.11133	0.099
5c-A-c	3.4	0.00321	0.003
5c-A-t	3.5	0.00271	0.002
5d-A-c	3.3	0.00380	0.003
5d-A-t	3.1	0.00533	0.005
$\Sigma_i e^{-\epsilon_i/kT} = 1.128309$			

Optimized Cartesian coordinates and energies of TSs, intermediates, products and reactants obtained at the B3LYP/6-31G* level (Energy in a. u.). Single-point energies (at the PCM_(CH₃CN)/B3LYP/6-311G**//B3LYP/6-31G* level, imaginary frequencies (in cm⁻¹), if any, are also given after the respective coordinates.

TSs for Epoxide Formation

1. *si,si-c[‡]* (-1445.24267214)

6	-2.543116	-2.757958	-1.128744
6	-1.215772	-3.253535	-1.785094
6	-0.177992	-3.263091	-0.635937
6	-1.047325	-3.523232	0.601179
6	-2.221145	-2.547025	0.382086
6	-1.841005	-1.094725	0.810979
16	-0.590670	-0.487530	-0.488046
6	0.561267	-1.934106	-0.491501
6	0.495451	0.869023	0.104701
1	0.708275	0.703766	1.163689
6	-3.029028	-0.096933	1.088519
6	-2.556671	0.972344	2.096154
6	-3.575858	0.597999	-0.174932
6	-4.197650	-0.855605	1.763459
6	2.004677	0.733822	-0.977264
8	1.724246	0.151239	-2.091625
1	-1.266642	-1.173867	1.741553
1	-3.070389	-2.838109	1.001577
1	-0.518016	-3.368337	1.548928
1	-1.423174	-4.554319	0.595703
1	-3.323345	-3.520561	-1.223350
1	-2.925231	-1.855885	-1.611348
1	0.589522	-4.031957	-0.784021
1	-1.340558	-4.266086	-2.182684
1	-0.896861	-2.617135	-2.616656
1	1.147332	-1.891795	0.430376
1	1.203996	-1.667667	-1.338131
1	2.170799	1.835463	-1.007008
1	-2.827479	1.231067	-0.660756
1	-3.948358	-0.120917	-0.911482
1	-4.415411	1.245169	0.104143
1	-3.865623	-1.433453	2.634740
1	-4.934633	-0.126214	2.116860
1	-4.714731	-1.532181	1.075782
1	-2.233947	0.509531	3.037476
1	-1.734892	1.573049	1.705966
1	-3.379397	1.658105	2.328770
6	-0.082832	2.215213	-0.177300
6	-0.075082	3.215761	0.809941

6	-0.492994	4.515491	0.520347
6	-0.931838	4.842519	-0.763077
6	-0.923363	3.862955	-1.760193
6	-0.495120	2.567256	-1.478164
1	0.266639	2.973334	1.814293
1	-0.478538	5.270890	1.301998
1	-1.265151	5.851935	-0.988257
1	-1.236277	4.114012	-2.770561
1	-0.420011	1.828046	-2.270476
6	3.115096	0.127829	-0.099432
6	3.874968	-0.929916	-0.609421
6	4.932807	-1.471738	0.123667
6	5.254164	-0.953755	1.379850
6	4.518410	0.120130	1.889279
6	3.464323	0.658204	1.150513
1	3.622081	-1.295914	-1.600279
1	5.514555	-2.292814	-0.289819
1	6.078452	-1.372071	1.952296
1	4.772391	0.542321	2.859089
1	2.915127	1.511594	1.545639

E (CH₃CN) = -1445.545991

NImag = 1 (-218.5)

2. *si,re-c[‡]* (-1445.24424981)

6	1.472532	-2.269749	-0.080376
6	2.932721	-2.647804	0.176374
6	3.846292	-1.956707	-0.845780
6	3.862226	-0.501283	-0.335003
6	2.577983	0.266838	-0.781113
16	1.158970	-0.472948	0.240560
6	4.047685	-0.697779	1.200699
6	3.468626	-2.110678	1.526379
6	2.636899	1.839292	-0.762057
6	4.007516	2.298393	-1.317044
6	-0.504898	-0.169297	-0.442525
6	-1.148666	1.002588	0.205676
6	1.561027	2.400740	-1.716770
6	2.444262	2.461779	0.635513
6	-1.433826	-1.753176	0.058700
8	-1.138713	-2.062618	1.264157
6	-2.876143	-1.420873	-0.289977
1	-0.449217	-0.100020	-1.531687

1	2.366667	-0.028070	-1.816161	6	-2.240827	0.194638	0.291121
1	4.709643	0.038229	-0.760734	16	-0.955678	-0.634967	-0.817878
1	3.498882	-2.054207	-1.881353	6	-0.182477	-1.901348	0.312087
1	4.859639	-2.374772	-0.795751	6	0.414037	0.557112	-1.146801
1	5.116134	-0.659603	1.437932	6	0.743102	1.616113	-0.164848
1	3.566159	0.085272	1.789761	6	-3.250531	1.105943	-0.501922
1	2.987651	-3.741426	0.121339	6	-2.516023	2.093814	-1.431774
1	4.257663	-2.770916	1.901048	6	-4.275353	0.330546	-1.352727
1	2.686410	-2.076680	2.291310	6	-4.014013	1.952398	0.546426
1	1.183109	-2.484231	-1.113041	6	1.705807	-0.626593	-1.903630
1	0.755698	-2.731884	0.609365	6	2.864962	-0.790154	-0.918831
1	1.463208	2.230869	1.062117	8	1.072253	-1.673107	-2.286467
1	3.214260	2.135963	1.341916	1	-1.668063	0.862152	0.943310
1	2.515076	3.552792	0.557112	1	-3.706974	-0.430647	1.715754
1	4.244102	1.820355	-2.275802	1	-1.178976	-0.707108	2.589640
1	3.977278	3.379717	-1.489116	1	-2.358871	-1.951947	3.020536
1	4.830927	2.104263	-0.622552	1	-4.355523	-2.495259	0.823429
1	1.684116	2.001251	-2.731489	1	-3.516414	-2.015462	-0.636822
1	0.548933	2.180875	-1.376114	1	-0.506414	-3.206339	1.938115
1	1.652586	3.491125	-1.777725	1	-2.686118	-4.041406	1.379815
1	-1.014634	-2.375031	-0.772003	1	-2.016376	-3.807660	-0.234099
6	-1.861923	1.935251	-0.569621	1	0.663051	-1.414883	0.797451
6	-2.566695	2.978864	0.028074	1	0.219435	-2.604235	-0.418450
6	-2.572611	3.119790	1.416879	1	0.078984	1.004776	-2.082315
6	-1.885997	2.189690	2.200467	1	2.010895	0.118662	-2.677646
6	-1.187596	1.138065	1.608150	1	-3.788352	-0.312242	-2.094187
1	-1.875806	1.828432	-1.651866	1	-4.945039	-0.285757	-0.745599
1	-3.110437	3.684550	-0.594976	1	-4.900141	1.045322	-1.900898
1	-3.114281	3.938224	1.883478	1	-3.326202	2.542992	1.163080
1	-1.904113	2.273999	3.284331	1	-4.684340	2.651404	0.033659
1	-0.708449	0.386154	2.226096	1	-4.632676	1.342712	1.212435
6	-3.317871	-1.368834	-1.617101	1	-1.743995	2.659642	-0.902434
6	-4.653399	-1.094843	-1.913895	1	-2.052898	1.587013	-2.284705
6	-5.565737	-0.876239	-0.878198	1	-3.237706	2.810327	-1.840613
6	-5.133788	-0.938858	0.449172	6	0.998968	2.913632	-0.663302
6	-3.797079	-1.210774	0.740485	6	1.434704	3.943842	0.166557
1	-2.610749	-1.556658	-2.424981	6	1.607729	3.722105	1.534870
1	-4.985536	-1.061058	-2.949142	6	1.351437	2.451307	2.051473
1	-6.608508	-0.667657	-1.105189	6	0.937654	1.413564	1.216964
1	-5.843502	-0.780381	1.258011	1	0.858520	3.106069	-1.724680
1	-3.435958	-1.287737	1.760985	1	1.627825	4.926751	-0.256041
				1	1.938424	4.525771	2.186668
				1	1.489194	2.257722	3.112335
				1	0.783713	0.431894	1.650494
				6	3.197040	-2.075306	-0.473345
				6	4.291749	-2.283657	0.366904
				6	5.082834	-1.204455	0.766701
6	-3.380409	-2.188836	0.430676	6	4.777605	0.079249	0.306903
6	-2.307527	-3.285361	0.682965	6	3.683222	0.281191	-0.534650
6	-1.127955	-2.535621	1.331779	1	2.595293	-2.904049	-0.833937
6	-1.845504	-1.473192	2.177468	1	4.538785	-3.290483	0.696991
6	-2.881746	-0.908249	1.180556	1	5.939529	-1.362939	1.417357
E (CH ₃ CN) = -1445.548329							
NImag = 1 (-238.1)							
3. <i>re,si-c</i> [‡] (-1445.24026914)							

1	5.397558	0.923705	0.599103
1	3.465782	1.281737	-0.899685

E (CH₃CN) = -1445.543201
NImag = 1 (-234.3)

4. *re, si-t[‡]* (-1445.23221915)

6	1.841428	-2.133328	-2.711835
6	2.179955	-0.652148	-2.453410
6	3.292674	-0.746655	-1.398031
6	2.710128	-1.768958	-0.398663
6	2.060004	-2.836711	-1.341217
6	0.998691	0.165068	-1.924713
16	0.207089	-0.479645	-0.376666
6	1.749360	-1.070165	0.600122
6	-0.655666	1.073587	0.176669
6	-2.199769	1.446492	-0.794757
8	-2.541010	2.601057	-0.392982
6	1.372474	-1.884782	1.887664
6	0.886038	-3.320864	1.607716
6	-3.108103	0.261256	-0.456203
6	-3.135157	-0.907650	-1.222507
6	-3.987101	-1.963635	-0.888121
6	-4.828028	-1.855845	0.221094
6	-4.819403	-0.682739	0.983029
6	-3.971015	0.369178	0.640942
6	0.239372	2.278030	0.310227
6	1.008264	2.500759	1.464209
6	1.847980	3.610745	1.577476
6	1.925935	4.533673	0.534664
6	1.148197	4.344095	-0.609621
6	0.310178	3.234476	-0.719138
6	2.645862	-1.954695	2.766083
6	0.280684	-1.175465	2.716044
1	2.215817	-0.135744	0.932231
1	3.507368	-2.222396	0.198873
1	3.547088	0.215868	-0.940017
1	4.204534	-1.149055	-1.856101
1	2.734049	-3.693070	-1.446972
1	1.121943	-3.224675	-0.945621
1	2.513918	-0.145071	-3.367039
1	2.524329	-2.537720	-3.466899
1	0.824130	-2.269130	-3.094496
1	1.307451	1.190430	-1.708441
1	0.172511	0.200715	-2.640732
1	-1.090797	0.787136	1.134571
1	-1.826223	1.325239	-1.849517
1	-0.012084	-3.334498	0.980624
1	1.653855	-3.937006	1.130226
1	0.626416	-3.803185	2.557167
1	3.008051	-0.953011	3.026549

1	2.420237	-2.480018	3.700955
1	3.463882	-2.495767	2.279390
1	0.554057	-0.144332	2.959395
1	-0.688516	-1.166002	2.207089
1	0.139846	-1.709698	3.662532
1	0.933442	1.807085	2.296957
1	2.431137	3.757112	2.483239
1	2.574017	5.402150	0.619153
1	1.179252	5.073413	-1.414905
1	-0.334089	3.129065	-1.583230
1	-3.967859	1.306591	1.190269
1	-5.486081	-0.586805	1.837303
1	-5.496065	-2.673248	0.481738
1	-4.003016	-2.864013	-1.498482
1	-2.495849	-0.986803	-2.101618

E (CH₃CN) = -1445.537486
NImag = 1 (-253.5)

5. *re, re-c[‡]* (-1445.24615275)

6	3.523742	-2.523218	-1.008523
6	2.695124	-1.630663	-1.955074
6	3.419489	-0.278883	-1.850150
6	3.598743	-0.121661	-0.324453
6	3.999929	-1.567488	0.122737
6	1.231422	-1.505480	-1.536224
16	0.972602	-0.858250	0.197969
6	2.314121	0.463471	0.331017
6	-0.691110	-0.102395	0.140851
6	-1.671577	-1.584883	-0.601394
6	-3.069132	-1.315974	-0.069622
6	2.496142	1.043548	1.781564
6	3.176931	0.074165	2.767640
6	-0.898302	1.247895	-0.422296
6	-0.342931	1.718939	-1.631160
6	-0.675245	2.972792	-2.145393
6	-1.585892	3.795115	-1.482119
6	-2.158233	3.344601	-0.289621
6	-1.816270	2.100488	0.232658
8	-1.079827	-2.661945	-0.249226
6	3.370779	2.314970	1.650115
6	1.151254	1.482257	2.396862
1	1.956784	1.290040	-0.292444
1	4.405029	0.583406	-0.104504
1	2.874821	0.553271	-2.311553
1	4.400988	-0.340987	-2.336535
1	5.086185	-1.624027	0.249311
1	3.560556	-1.844322	1.080980
1	2.684740	-2.024468	-2.979012
1	4.381504	-2.935042	-1.551375
1	2.945142	-3.370387	-0.626555

1	0.686742	-0.845190	-2.211057	6	-1.087635	-0.561341	3.451432
1	0.689150	-2.453117	-1.471478	6	2.756171	1.114967	2.456689
1	-1.018148	-0.165434	1.177784	6	3.894616	-0.905696	1.473040
1	2.611104	-0.856934	2.882497	8	0.718319	-1.644491	2.339413
1	4.199585	-0.176472	2.469978	6	-2.123065	0.059675	0.429099
1	3.231612	0.546020	3.755508	7	-2.329264	-0.800623	-0.606567
1	2.909248	3.050560	0.980815	16	-2.256627	-2.389752	-0.223877
1	3.481919	2.784873	2.633713	6	-3.624401	-3.062214	-1.188298
1	4.378330	2.100438	1.279995	6	-2.465083	1.498525	0.118174
1	0.590323	2.145027	1.731957	8	-1.015291	-2.980955	-0.779576
1	0.515390	0.626726	2.645424	8	-2.551985	-2.647459	1.208356
1	1.341234	2.023033	3.331198	1	-0.203203	1.205242	1.359112
1	-1.600499	-1.246287	-1.663865	1	2.196037	1.758551	-0.048238
1	-2.272663	1.766591	1.160456	1	4.265410	0.844539	-1.360736
1	-2.871660	3.968737	0.242623	1	2.180545	2.209522	-2.317301
1	-1.846459	4.768964	-1.886909	1	3.126626	1.249241	-3.465501
1	-0.221956	3.302330	-3.077173	1	4.166924	-1.188566	-2.511514
1	0.358092	1.106626	-2.187845	1	3.229681	-1.738456	-1.131950
6	-3.946128	-0.426188	-0.700311	1	0.773144	0.462245	-3.754498
6	-5.230591	-0.215942	-0.193594	1	2.309026	-1.375894	-3.902039
6	-5.650967	-0.897190	0.950632	1	1.325148	-1.951277	-2.553891
6	-4.783143	-1.795908	1.579188	1	-0.013463	1.377078	-1.512082
6	-3.503154	-2.005997	1.068932	1	-0.599784	-0.266834	-1.846200
1	-3.623042	0.098300	-1.597070	1	-2.515520	-0.243392	1.403209
1	-5.904731	0.474674	-0.695010	1	3.031150	-1.557463	1.633412
1	-6.651989	-0.737456	1.344156	1	4.497010	-1.308298	0.652016
1	-5.112109	-2.340011	2.461835	1	4.512338	-0.944293	2.378067
1	-2.818246	-2.720149	1.516884	1	4.493622	2.444334	0.705685
E (CH ₃ CN) = -1445.547268				1	5.286946	1.473280	1.951836
NImag = 1 (-244.5)				1	5.426538	0.998566	0.264020
<u>TSs for Aziridine formation</u>				1	2.399738	2.139375	2.288612
Addition of Stabilized ylide (R = COMe)				1	1.917104	0.494574	2.767015
<u>System 1 (R = COMe; X = Ph; Y = SO₂Me)</u>				1	3.459210	1.145171	3.296560
6. 1a-A-c[‡] (-1934.86292407)				1	-3.599050	-4.148272	-1.074198
6	0.293749	0.342338	-1.687145	1	-4.561360	-2.656262	-0.803591
6	1.311883	0.235844	-2.826918	1	-3.483628	-2.785446	-2.234358
6	2.488089	1.188956	-2.575143	1	-0.599877	-0.885741	4.373857
6	3.245088	0.467078	-1.441795	1	-1.438039	0.470360	3.556878
6	2.562289	0.724537	-0.058911	1	-1.953487	-1.211449	3.275012
16	0.980045	-0.340553	-0.113786	6	-2.522396	2.455305	1.142952
6	3.246099	-1.011219	-1.945947	6	-2.871299	3.778213	0.874013
6	1.999318	-1.151114	-2.876160	6	-3.176768	4.169372	-0.431464
6	3.469183	0.551267	1.207881	6	-3.143037	3.222342	-1.456418
6	4.739371	1.417509	1.004900	6	-2.796830	1.898147	-1.183178
6	-0.276738	0.147287	1.109250	1	-2.303041	2.160596	2.167058
6	-0.125117	-0.756306	2.294869	1	-2.913216	4.500941	1.684830
E (CH ₃ CN) = -1935.220688				1	-3.450900	5.199259	-0.644277
NImag = 1 (-255.4)				1	-3.399082	3.512021	-2.472570
				1	-2.801658	1.148397	-1.966702

7. 1a-A-$t^{\ddagger}$ (-1934.87160696)				1	-1.707050	-2.600494	2.849483
				1	-2.757679	-1.308108	2.244930
				6	-3.616709	-1.062494	-1.025150
6	0.923695	-1.076159	-1.823123	6	-4.922483	-1.540712	-0.917926
6	2.293753	-1.059659	-2.507687	6	-5.810396	-0.955956	-0.012693
6	3.072699	0.193054	-2.073253	6	-5.384646	0.113018	0.780019
6	3.500598	-0.179291	-0.637644	6	-4.080136	0.592955	0.671773
6	2.357640	0.103215	0.386825	1	-2.928054	-1.526221	-1.726309
16	1.056342	-1.220220	0.024853	1	-5.246667	-2.366874	-1.545097
6	3.949285	-1.669786	-0.796668	1	-6.828993	-1.326065	0.069422
6	3.218315	-2.212802	-2.061373	1	-6.074074	0.579995	1.478884
6	2.809562	0.200530	1.888475	1	-3.744564	1.439047	1.262169
6	3.633434	1.508837	2.003387	E (CH ₃ CN) = -1935.223192			
6	-0.618364	-0.790380	0.655017	NImag = 1 (-255.5)			
6	-1.297892	-2.089806	0.819280	8. 1b-A-$c^{\ddagger}$ (-1934.8622016)			
6	-2.269340	-2.246880	1.974067	6	1.050991	1.126105	1.504962
6	1.609581	0.351098	2.847074	6	2.399657	1.764605	1.855448
6	3.667597	-0.984648	2.370061	6	3.413904	0.689159	2.260185
8	-1.083888	-3.019077	0.036892	6	3.749816	0.041983	0.902463
6	-1.793560	0.548337	-0.394464	6	2.643037	-0.976867	0.482162
7	-1.607009	1.791734	0.103611	16	1.158379	0.110807	-0.042747
16	-0.348360	2.649049	-0.464949	6	3.926120	1.289468	-0.019251
6	-1.109106	4.243600	-0.816224	6	3.067989	2.425257	0.623934
6	-3.178670	0.004255	-0.227007	6	3.057651	-2.081805	-0.556426
8	0.657700	2.895401	0.600509	6	4.438522	-2.655154	-0.147218
8	0.193966	2.118242	-1.749046	6	-0.399416	-0.818584	-0.008513
1	-0.527658	-0.169474	1.537474	6	-0.647798	-1.421964	-1.345680
1	1.885824	1.054612	0.137432	6	-1.631483	-2.579591	-1.431828
1	4.342413	0.437222	-0.313791	6	2.066441	-3.264438	-0.481182
1	2.482191	1.111843	-2.130816	6	3.152146	-1.572524	-2.008951
1	3.963719	0.312300	-2.702662	8	-0.125533	-0.984791	-2.363968
1	5.034879	-1.703291	-0.937322	6	-1.908414	0.386714	0.326747
1	3.730255	-2.276490	0.082770	7	-2.156914	1.241514	-0.701763
1	2.097628	-1.081247	-3.586552	16	-1.391446	2.678933	-0.636121
1	3.937928	-2.436788	-2.856014	6	-2.502005	3.683227	-1.631442
1	2.664535	-3.136158	-1.859441	6	-3.025130	-0.580892	0.634970
1	0.391259	-0.149638	-2.038645	8	-1.362135	3.244528	0.743745
1	0.318784	-1.948422	-2.084449	8	-0.073148	2.679081	-1.325523
1	-1.365841	0.305418	-1.366900	1	-0.430226	-1.509145	0.834093
1	3.131711	-1.938256	2.295340	1	2.305985	-1.497158	1.387263
1	4.606357	-1.073135	1.814671	1	4.680604	-0.521895	0.970347
1	3.925513	-0.838107	3.425378	1	3.032938	-0.022022	3.003442
1	3.045079	2.369598	1.670018	1	4.314218	1.155955	2.678903
1	3.910275	1.669089	3.051702	1	4.984562	1.569911	-0.034724
1	4.564277	1.476923	1.427305	1	3.635071	1.097750	-1.054095
1	0.940582	1.155935	2.526957	1	2.200916	2.488647	2.653717
1	1.041254	-0.580446	2.943404	1	3.707935	3.251304	0.950676
1	1.979307	0.599613	3.848659	1	2.326210	2.834872	-0.068425
1	-0.311804	4.924291	-1.122949	1	0.688006	0.479169	2.311232
1	-1.839691	4.117147	-1.616823				
1	-1.591568	4.603099	0.093839				
1	-3.020134	-2.998798	1.720750				

1	0.308046	1.898259	1.291462	6	-3.696517	1.530551	-0.712095
1	2.197504	-1.187525	-2.378626	6	-4.649353	0.383302	1.318156
1	3.908911	-0.788329	-2.113339	6	-2.609200	1.798021	1.514341
1	3.451502	-2.400632	-2.662267	7	1.831613	1.422073	-0.891218
1	4.472440	-2.937025	0.912759	16	1.281452	2.950864	-0.683344
1	4.633543	-3.559875	-0.733242	8	-0.203103	3.007473	-0.804588
1	5.259767	-1.960463	-0.346713	8	1.851782	3.612707	0.514960
1	2.015538	-3.675404	0.535171	6	1.945500	3.753873	-2.150846
1	1.058208	-2.991397	-0.789179	6	0.810915	0.314597	3.545180
1	2.399543	-4.068266	-1.146915	1	-2.333127	-0.956499	1.379607
1	-1.518250	0.810732	1.257338	1	-4.189234	-1.670425	-0.240612
1	-2.591427	3.223722	-2.616890	1	-2.183596	-3.168367	0.742621
1	-3.473326	3.734171	-1.137422	1	-3.085643	-3.780090	-0.657143
1	-2.053832	4.675992	-1.709306	1	-3.917123	-1.673923	-2.562520
1	-1.819429	-3.069365	-0.473561	1	-2.811406	-0.337822	-2.315581
1	-2.587296	-2.203609	-1.810963	1	-0.709293	-3.815598	-1.379251
1	-1.247632	-3.303157	-2.157437	1	-2.173112	-3.112633	-3.142008
6	-2.996768	-1.355912	1.803047	1	-1.069385	-1.739984	-3.117993
6	-4.048313	-2.216219	2.117860	1	0.178877	-2.318023	0.379075
6	-5.153135	-2.308662	1.268212	1	0.706742	-1.793413	-1.243548
6	-5.200402	-1.525220	0.113404	1	0.079860	1.390463	1.226450
6	-4.147652	-0.664548	-0.198720	1	2.373149	1.313499	1.139449
1	-2.149429	-1.276087	2.482081	1	-2.798357	1.829445	-1.262986
1	-4.010261	-2.805617	3.030422	1	-4.339324	0.933237	-1.366202
1	-5.975571	-2.975832	1.512335	1	-4.244688	2.448059	-0.468465
1	-6.064794	-1.577891	-0.543733	1	-4.442415	-0.152691	2.252540
1	-4.180536	-0.031606	-1.079306	1	-5.219053	1.283724	1.572190
E (CH ₃ CN) = -1935.224761				1	-5.299241	-0.244481	0.700742
NImag = 1 (-253.3)				1	-2.228820	1.317496	2.423801
9. 1c-A-<i>c</i>[‡] (-1934.8749254)				1	-1.789009	2.302888	0.996451
6	3.210265	-0.982331	-1.174203	1	-3.313012	2.577644	1.827080
6	2.833195	-0.538243	0.101742	1	1.562053	4.776388	-2.161645
6	3.258112	-1.269909	1.219151	1	3.034897	3.750305	-2.090932
6	4.016039	-2.430923	1.067409	1	1.604627	3.206858	-3.031130
6	4.368197	-2.876406	-0.208272	1	-0.010112	0.885015	3.999965
6	3.967001	-2.144128	-1.327822	1	1.172717	-0.406999	4.282029
6	2.051852	0.737030	0.263827	1	1.599084	1.032118	3.294628
6	0.304031	0.339307	1.072125	1	3.004029	-0.927486	2.218552
6	0.276146	-0.430605	2.327737	1	4.335485	-2.984283	1.946511
8	-0.130044	-1.589600	2.439364	1	4.960845	-3.779642	-0.327384
16	-0.761164	-0.204602	-0.281261	1	4.254612	-2.471872	-2.323814
6	-0.152143	-1.938771	-0.586096	1	2.913474	-0.388357	-2.032264
6	-1.205916	-2.851237	-1.216551	E (CH ₃ CN) = -1935.22858			
6	-2.436088	-2.969474	-0.304122	NImag = 1 (-252.4)			
6	-3.134613	-1.608604	-0.519426	10. 1c-A-<i>t</i>[‡] (-1934.87179279)			
6	-2.506038	-0.518003	0.392572	6	-1.018640	-1.814093	-0.495655
6	-2.988456	-1.383310	-2.060775	6	-2.366444	-2.449939	-0.832459
6	-1.806994	-2.287683	-2.521425	6	-3.426204	-2.083780	0.218731
6	-3.342515	0.795628	0.595408	6	-3.769216	-0.624085	-0.154772

6	-2.742559	0.357474	0.472642	1	1.087273	1.986075	-2.115726
16	-1.089224	0.050752	-0.424990	1	1.976738	4.275432	-2.422847
6	-3.819921	-0.672846	-1.717445	1	3.926811	5.045859	-1.080951
6	-2.989734	-1.920520	-2.141604	1	4.988901	3.493711	0.546721
6	-3.152759	1.867695	0.533313	1	4.098137	1.183922	0.827655
6	-4.325424	1.969243	1.540540				
6	0.351749	0.423446	0.615934				
6	0.301254	-0.140386	2.004359				
6	1.497739	0.186742	2.861100				
8	-0.622817	-0.835791	2.416010				
6	-2.005324	2.739828	1.086808				
6	-3.601511	2.461631	-0.815269	6	3.508072	-0.402008	-1.128031
6	1.961474	0.051001	-0.419050	6	2.984521	-0.535996	0.165060
7	2.826311	-0.826806	0.166878	6	3.744858	-1.202518	1.134434
16	2.481155	-2.405204	-0.068949	6	4.993202	-1.744326	0.817035
8	1.933363	-2.677936	-1.427468	6	5.497211	-1.622382	-0.478713
6	2.517611	1.443095	-0.594859	6	4.752014	-0.945762	-1.448281
6	4.130414	-3.123027	0.002678	6	1.619126	0.046851	0.518281
8	1.707224	-2.974279	1.063691	6	0.420418	-0.953844	0.171416
1	-2.525148	0.030271	1.491183	6	0.598251	-1.913175	-1.010662
1	-4.745183	-0.341108	0.250007	8	0.168697	-1.701918	-2.130151
1	-3.073564	-2.198843	1.248301	16	-1.037152	0.207639	0.085109
1	-4.313477	-2.715760	0.088808	6	-1.087695	0.979018	-1.641469
1	-4.860559	-0.771824	-2.043364	6	-2.426573	0.908475	-2.381556
1	-3.437020	0.237678	-2.180583	6	-3.081957	-0.474309	-2.275901
1	-2.175699	-3.528530	-0.877752	6	-3.607788	-0.475452	-0.819730
1	-3.642049	-2.685891	-2.575204	6	-2.516854	-1.004590	0.143475
1	-2.231389	-1.683786	-2.895679	6	-4.055517	1.009045	-0.581039
1	-0.647251	-2.142814	0.474506	6	-3.505891	1.822392	-1.779390
1	-0.253906	-2.025944	-1.247185	6	-2.972155	-1.324726	1.617002
1	0.436814	1.505868	0.642690	6	-3.546716	-0.120931	2.391850
1	1.461953	-0.293280	-1.333065	6	-4.055453	-2.427706	1.535728
1	-2.817535	2.385532	-1.577112	6	-1.808646	-1.898834	2.455546
1	-4.505022	1.980199	-1.201249	7	1.299846	1.270700	-0.167883
1	-3.828210	3.526295	-0.686028	16	1.241387	2.618736	0.722150
1	-4.043104	1.577434	2.524510	8	0.221922	3.505440	0.110267
1	-4.606817	3.020611	1.667870	8	1.141865	2.352059	2.180978
1	-5.218391	1.433846	1.203927	6	2.823749	3.472017	0.481483
1	-1.582375	2.323872	2.007869	6	1.294944	-3.219789	-0.675721
1	-1.197784	2.870474	0.358692	1	-2.141039	-1.942029	-0.281087
1	-2.386688	3.740681	1.318141	1	-4.459429	-1.154749	-0.727656
1	4.014054	-4.206298	-0.072735	1	-2.396754	-1.299305	-2.493571
1	4.719545	-2.737964	-0.830874	1	-3.923467	-0.539499	-2.976101
1	4.587058	-2.852936	0.956070	1	-5.145398	1.080224	-0.506192
1	1.302143	-0.111269	3.893165	1	-3.657421	1.408455	0.352754
1	2.348599	-0.377083	2.453001	1	-2.193507	1.183922	-3.418162
1	1.759816	1.249728	2.809630	1	-4.291624	1.993715	-2.524662
6	1.934114	2.321299	-1.519416	1	-3.116724	2.800576	-1.480137
6	2.435610	3.611185	-1.694807	1	-0.303133	0.464823	-2.184383
6	3.532380	4.042250	-0.945214	1	-0.770999	1.996953	-1.408114
6	4.126381	3.170047	-0.030595	1	0.217729	-1.578469	1.042822
6	3.626695	1.878536	0.140810	1	1.574227	0.161822	1.611312

E (CH₃CN) = -1935.227477

NImag = 1 (-230.5)

11. **1c-c** (-1934.8742231)

1	-2.844045	0.718328	2.428537	6	-3.626718	-3.164009	0.901509
1	-4.491405	0.233094	1.970850	8	3.878984	-2.525279	0.445572
1	-3.747473	-0.423312	3.426199	8	4.250990	-0.782431	-1.341891
1	-3.704081	-3.300053	0.970712	1	-2.264480	-1.716701	-0.835558
1	-4.308507	-2.768092	2.546079	1	-4.650623	-1.014261	-0.275063
1	-4.981033	-2.072209	1.073769	1	-3.239674	-0.439423	-2.494436
1	-1.340601	-2.765393	1.971625	1	-4.731967	0.466949	-2.179323
1	-1.040123	-1.148263	2.670583	1	-5.191363	1.035865	0.709539
1	-2.192135	-2.239075	3.423620	1	-3.608383	0.972176	1.453311
1	2.786972	4.419333	1.024854	1	-2.993490	2.212744	-2.471747
1	3.627799	2.843269	0.870826	1	-4.538613	2.759626	-0.723918
1	2.961402	3.650402	-0.586495	1	-3.027169	2.885436	0.170971
1	0.565787	-3.889247	-0.197218	1	-1.014129	0.792752	-2.202615
1	1.643341	-3.687701	-1.598625	1	-0.923477	2.202642	-1.104045
1	2.128620	-3.083929	0.017463	1	0.664127	-1.291779	0.531282
1	3.362065	-1.286526	2.149971	1	2.219711	0.386263	-1.267760
1	5.574007	-2.250940	1.583725	1	-2.497069	-0.499624	2.850855
1	6.469198	-2.039597	-0.728565	1	-4.166002	-0.956497	2.446446
1	5.146347	-0.832942	-2.455124	1	-3.146006	-2.052709	3.378549
1	2.938140	0.156158	-1.864255	1	-3.302123	-3.700532	0.002294
E (CH ₃ CN) = -1935.234581				1	-3.670972	-3.887888	1.722332
NImag = 0				1	-4.645720	-2.801619	0.734861
12. 1c-R[‡] (-1934.8630892)				1	-0.835526	-3.167477	0.713702
6	-3.669894	2.189208	-0.378499	1	-0.564806	-1.991042	2.022384
6	-2.954553	1.559489	-1.591339	1	-1.434297	-3.481643	2.343300
6	-3.727496	0.248346	-1.797189	1	6.250513	-1.045052	0.772360
6	-3.825201	-0.302457	-0.357271	1	5.526667	0.599532	0.786413
6	-4.120335	0.979439	0.490326	1	5.152055	-0.559368	2.103535
6	-2.542959	-1.094317	0.016965	1	1.838357	-2.981904	-0.995623
16	-1.132607	0.183923	0.120334	1	1.246655	-3.082255	-2.700830
6	-1.468472	1.289939	-1.348077	1	2.437305	-1.852598	-2.164845
6	0.494572	-0.640506	-0.323636	1	1.775262	2.599366	-1.786520
6	0.397989	-1.477752	-1.604654	1	1.299084	4.933323	-1.102406
6	1.536793	-2.417440	-1.883980	1	0.749050	5.448659	1.269878
6	-2.639339	-2.029281	1.274437	1	0.730006	3.615894	2.953271
6	-1.284851	-2.696120	1.594848	1	1.261297	1.287369	2.260875
6	1.839067	0.349922	-0.236358	E (CH ₃ CN) = -1935.228475			
7	2.739996	-0.228947	0.688102	NImag = 1 (-26.9)			
16	3.970227	-1.083298	0.095690	13. 1c-t (-1934.8687874)			
6	5.373818	-0.450824	1.040361	6	-1.818775	2.208055	-1.503825
6	1.491914	1.774152	0.183123	6	-1.665113	1.701628	-0.204136
6	1.217780	2.083467	1.523975	6	-1.534564	2.608993	0.853734
6	0.941115	3.394086	1.910068	6	-1.532413	3.988531	0.622352
6	0.954163	4.425529	0.965751	6	-1.661107	4.478015	-0.676440
6	1.256929	4.135470	-0.365096	6	-1.810372	3.581025	-1.739788
6	1.523785	2.818109	-0.750626	6	-1.694947	0.193553	0.045713
8	-0.558748	-1.384318	-2.366039	6	-0.397587	-0.485220	-0.582161
6	-3.144092	-1.332343	2.552744	6	-0.339952	-2.028330	-0.491436

8	0.321827	-2.576109	0.378886	E (CH ₃ CN) = -1935.236745		
16	1.161374	0.325074	0.140358	NImag = 0		
6	0.924209	-0.044890	1.958095			
6	2.231489	-0.149208	2.745500	14. 1c -E [‡] (-1934.8668712)		
6	3.150123	-1.227336	2.149299	6	-1.078009	0.660966 -1.776396
6	3.697721	-0.527266	0.885157	6	-2.393780	0.762079 -2.551373
6	2.703806	-0.687974	-0.297170	6	-3.247380	-0.498202 -2.337918
6	3.962083	0.933357	1.378255	6	-3.796859	-0.281673 -0.910513
6	3.104463	1.119928	2.663712	6	-2.751462	-0.737676 0.145064
6	3.249632	-0.379584	-1.734028	6	-1.284753	0.442536 0.061024
6	3.941724	0.989648	-1.872372	16	-4.160479	1.237985 -0.909196
6	4.272200	-1.494306	-2.066261	6	-3.323041	1.886763 -2.050449
6	2.126741	-0.460345	-2.789924	6	-3.268306	-0.944879 1.611508
7	-2.797225	-0.443278	-0.605531	6	-4.226728	-2.160161 1.590980
16	-3.772755	-1.300493	0.351169	6	0.569649	-0.588477 0.456147
8	-4.055078	-2.624429	-0.262143	6	0.427003	-2.010330 -0.106859
8	-3.340799	-1.298674	1.778352	6	0.795680	-3.168736 0.785143
6	-5.361413	-0.430478	0.299657	6	0.028379	-2.178654 -1.248880
6	-1.095059	-2.814068	-1.526124	8	-2.101739	-1.294510 2.557675
1	2.346424	-1.719425	-0.295515	6	-4.015694	0.268550 2.197436
1	4.629389	-0.996989	0.557563	6	1.730186	0.231485 -0.089161
1	2.635623	-2.169584	1.938527	7	2.721298	-0.620802 0.544314
1	3.972761	-1.435028	2.843990	16	3.788759	-1.353344 -0.464695
1	5.026662	1.059332	1.599873	8	3.624393	-0.938059 -1.878955
1	3.713034	1.682213	0.625498	6	1.778170	1.684666 0.357433
1	1.934689	-0.375599	3.776675	6	5.376223	-0.689927 0.097737
1	3.746111	1.177743	3.549218	8	3.844969	-2.805140 -0.173735
1	2.508695	2.038916	2.640100	1	-2.347941	-1.698992 -0.189176
1	0.357716	-0.973602	2.002255	1	-4.688773	-0.893173 -0.744407
1	0.310091	0.787937	2.307086	1	-2.684495	-1.430328 -2.454403
1	-0.371041	-0.182426	-1.629544	1	-4.076065	-0.512306 -3.056357
1	-1.682536	0.009183	1.128561	1	-5.232434	1.356839 -1.099018
1	3.268004	1.818037	-1.626244	1	-3.957525	1.715564 0.049393
1	4.832827	1.068916	-1.242804	1	-2.112928	0.901076 -3.602564
1	4.263148	1.128981	-2.910847	1	-3.974503	2.214694 -2.867585
1	3.816866	-2.489457	-2.003184	1	-2.766429	2.766959 -1.710975
1	4.637752	-1.359585	-3.090195	1	-0.488468	-0.191923 -2.114652
1	5.145380	-1.476015	-1.406615	1	-0.491454	1.579197 -1.859082
1	1.558928	-1.394853	-2.718470	1	0.530646	-0.545267 1.541286
1	1.430181	0.382385	-2.718151	1	1.759210	0.180097 -1.184176
1	2.565316	-0.420717	-3.792833	1	-3.392367	1.169420 2.205129
1	-6.089981	-1.015692	0.866439	1	-4.937229	0.491048 1.651449
1	-5.236923	0.559571	0.744012	1	-4.295562	0.054833 3.235471
1	-5.671939	-0.343885	-0.743317	1	-3.731053	-3.055900 1.198455
1	-0.632122	-3.801236	-1.626804	1	-4.558561	-2.383741 2.610999
1	-2.135713	-2.930425	-1.178597	1	-5.123729	-1.977062 0.991466
1	-1.144005	-2.298652	-2.489615	1	-1.517019	-2.143310 2.188090
1	-1.468873	2.236310	1.874459	1	-1.427832	-0.444258 2.712004
1	-1.441243	4.677007	1.458918	1	-2.495010	-1.570538 3.542171
1	-1.661570	5.549394	-0.860480	1	6.164026	-1.188331 -0.472677
1	-1.935333	3.956249	-2.752662			
1	-1.990579	1.511978	-2.320600			

1	5.393017	0.386440	-0.083336	1	-3.326116	2.880886	-1.397951
1	5.482284	-0.902793	1.162581	1	-0.907741	0.045961	-1.634329
1	0.210551	-4.049694	0.504901	1	-0.990029	1.784932	-1.304968
1	1.861702	-3.372393	0.606077	1	1.643452	-0.506814	1.703970
1	0.679038	-2.940583	1.847980	1	2.288342	0.273731	-1.229047
6	1.777223	2.720284	-0.584807	1	-4.428612	1.018602	2.238118
6	1.835688	4.057366	-0.181868	1	-5.879132	0.391357	1.432639
6	1.898387	4.374152	1.174598	1	-5.441882	-0.192280	3.040057
6	1.919260	3.347408	2.123640	1	-4.579986	-3.075234	0.769419
6	1.866434	2.015485	1.717593	1	-5.567077	-2.574699	2.151665
1	1.759089	2.476868	-1.645201	1	-5.958578	-1.984461	0.536595
1	1.842429	4.847323	-0.928586	1	-2.516212	-2.277324	2.111607
1	1.944420	5.412516	1.492303	1	-2.491629	-0.648517	2.808757
1	1.988019	3.587434	3.181719	1	-3.645335	-1.848758	3.408576
1	1.927300	1.217936	2.453331	1	6.492274	-2.181652	-0.507170
E (CH ₃ CN) = -1935.228843				1	6.134065	-0.463453	-0.134134
NImag = 1 (-197.6)				1	5.868912	-1.729164	1.117204
15. 1c -PC (-1934.92270128)				1	-0.128233	-3.526577	0.302364
6	-1.578384	0.861241	-1.343883	1	1.357467	-3.420388	1.291044
6	-2.729683	0.987651	-2.351811	1	-0.048460	-2.425289	1.714029
6	-3.560519	-0.307265	-2.381949	6	2.130887	2.849650	-0.524029
6	-4.369799	-0.214558	-1.068265	6	2.191320	4.178469	-0.102435
6	-3.478189	-0.654473	0.124943	6	2.720081	4.490926	1.150474
16	-2.122801	0.597856	0.402164	6	3.190731	3.467892	1.977506
6	-4.816491	1.277775	-1.065225	6	3.127749	2.140200	1.557986
6	-3.779876	2.044473	-1.939996	1	1.727962	2.608662	-1.504996
6	-4.198117	-1.025745	1.466745	1	1.830607	4.968302	-0.755726
6	-5.129102	-2.232094	1.206757	1	2.770203	5.525297	1.479441
6	1.902912	-0.701155	0.664303	1	3.610777	3.705501	2.951316
6	1.049134	-1.767868	-0.020907	1	3.509790	1.346223	2.193578
6	0.513427	-2.856047	0.877043	E (CH ₃ CN) = -1935.267601			
8	0.823292	-1.715994	-1.214278	NImag = 0			
6	-3.146800	-1.471832	2.507402	16. 1d -A-c [‡] (-1934.8744851)			
6	-5.032559	0.120482	2.071568	6	-2.131196	-1.466135	-2.890977
6	2.477538	0.407481	-0.164678	6	-1.428735	-2.286675	-1.790518
7	3.361636	-0.602539	0.442353	6	-2.586067	-2.628984	-0.838993
16	4.173375	-1.754574	-0.561458	6	-3.307763	-1.269540	-0.697887
8	4.135293	-1.348327	-1.968954	6	-3.264268	-0.694903	-2.153148
6	2.590799	1.818562	0.304489	6	-2.628613	-0.406836	0.399875
6	5.846930	-1.499692	0.051468	16	-0.907421	0.060773	-0.261252
8	3.720240	-3.086492	-0.141671	6	-0.323954	-1.526121	-1.061491
1	-2.969187	-1.575675	-0.189075	6	-3.439319	0.820723	0.940890
1	-5.236858	-0.882493	-1.104962	6	-3.948514	1.780193	-0.151796
1	-2.949428	-1.215005	-2.454507	6	0.269905	0.241534	1.098744
1	-4.241167	-0.295064	-3.243078	6	0.246137	-0.828308	2.133917
1	-5.819902	1.356457	-1.499986	8	-0.378225	-1.879986	2.008084
1	-4.866792	1.694024	-0.059080	6	-4.655531	0.246698	1.709363
1	-2.285174	1.212136	-3.330169	6	-2.611913	1.643214	1.952258
1	-4.259483	2.458088	-2.834778	6	1.099892	-0.575266	3.361496

6	2.037464	0.596733	0.329815
6	1.838645	1.987308	-0.221518
7	2.485460	-0.309575	-0.577817
16	3.215297	-1.648058	0.021195
8	3.601126	-1.500384	1.448959
8	2.457789	-2.864527	-0.350945
6	4.742719	-1.692060	-0.939310
1	-2.399285	-1.053550	1.249083
1	-4.342681	-1.413618	-0.374562
1	-2.251579	-3.044261	0.116387
1	-3.255718	-3.356666	-1.313841
1	-4.229895	-0.857556	-2.643082
1	-3.087202	0.381354	-2.172157
1	-0.941343	-3.181508	-2.195534
1	-2.554068	-2.144084	-3.640302
1	-1.442379	-0.796812	-3.417908
1	0.123565	-2.126894	-0.273152
1	0.475734	-1.187410	-1.721184
1	0.115027	1.227426	1.526487
1	-3.127329	2.196386	-0.746078
1	-4.656475	1.296589	-0.831278
1	-4.470763	2.621732	0.318352
1	-4.340564	-0.435057	2.508122
1	-5.215967	1.066928	2.172074
1	-5.349875	-0.291469	1.056831
1	-2.160305	1.009809	2.723658
1	-1.819638	2.220836	1.464581
1	-3.265929	2.364572	2.454914
1	2.523026	0.605977	1.312084
1	4.486655	-1.689281	-1.999996
1	5.346766	-0.819212	-0.686111
1	5.266766	-2.613531	-0.675440
1	0.708711	-1.163259	4.195357
1	2.117215	-0.919402	3.133209
1	1.147097	0.483895	3.636920
6	1.773896	3.087032	0.646250
6	1.605870	4.380580	0.152581
6	1.498872	4.594328	-1.223513
6	1.574775	3.507283	-2.096591
6	1.749282	2.214866	-1.600660
1	1.872181	2.929783	1.719186
1	1.568161	5.221180	0.840727
1	1.369250	5.601148	-1.611732
1	1.508164	3.667164	-3.169891
1	1.843411	1.367573	-2.271587

E (MeCN) = -1935.229815
NImag = 1 (-251.8)

17. **1d-A- $t^{\ddagger}$** (-1934.87095792)

6	1.162492	1.930973	-0.140296
6	2.560724	2.539908	-0.250694
6	3.527699	1.871628	0.739351
6	3.810018	0.515692	0.055893
6	2.694484	-0.509488	0.393999
16	1.110165	0.096334	-0.475659
6	3.953701	0.908200	-1.451276
6	3.240038	2.282445	-1.612427
6	3.012595	-2.020830	0.121808
6	4.156825	-2.412175	1.091057
6	-0.358600	-0.437380	0.433339
6	-0.328861	-0.221134	1.902740
6	-1.344845	-1.026976	2.680317
8	0.447085	0.555859	2.466355
6	1.807500	-2.926085	0.457827
6	3.457457	-2.324689	-1.321814
6	-1.997723	0.114124	-0.456127
7	-3.004328	-0.707142	-0.036125
16	-2.957208	-2.203826	-0.718034
8	-1.991544	-3.095303	-0.009034
6	-2.241368	1.574515	-0.199088
6	-4.607749	-2.788805	-0.308857
8	-2.829054	-2.165814	-2.193345
1	2.443478	-0.409212	1.453179
1	4.742688	0.083568	0.427901
1	3.115780	1.772796	1.748601
1	4.454053	2.455551	0.804856
1	5.014421	0.990289	-1.709247
1	3.529467	0.159122	-2.120735
1	2.434275	3.611588	-0.054214
1	3.970064	3.073897	-1.812819
1	2.526476	2.289414	-2.443832
1	0.750454	2.053122	0.859916
1	0.475179	2.349405	-0.877472
1	-0.512932	-1.483263	0.176134
1	2.697881	-2.031539	-2.055240
1	4.399490	-1.831403	-1.580554
1	3.613473	-3.403785	-1.432063
1	3.882345	-2.219109	2.134864
1	4.361294	-3.484041	0.994404
1	5.092630	-1.884902	0.880343
1	1.393067	-2.706923	1.447888
1	0.999073	-2.855990	-0.275243
1	2.133112	-3.972165	0.462541
1	-1.614851	-0.052223	-1.471691
1	-4.735330	-2.755899	0.774029
1	-5.338992	-2.148113	-0.803723
1	-4.683007	-3.815109	-0.674243

1	-1.343263	-0.705770	3.724564	1	-0.007129	-2.373655	-0.871601
1	-2.336565	-0.925471	2.221094	1	0.061013	1.200524	1.481261
1	-1.104423	-2.095054	2.612744	1	-2.114417	2.133046	-1.744728
6	-2.098370	2.483593	-1.256630	1	-3.860162	1.802243	-1.714262
6	-2.352299	3.844664	-1.072773	1	-3.241005	3.352372	-1.146196
6	-2.755250	4.315258	0.177292	1	-4.224238	1.574396	2.028886
6	-2.916307	3.414532	1.233622	1	-4.496221	3.017839	1.041539
6	-2.669309	2.055348	1.045606	1	-5.095294	1.457489	0.488041
1	-1.805979	2.116202	-2.238560	1	-1.712565	2.301793	2.036019
1	-2.244985	4.532287	-1.907871	1	-0.919785	2.690147	0.482518
1	-2.953258	5.373436	0.326108	1	-2.261284	3.663086	1.058661
1	-3.241323	3.771751	2.207316	1	2.530798	0.125418	1.234184
1	-2.819821	1.359557	1.863969	1	4.008656	-1.596864	-2.338042
E (MeCN) = -1935.230318				1	4.789910	-0.862265	-0.899789
NImag = 1 (-243.8)				1	4.907095	-2.628834	-1.179446
18. 1d-c (-1934.88266)				1	1.083416	-1.181439	4.292937
6	-2.586898	-2.215918	-2.135468	1	2.169981	-1.388215	2.871989
6	-2.187522	-2.688615	-0.723960	1	1.868098	0.232095	3.516033
6	-3.355858	-2.194655	0.140594	6	2.156995	2.789675	0.757023
6	-3.533221	-0.742577	-0.354083	6	2.356968	4.079149	0.263331
6	-3.340994	-0.875168	-1.902817	6	2.402139	4.299031	-1.115737
6	-2.553516	0.219259	0.377685	6	2.253397	3.220365	-1.988312
16	-0.808185	-0.235094	-0.234308	6	2.056875	1.929685	-1.490371
6	-0.858453	-2.110539	-0.241447	1	2.140736	2.628665	1.834718
6	-2.907538	1.749313	0.271606	1	2.487259	4.909006	0.953512
6	-3.037189	2.275689	-1.171483	1	2.560704	5.301773	-1.504038
6	0.380808	0.207586	1.154570	1	2.296048	3.381520	-3.062829
6	0.226448	-0.664277	2.417538	1	1.958892	1.075461	-2.151899
8	-0.835720	-1.205961	2.676935	E (CH ₃ CN) = -1935.24136			
6	-4.261891	1.948376	0.998789	NImag = 0			
6	-1.880050	2.637292	1.005196	19. 1d-R[‡] (-1934.8615465)			
6	1.409833	-0.748956	3.345046	6	-3.374286	2.477213	-0.822374
6	1.782871	0.285625	0.445417	6	-2.372039	1.775405	-1.759137
6	2.000004	1.699785	-0.112549	6	-3.135919	0.512616	-2.181807
7	1.817006	-0.727960	-0.575624	6	-3.690822	0.002625	-0.832505
16	2.751216	-2.007823	-0.341787	6	-4.111615	1.317681	-0.095133
8	3.202120	-2.152582	1.074975	6	-2.637825	-0.877988	-0.107985
8	2.104914	-3.181296	-0.975778	16	-1.205642	0.272479	0.389441
6	4.275940	-1.743851	-1.289905	6	-1.045366	1.427218	-1.083179
1	-2.544415	-0.043674	1.437756	6	-3.169379	-1.777266	1.064778
1	-4.539248	-0.383490	-0.125838	6	-3.980779	-1.018358	2.132441
1	-3.164943	-2.267798	1.216037	6	0.373734	-0.752471	0.296530
1	-4.259616	-2.774806	-0.083652	6	0.483532	-1.588626	-1.019005
1	-4.319298	-0.886705	-2.394428	8	-0.075134	-1.230953	-2.046011
1	-2.792213	-0.035125	-2.330499	6	-4.079220	-2.850514	0.414792
1	-2.057441	-3.776869	-0.680098	6	-2.028507	-2.530246	1.781031
1	-3.250541	-2.955432	-2.596349	6	1.080020	-2.973454	-0.887474
1	-1.721240	-2.103709	-2.796225	6	1.738878	0.023591	0.538359
1	-0.654497	-2.424537	0.779664	6	1.649833	1.549048	0.615211

7	2.573854	-0.461006	-0.536697	6	3.763382	0.432789	0.114717
16	3.867924	-1.324541	-0.089236	6	3.945336	0.908751	-1.363866
8	3.708922	-1.923526	1.267118	6	2.608970	-0.572886	0.377351
8	4.236760	-2.220381	-1.203398	16	1.068323	0.160044	-0.464547
6	5.253332	-0.159006	0.068107	6	1.179827	1.974999	-0.033019
1	-2.183358	-1.536794	-0.850919	6	2.873342	-2.073784	0.003650
1	-4.559318	-0.640975	-0.993399	6	3.269263	-2.305050	-1.467258
1	-2.509911	-0.218558	-2.701387	6	-0.471122	-0.402543	0.418275
1	-3.965886	0.786446	-2.844237	6	-0.412189	-0.233054	1.928619
1	-5.197205	1.445854	-0.152007	8	0.452336	0.434213	2.488168
1	-3.859899	1.297298	0.966144	6	4.031735	-2.554287	0.915137
1	-2.101184	2.407799	-2.613670	6	1.651433	-2.961749	0.323591
1	-4.078658	3.066694	-1.419040	6	-1.461205	-0.994865	2.693910
1	-2.886225	3.168252	-0.126590	6	-1.810967	0.113636	-0.390655
1	-0.370742	0.914976	-1.766487	6	-2.109561	1.594179	-0.218986
1	-0.566829	2.308551	-0.656489	7	-2.936088	-0.673583	-0.008292
1	0.230105	-1.445076	1.126135	16	-2.902050	-2.151255	-0.670097
1	-3.391104	-0.230406	2.614474	8	-2.816150	-2.151226	-2.153560
1	-4.890551	-0.568620	1.724461	8	-1.904010	-3.060486	-0.003646
1	-4.287940	-1.719816	2.916278	6	-4.532128	-2.756661	-0.205011
1	-3.538831	-3.431705	-0.341482	1	2.357986	-0.535109	1.439935
1	-4.424058	-3.548389	1.185511	1	4.672441	-0.055465	0.473789
1	-4.969747	-2.422988	-0.055905	1	3.090398	1.610397	1.872160
1	-1.390030	-3.080117	1.081015	1	4.472933	2.291946	0.994268
1	-1.402179	-1.860717	2.380694	1	5.012174	0.957644	-1.604069
1	-2.456480	-3.262387	2.474096	1	3.498188	0.221952	-2.083716
1	2.078507	-0.324320	1.525024	1	2.521584	3.587459	0.176681
1	5.400526	0.336296	-0.893499	1	4.065152	3.089682	-1.586335
1	5.021493	0.573760	0.844852	1	2.599407	2.413795	-2.288053
1	6.145338	-0.727726	0.342161	1	0.748539	2.071906	0.961134
1	0.290901	-3.709882	-1.095773	1	0.528037	2.454504	-0.765607
1	1.873232	-3.085648	-1.630155	1	-0.506633	-1.474813	0.203702
1	1.518912	-3.158931	0.094525	1	2.505647	-1.936526	-2.161218
6	1.106327	2.181928	1.743358	1	4.225805	-1.837634	-1.720425
6	1.028593	3.574666	1.815558	1	3.374788	-3.380864	-1.646344
6	1.510745	4.356013	0.762764	1	3.800833	-2.400104	1.975881
6	2.080677	3.734576	-0.351963	1	4.185803	-3.627802	0.762751
6	2.152685	2.342364	-0.422956	1	4.981936	-2.058215	0.694903
1	0.753435	1.582086	2.580561	1	1.264673	-2.780471	1.332846
1	0.608881	4.048479	2.699485	1	0.828565	-2.846628	-0.386916
1	1.458983	5.440280	0.819291	1	1.949382	-4.014697	0.276242
1	2.475503	4.337379	-1.166243	1	-1.517990	-0.043559	-1.443323
1	2.600854	1.835732	-1.271951	1	-4.626067	-2.728512	0.881524
				1	-5.286766	-2.123352	-0.673297
				1	-4.608360	-3.782976	-0.570093
				1	-1.396002	-0.743373	3.755010
				1	-2.451179	-0.794611	2.264740
				1	-1.310212	-2.070952	2.540302
				6	-2.078984	2.433841	-1.340741
6	3.296762	2.321741	-1.448242	6	-2.364546	3.796988	-1.230176
6	2.605968	2.525334	-0.083548	6	-2.689716	4.342728	0.012030
6	3.523847	1.754809	0.877595	6	-2.741804	3.512622	1.134365
E (CH ₃ CN) = -1935.232597							
NImag = 1 (-24.8)							
20. 1d -t (-1934.8735872)							

6	-2.461144	2.150929	1.018236	1	-0.557403	-1.483929	-0.140276
1	-1.845940	2.008989	-2.314991	1	2.839295	-1.258088	-2.620985
1	-2.341249	4.427413	-2.115556	1	4.453031	-1.554502	-1.936355
1	-2.913025	5.402373	0.104065	1	3.485354	-2.897680	-2.539624
1	-3.009846	3.925083	2.103727	1	3.344462	-3.258129	1.219443
1	-2.535158	1.516175	1.895091	1	3.861171	-4.039159	-0.279735
				1	4.745159	-2.637443	0.321590
E (CH ₃ CN) = -1935.238176				1	0.972862	-3.171656	0.119511
NImag = 0				1	0.781429	-2.457196	-1.494823
21. 1d-E[‡] (-1934.86921945)				1	1.710223	-3.932381	-1.288371
				1	-1.804585	-0.146381	-1.525239
				1	-5.592579	-1.235802	-0.062105
6	-1.545061	2.442130	-1.579061	1	-4.912103	-0.993376	-1.705301
6	-1.946658	1.700559	-0.459505	1	-5.372797	-2.638859	-1.159395
6	-2.483342	2.381333	0.641034	1	0.087307	-2.377117	2.203841
6	-2.581828	3.772700	0.630820	1	-0.642455	-1.489702	3.574437
6	-2.156072	4.505687	-0.480208	1	-1.665085	-2.172031	2.258476
6	-1.641824	3.835930	-1.591388	1	-1.167438	1.921046	-2.457525
6	-1.824251	0.188029	-0.478105	1	-1.333835	4.392989	-2.472861
7	-2.828785	-0.471703	0.339024	1	-2.240362	5.589438	-0.485868
16	-3.309440	-1.934824	-0.185948	1	-2.999381	4.287526	1.492392
8	-3.483453	-2.832900	0.977531	1	-2.832575	1.806391	1.490644
6	-0.612406	-0.456925	0.211617				
16	1.188299	0.206832	-0.562320	E (CH ₃ CN) = -1935.231345			
6	2.536551	-0.870374	0.215329	NImag = 1 (-123.0)			
6	3.753314	0.027658	0.554024	22. 1d-PC (-1934.92500615)			
6	3.360667	1.093767	1.604325	6	1.504047	1.702380	1.913323
6	2.791487	2.223025	0.732643	6	2.179301	1.310339	0.748628
6	1.382282	1.887403	0.238848	6	2.201643	2.174593	-0.354410
6	4.327993	0.878619	-0.625533	6	1.558535	3.410577	-0.285370
6	3.841222	2.335114	-0.388878	6	0.884767	3.795141	0.876481
6	2.796557	-2.176635	-0.620650	6	0.855397	2.935198	1.976728
6	3.745005	-3.069409	0.216066	6	2.876256	-0.009025	0.750772
6	-0.591856	-0.379683	1.750667	7	3.785929	-0.335400	-0.349908
8	-0.427695	0.683281	2.330004	16	5.286539	-1.102124	0.034246
6	-0.712814	-1.685416	2.501919	8	5.528199	-2.092932	-1.014478
6	1.484836	-2.965022	-0.826797	6	2.602226	-1.182558	-0.181203
6	3.432804	-1.942617	-2.005092	16	-2.251606	-0.027646	0.588860
6	-4.974433	-1.669473	-0.849882	6	-3.693921	-0.911331	-0.199890
8	-2.485956	-2.439803	-1.322351	6	-4.617169	0.112497	-0.914318
1	2.108080	-1.198801	1.168581	6	-3.881153	0.705494	-2.137387
1	4.517481	-0.641425	0.959375	6	-2.971087	1.767414	-1.495101
1	2.654579	0.728955	2.358449	6	-1.778012	1.104042	-0.793053
1	4.256926	1.445884	2.128534	6	-4.972341	1.390390	-0.097439
1	5.421440	0.824028	-0.629264	6	-3.931519	2.473841	-0.510721
1	3.996788	0.511949	-1.596934	6	-4.357306	-1.918672	0.801291
1	2.688816	3.164245	1.286572	6	-5.397205	-2.764951	0.032153
1	4.669071	2.966469	-0.047428	6	1.555213	-1.149606	-1.269855
1	3.439582	2.797364	-1.296999	8	1.532509	-0.276011	-2.115305
1	0.665027	1.897464	1.060387				
1	1.046091	2.576669	-0.538669				

6	0.509378	-2.241083	-1.191426	16	-0.444183	-0.078237	0.147192
6	-3.280365	-2.886905	1.339940	6	-0.062960	-1.318245	1.471168
6	-5.058597	-1.244908	1.997566	6	-3.160687	0.921032	-0.518824
6	6.388061	0.300629	-0.193574	6	-2.745658	0.915337	-2.002940
8	5.313158	-1.503872	1.448817	6	0.397056	1.363335	0.856295
1	-3.261495	-1.542201	-0.988612	6	2.257166	0.968494	1.016830
1	-5.523717	-0.414004	-1.231104	6	2.517307	1.322066	2.477595
1	-3.331346	-0.044090	-2.719769	6	-4.665668	0.558168	-0.425911
1	-4.600970	1.186391	-2.812369	6	-3.030159	2.347166	0.059957
1	-5.987641	1.713820	-0.355258	6	0.363624	2.535130	-0.056291
1	-4.952538	1.213522	0.978024	6	0.795369	3.865083	0.544997
1	-2.565226	2.464190	-2.240001	8	0.077601	2.445966	-1.243831
1	-4.426454	3.313085	-1.013199	7	2.633099	-0.313226	0.711335
1	-3.397896	2.881477	0.354093	16	3.030386	-0.617240	-0.850557
1	-1.166611	0.556962	-1.518988	8	3.319682	0.610191	-1.627150
1	-1.134585	1.853656	-0.321790	6	4.585131	-1.515445	-0.652827
1	2.752958	-2.152134	0.292737	8	2.078359	-1.591753	-1.440470
1	-4.378017	-0.587689	2.548774	1	0.046401	1.560190	1.870487
1	-5.925075	-0.653899	1.683734	1	-2.504150	0.205838	1.414433
1	-5.420928	-2.011935	2.692942	1	-3.808840	-1.632854	0.091825
1	-4.948745	-3.259432	-0.838512	1	-2.559695	-1.860803	2.435626
1	-5.799486	-3.546889	0.687047	1	-2.870581	-3.344486	1.520002
1	-6.245377	-2.167554	-0.317059	1	-2.697418	-3.144428	-1.298037
1	-2.735032	-3.370611	0.520014	1	-1.682074	-1.777880	-1.724427
1	-2.548903	-2.377282	1.974693	1	-0.405281	-3.356212	1.960925
1	-3.750281	-3.675106	1.940293	1	-0.917554	-4.199433	-0.229807
1	3.197815	-0.349497	1.735423	1	0.161659	-2.872992	-0.684312
1	6.308881	0.637703	-1.227620	1	-0.304664	-0.851042	2.432978
1	6.102735	1.091508	0.502583	1	1.022573	-1.429382	1.378496
1	7.397936	-0.053821	0.024806	1	2.628293	1.731388	0.323722
1	-0.169925	-2.024714	-0.354535	1	2.120500	2.305808	2.750942
1	-0.068454	-2.257889	-2.117834	1	2.084752	0.567940	3.143480
1	0.961016	-3.223631	-1.013489	1	3.600293	1.328236	2.645000
1	1.488904	1.038729	2.774887	1	-1.703612	1.216711	-2.137660
1	0.335932	3.225646	2.885653	1	-2.891711	-0.068885	-2.459869
1	0.388026	4.760503	0.925814	1	-3.370721	1.626432	-2.555858
1	1.584740	4.076134	-1.144109	1	-4.997747	0.425847	0.611670
1	2.711513	1.864710	-1.258677	1	-5.252128	1.377245	-0.855568
				1	-4.918166	-0.345662	-0.988095
E (CH ₃ CN) = -1935.271558				1	-3.341014	2.378660	1.112207
NImag = 0				1	-2.018379	2.738907	-0.020820
				1	-3.680722	3.030808	-0.496656
<u>System 2: (R = COMe; X = Me, Y = SO₂Me)</u>				1	4.890683	-1.860653	-1.643237
				1	5.334429	-0.841714	-0.233683
23. 2- <i>si,si</i> -c [‡] (-1743.1260957)				1	4.416825	-2.364842	0.011275
				1	0.609166	4.656259	-0.183934
6	-0.790414	-3.112056	-0.201028	1	0.257087	4.080379	1.475586
6	-0.835607	-2.623824	1.267731	1	1.866431	3.851873	0.780351
6	-2.333324	-2.388020	1.500613				
6	-2.728778	-1.600103	0.235458	E (CH ₃ CN) = -1743.443892			
6	-2.001530	-2.404515	-0.888989	NImag = 1 (-223.3)			
6	-2.349322	-0.087981	0.369345				

24. $2-si,si-t^{\ddagger}$ (-1743.13368421)				1	-5.461945	0.119810	-1.382478
				1	-1.756836	4.068855	0.648901
6	2.686525	-2.533020	1.543446	1	-1.404143	3.317759	-0.929856
6	1.479690	-2.787606	0.608330	1	-2.641955	2.593520	0.087623
6	2.085143	-2.604221	-0.788730	E (CH ₃ CN) = -1743.446776			
6	2.919598	-1.319170	-0.616662	NImag = 1 (-250.6)			
6	3.610039	-1.548226	0.761306	25. $2-si,re-c^{\ddagger}$ (-1743.12349096)			
6	2.029819	-0.049646	-0.732861	6	-0.007076	-1.437630	1.247270
16	0.878352	-0.023473	0.792230	6	-0.868006	-2.692442	1.068040
6	0.329075	-1.800975	0.818160	6	-2.318927	-2.409889	1.474493
6	2.760516	1.329753	-0.970856	6	-2.819094	-1.554684	0.293645
6	3.256598	2.016598	0.318617	6	-2.353204	-0.072224	0.440560
6	-0.653211	0.834765	0.385965	16	-0.479370	-0.103086	0.051970
6	-2.294855	0.098827	1.278053	6	-2.257104	-2.335887	-0.935735
6	-2.414338	0.813899	2.608201	6	-0.997389	-3.101773	-0.420154
6	3.974973	1.104953	-1.903695	6	-3.171976	1.007357	-0.357993
6	1.804327	2.289089	-1.714628	6	-4.683884	0.708483	-0.197388
6	-0.611371	2.260471	0.765434	6	0.368575	1.343403	0.729456
6	-1.679950	3.119135	0.114160	6	0.413508	2.422691	-0.284263
8	0.182417	2.723133	1.585466	6	0.680731	3.845327	0.195476
7	-3.332120	0.280378	0.426132	6	-2.942820	2.400135	0.270097
16	-3.305947	-0.742544	-0.863392	6	-2.842848	1.055619	-1.864100
8	-2.795022	-2.099169	-0.517752	8	0.292878	2.205740	-1.484525
6	-5.061374	-0.883105	-1.227815	6	2.264360	0.908120	1.131616
8	-2.663348	-0.100909	-2.039804	7	3.028879	0.705052	0.031328
1	-0.953971	0.620751	-0.639284	16	3.087075	-0.836796	-0.513378
1	1.343706	-0.205902	-1.573397	6	4.627694	-0.792454	-1.438745
1	3.661071	-1.244587	-1.413687	6	2.710491	2.095996	1.970681
1	1.335093	-2.540694	-1.585016	8	3.236236	-1.826065	0.592659
1	2.750284	-3.444409	-1.023344	8	2.006169	-1.159752	-1.483448
1	4.595387	-1.997561	0.600167	1	-0.025682	1.617583	1.708855
1	3.775744	-0.619926	1.311680	1	-2.418274	0.196187	1.502394
1	1.052374	-3.786643	0.753295	1	-3.909488	-1.537983	0.273805
1	3.208614	-3.475552	1.737545	1	-2.416887	-1.914148	2.448159
1	2.379184	-2.133960	2.516335	1	-2.889546	-3.345896	1.519634
1	-0.466197	-1.934666	0.077899	1	-3.019090	-3.041492	-1.283250
1	-0.103659	-1.918138	1.815544	1	-2.019272	-1.686806	-1.780986
1	-1.919735	-0.919660	1.380846	1	-0.399500	-3.477861	1.671871
1	-1.468784	0.811121	3.159186	1	-1.148988	-4.183557	-0.494164
1	-2.745585	1.848196	2.484638	1	-0.095082	-2.855181	-0.988096
1	-3.170856	0.293657	3.208482	1	-0.090871	-1.030899	2.261174
1	2.435113	2.270703	0.995484	1	1.038956	-1.661861	1.027434
1	3.982410	1.402153	0.861018	1	-1.795337	1.306542	-2.054620
1	3.761814	2.952273	0.052050	1	-3.069664	0.105163	-2.357690
1	3.698456	0.571518	-2.821478	1	-3.460652	1.824330	-2.343343
1	4.376206	2.079721	-2.201286	1	-4.966359	0.550428	0.851043
1	4.785711	0.556328	-1.413841	1	-5.254974	1.567948	-0.565061
1	1.445534	1.848263	-2.652530	1	-5.004725	-0.161970	-0.777298
1	0.938169	2.562461	-1.112109	1	-3.225082	2.407412	1.330713
1	2.331522	3.217311	-1.961668				
1	-5.156821	-1.479878	-2.137420				
1	-5.559145	-1.372772	-0.389445				

1	-1.908788	2.732547	0.190741	1	-0.866881	-0.809499	-1.987579
1	-3.562688	3.143684	-0.242985	1	-0.801881	1.633330	1.057678
1	2.046478	0.047574	1.771704	1	-2.827010	1.681348	0.265570
1	4.549724	-0.016060	-2.201137	1	-2.288117	2.824519	-1.895614
1	5.448761	-0.579754	-0.752671	1	-2.022888	1.260840	-2.700270
1	4.752210	-1.774435	-1.899973	1	-3.648339	1.723428	-2.190601
1	0.608896	3.972440	1.278294	1	1.427616	-1.149485	2.588694
1	1.682739	4.144495	-0.130999	1	3.075748	-1.697174	2.217077
1	-0.031492	4.513330	-0.299390	1	2.798690	-0.543396	3.522666
1	2.973043	2.950464	1.344139	1	4.331477	1.578112	0.818660
1	3.618921	1.791327	2.504137	1	4.520744	0.990113	2.477939
1	1.966835	2.398939	2.715571	1	4.775557	-0.111628	1.126967
E (CH ₃ CN) = -1743.441566				1	1.967779	2.449762	1.502724
NImag = 1 (-260.4)				1	0.889564	1.366146	2.413662
26. 2- <i>re</i> , <i>si</i> - <i>c</i> [‡] (-1743.1378476)				1	2.428525	1.862407	3.106682
6	0.176625	-0.497757	-1.898241	1	-4.923703	-1.982967	1.683099
6	1.162757	-1.587690	-2.317284	1	-5.293401	-0.509171	0.729233
6	2.609651	-1.104137	-2.128390	1	-4.832981	-2.030257	-0.107632
6	2.779364	-1.178482	-0.596011	1	0.238471	4.331218	0.659482
6	2.173977	0.082223	0.092806	1	-0.306725	4.724700	-0.981263
16	0.302153	-0.101963	-0.087401	1	-1.431711	3.981794	0.201760
6	2.104888	-2.547992	-0.256054	E (CH ₃ CN) = -1743.447772			
6	1.088639	-2.833446	-1.403383	NImag = 1 (-252.2)			
6	2.653913	0.360552	1.559439	27. 2- <i>re</i> , <i>si</i> - <i>t</i> [‡] (-1743.134269)			
6	4.158582	0.720393	1.479594	6	2.985035	2.160298	-0.865404
6	-0.539208	1.483822	0.013826	6	1.726669	3.078496	-0.871568
6	-2.421452	1.099299	-0.568081	6	0.912387	2.644988	0.365581
7	-2.665078	-0.234610	-0.587316	6	2.008024	2.223840	1.357225
16	-2.939191	-0.952557	0.872189	6	2.929446	1.353497	0.474345
8	-2.794308	-0.000411	2.003793	6	2.383388	-0.096743	0.380267
6	0.077585	2.633825	-0.649295	16	0.781801	-0.006261	-0.650288
6	-0.401587	3.999637	-0.169033	6	-0.051379	1.491993	0.091588
8	0.913853	2.551775	-1.554447	6	-0.399330	-1.302576	-0.230360
6	1.933789	1.581626	2.170191	6	-0.603686	-1.551899	1.223776
6	2.474188	-0.833701	2.516567	6	3.386729	-1.195424	-0.108624
6	-2.587141	1.772997	-1.916988	6	2.687442	-2.561015	-0.276631
6	-4.685241	-1.414448	0.781064	6	4.107580	-0.854435	-1.426742
8	-2.182863	-2.219418	0.931119	6	4.443864	-1.361265	1.011557
1	2.412371	0.963870	-0.509087	6	-2.087956	-0.982312	-1.280689
1	3.838083	-1.196478	-0.324697	6	-2.077547	-2.206083	-2.183886
1	2.795423	-0.106163	-2.540354	7	-3.207662	-0.879827	-0.528840
1	3.304505	-1.803191	-2.610433	16	-3.516221	0.618956	0.072083
1	2.877318	-3.323731	-0.224704	6	-5.314544	0.579375	0.143327
1	1.614274	-2.554387	0.717850	8	-3.026339	0.758268	1.464951
1	0.932720	-1.828456	-3.362224	8	-3.128458	1.705604	-0.869278
1	1.381768	-3.726300	-1.965527	1	2.013141	-0.397166	1.362343
1	0.076851	-3.002500	-1.020798	1	3.928103	1.276275	0.913995
1	0.354890	0.441883	-2.422433	1	1.620132	1.696592	2.234313

1	2.556241	3.108174	1.705206	6	1.401639	-2.911481	-1.336541
1	3.901488	2.758904	-0.892582	8	0.165348	-0.978556	-2.011465
1	3.012452	1.513882	-1.744112	6	-2.719879	-2.523681	0.400410
1	0.288639	3.460267	0.750494	6	-4.146549	-0.728940	1.392601
1	2.018502	4.129256	-0.770166	6	1.626072	-1.094354	2.775715
1	1.150236	2.995801	-1.799343	6	5.096961	1.132634	0.439546
1	-0.538351	1.146338	1.003415	8	4.017507	-0.972311	-0.764856
1	-0.824109	1.759713	-0.632632	1	-1.960114	-0.477273	-1.352452
1	-0.089699	-2.201005	-0.757396	1	-3.852527	1.244348	-1.090783
1	-1.745873	-0.077181	-1.795552	1	-1.474043	1.543987	-2.323723
1	-1.136224	-2.303994	-2.735363	1	-2.420374	2.997312	-1.946501
1	-2.259674	-3.121501	-1.612033	1	-3.894162	2.822561	0.633708
1	-2.891881	-2.103419	-2.910360	1	-3.028909	1.635625	1.586343
1	3.403624	-0.706324	-2.253503	1	-0.199472	3.400311	-0.909229
1	4.727566	0.042807	-1.338763	1	-2.006286	4.186089	0.464762
1	4.768901	-1.683152	-1.705420	1	-1.187691	3.140528	1.621029
1	3.976218	-1.632987	1.964899	1	0.640718	1.096572	-0.950481
1	5.141001	-2.162191	0.740587	1	0.813454	1.768121	0.669396
1	5.036930	-0.455064	1.168717	1	0.076063	-2.161728	0.955597
1	2.092151	-2.825234	0.603917	1	-3.465500	-0.538255	2.229793
1	2.035444	-2.582161	-1.156297	1	-4.751694	0.168161	1.230431
1	3.440781	-3.343840	-0.420085	1	-4.827234	-1.530766	1.701689
1	-5.638225	1.514584	0.605234	1	-3.920996	-1.718215	-1.939050
1	-5.707978	0.492767	-0.870575	1	-5.129397	-2.159620	-0.722352
1	-5.619998	-0.273793	0.750880	1	-4.990606	-0.482847	-1.249631
8	-0.079780	-0.878958	2.109316	1	-2.111794	-2.861297	-0.445549
6	-1.561188	-2.676011	1.542252	1	-2.086895	-2.494615	1.293397
1	-1.560459	-2.862236	2.618127	1	-3.491344	-3.280668	0.581451
1	-2.560818	-2.361288	1.209305	1	2.558041	-1.823392	0.921305
1	-1.306884	-3.594804	0.999911	1	2.522113	-1.123815	3.406623
E (CH ₃ CN) = -1743.445760				1	1.023853	-0.242467	3.106265
NImag = 1 (-233.7)				1	1.062152	-2.018635	2.939149
28. 2- <i>re</i> , <i>re</i> -c [‡] (-1743.1361678)				1	4.808604	2.063191	0.930907
6	0.089329	1.485310	-0.096293	1	5.559433	0.447100	1.151660
6	-0.849722	2.619901	-0.496454	1	5.772617	1.334236	-0.394820
6	-1.900102	2.136535	-1.508353	1	1.127837	-3.323082	-2.311221
6	-2.873398	1.337999	-0.612390	1	2.457000	-2.610561	-1.366454
6	-2.353858	-0.109974	-0.402640	1	1.281541	-3.673382	-0.558937
16	-0.789564	0.027079	0.675741	E (CH ₃ CN) = -1743.447939			
6	-2.975794	2.227495	0.671241	NImag = 1 (-249.5)			
6	-1.719507	3.147711	0.663248	29. 2- <i>re</i> , <i>re</i> -t [‡] (-1743.1362782)			
6	-3.390186	-1.161439	0.121922	6	-3.440916	-0.160800	-1.822704
6	-4.414132	-1.384085	-1.018903	6	-3.047992	-1.634198	-2.140982
6	0.372194	-1.309478	0.349213	6	-2.715459	-2.264172	-0.771039
6	2.073584	-0.930299	1.330219	6	-3.646826	-1.503571	0.186910
7	2.655797	0.264840	1.087617	6	-3.456055	-0.038802	-0.263895
16	3.616281	0.360374	-0.244975	6	-2.188700	0.576427	0.389451
8	3.055966	1.325908	-1.216889	16	-0.693463	-0.303918	-0.387150
6	0.577846	-1.664019	-1.076245	6	-1.254231	-2.076669	-0.354853

6	0.713271	-0.331905	0.730578	System 3 (R = COMe; X = Ph; Y = CO₂Me)			
6	0.458509	-0.687569	2.134747				
6	-2.061825	2.139135	0.361521	30. 3a-A-c[‡] (-1574.8491993)			
6	-0.733326	2.609523	0.995115	6	-2.580943	-2.058419	-1.576254
6	-2.169003	2.760075	-1.044698	6	-2.578855	-1.279575	-0.408401
6	-3.209248	2.692460	1.243154	6	-3.049301	-1.860809	0.777653
6	2.184896	-1.400908	-0.057685	6	-3.471505	-3.190832	0.802055
6	2.170938	-2.754955	0.627504	6	-3.445424	-3.961680	-0.361575
7	3.338184	-0.710944	0.119946	6	-3.004832	-3.386407	-1.556000
16	3.503332	0.575993	-0.892383	6	-2.190158	0.177477	-0.445684
6	5.259801	0.909263	-0.701408	7	-2.293366	0.860268	0.719174
8	3.245449	0.241820	-2.312642	6	-2.421553	2.204930	0.550637
8	2.776263	1.767673	-0.364287	8	-2.533986	2.829135	1.763873
1	-2.146893	0.259296	1.435171	6	-2.683858	4.244960	1.693020
1	-4.297834	0.577518	0.062975	8	-2.437671	2.850315	-0.502337
1	-3.413280	-1.668383	1.243793	6	-0.321409	0.182550	-1.158636
1	-4.685523	-1.811919	0.016003	6	-0.140451	1.387511	-2.012783
1	-4.438767	0.063377	-2.213350	16	0.874221	0.261780	0.199356
1	-2.757251	0.545604	-2.294858	6	2.484786	-0.715258	-0.120843
1	-2.898273	-3.345553	-0.762618	6	3.102133	-0.931233	1.297377
1	-3.889588	-2.167567	-2.595295	6	2.303364	-1.981580	2.096216
1	-2.211108	-1.700600	-2.844872	6	1.114780	-1.155452	2.607474
1	-1.084585	-2.418439	0.666023	6	0.138428	-0.869369	1.463233
1	-0.568754	-2.578000	-1.043953	6	3.073117	0.300096	2.256800
1	1.240101	0.607540	0.583783	6	1.801933	0.122698	3.145448
1	-1.400980	2.373514	-1.723684	6	3.438518	-0.132362	-1.220484
1	-3.151386	2.597154	-1.499013	6	4.733437	-0.985866	-1.228831
1	-2.019498	3.843160	-0.971725	6	2.799500	-0.294730	-2.617090
1	-3.169485	2.281502	2.258929	6	3.817776	1.344720	-0.998121
1	-3.112872	3.780911	1.321302	1	-0.285856	-0.767895	-1.687817
1	-4.201104	2.485314	0.828828	1	2.136025	-1.688330	-0.487274
1	-0.559367	2.141954	1.971123	1	4.127121	-1.270059	1.141174
1	0.135300	2.419875	0.357630	1	2.008890	-2.854620	1.501751
1	-0.776010	3.693006	1.153465	1	2.907290	-2.341317	2.938705
1	1.767385	-1.429287	-1.073582	1	3.976456	0.289580	2.875513
1	2.853549	-3.418777	0.083491	1	3.067821	1.252390	1.723028
1	2.536842	-2.679391	1.655030	1	0.541778	-1.672516	3.385972
1	1.178542	-3.213655	0.637020	1	2.083424	-0.022136	4.193589
1	5.470688	1.087929	0.353780	1	1.139008	0.993089	3.107198
1	5.821926	0.048947	-1.067769	1	-0.177191	-1.788647	0.964226
1	5.483876	1.797743	-1.295448	1	-0.751175	-0.312954	1.777614
8	-0.556795	-1.266527	2.535625	1	-2.574002	0.672285	-1.342555
6	1.584459	-0.315099	3.082742	1	2.937344	1.993396	-1.001725
1	1.530840	-0.938184	3.979145	1	4.365139	1.486711	-0.060276
1	2.562154	-0.399854	2.594490	1	4.476518	1.675021	-1.809945
1	1.467088	0.735525	3.380748	1	4.518915	-2.061305	-1.270768
E (CH ₃ CN) = -1743.449927				1	5.319295	-0.732860	-2.118901
NImag = 1 (-244.9)				1	5.372081	-0.795297	-0.361377
				1	2.485916	-1.330961	-2.797402
				1	1.943723	0.363530	-2.756047

1	3.533708	-0.034018	-3.387538	1	4.902943	-0.886004	-1.983786
1	-1.827003	4.711477	1.196007	1	3.600866	-1.787397	-1.230477
1	-3.590681	4.522548	1.145577	1	2.003103	1.387120	-3.486569
1	-2.752046	4.586771	2.728639	1	3.568867	-0.389951	-3.822598
1	-3.100074	-1.238149	1.664461	1	2.248607	-1.333367	-3.142804
1	-3.835907	-3.622088	1.731300	1	0.458514	1.544379	-1.515449
1	-3.779859	-4.995679	-0.343090	1	0.181670	0.090758	-2.509468
1	-3.000581	-3.968922	-2.473837	1	-1.519772	0.695991	-1.390885
1	-2.262228	-1.616833	-2.518586	1	1.922845	-2.503707	1.377000
8	0.683264	2.262853	-1.756104	1	3.569285	-2.562605	0.699349
6	-1.050618	1.519460	-3.219723	1	3.321606	-2.668330	2.440850
1	-1.401569	0.556402	-3.604998	1	4.718184	0.772965	2.078305
1	-1.918797	2.111451	-2.907079	1	4.817484	-0.748326	2.970473
1	-0.523511	2.066176	-4.005824	1	5.249011	-0.715161	1.261825
E (CH ₃ CN) = -1575.187958				1	2.312497	0.866775	3.075221
NImag = 1 (-288.5)				1	1.200462	-0.496298	2.828077
31. 3a-A-<i>t</i>[‡] (-1574.85460390)				1	2.637452	-0.708109	3.815180
6	-2.365759	-1.907935	-1.311177	1	-1.194894	4.997917	1.091844
6	-2.855011	-0.808218	-0.592326	1	-1.951543	5.276624	-0.489529
6	-4.141967	-0.883016	-0.043580	1	-2.860423	5.655008	1.008334
6	-4.913971	-2.034459	-0.202327	1	-4.522716	-0.014616	0.482545
6	-4.414642	-3.125426	-0.915231	1	-5.912442	-2.075545	0.225828
6	-3.135476	-3.057749	-1.472817	1	-5.017378	-4.021319	-1.040013
6	-2.046229	0.452840	-0.465717	1	-2.737430	-3.901309	-2.030737
7	-2.647823	1.487113	0.179125	1	-1.368400	-1.870949	-1.745592
6	-2.008528	2.669435	0.062809	8	-0.425525	-2.138656	1.561870
8	-2.745935	3.684076	0.606258	6	-1.773002	-0.470229	2.648345
6	-2.143833	4.972987	0.544964	1	-2.491115	0.246250	2.234202
8	-0.882951	2.901428	-0.421078	1	-2.279146	-1.321425	3.109172
6	-0.425887	0.028047	0.568214	1	-1.197689	0.057077	3.422071
6	-0.816712	-0.972758	1.584378	E (CH ₃ CN) = -1575.194111			
16	1.021317	-0.517674	-0.382782	NImag = 1 (-267.6)			
6	2.614712	0.170077	0.422805	32. 3b-A-<i>c</i>[‡] (-1574.85181509)			
6	3.655360	0.372773	-0.714011	6	2.794097	-1.677974	-1.602330
6	3.231518	1.510017	-1.664796	6	3.040986	-0.637432	-0.694313
6	2.231067	0.803296	-2.586921	6	4.291376	-0.583617	-0.063527
6	0.899351	0.603254	-1.862700	6	5.254886	-1.561780	-0.311628
6	3.850475	-0.828017	-1.687788	6	4.990283	-2.603914	-1.202260
6	2.953189	-0.522664	-2.926986	6	3.755574	-2.655589	-1.854073
6	3.077423	-0.654953	1.686921	6	2.023454	0.451122	-0.463245
6	4.553149	-0.308979	2.002668	7	2.428711	1.474115	0.329286
6	2.249709	-0.216683	2.915919	6	1.630076	2.557273	0.284837
6	2.958781	-2.185125	1.526064	8	2.141997	3.584734	1.021449
1	-0.257392	1.048638	0.902819	6	1.338897	4.759495	1.067065
1	2.317130	1.165270	0.772724	8	0.543075	2.691643	-0.313779
1	4.595235	0.627822	-0.222374	6	0.497597	-0.509900	0.331885
1	2.809966	2.381096	-1.150918	6	0.738148	-0.412563	1.796704
1	4.101284	1.849859	-2.240640	16	-1.100270	0.248315	-0.067059
				6	-0.953969	0.599219	-1.878197

1	-1.023874	4.674459	-1.256949	1	3.422777	2.522778	-2.821900
1	0.448360	5.561981	-0.818052	1	1.991181	1.506225	-2.943785
1	0.013294	5.364070	-2.546137	1	0.750212	2.148620	0.545172
1	3.241568	-0.446692	2.174091	1	0.111311	2.072325	-1.104264
1	4.906581	-2.220365	1.776943	1	-0.522626	-1.495500	0.587766
1	5.642880	-2.750379	-0.540797	1	-1.503523	0.409845	-1.315972
1	4.706991	-1.459393	-2.452171	1	2.750422	-2.475598	-1.375718
1	3.026726	0.343729	-2.028672	1	4.434448	-2.009723	-1.062961
8	0.180897	-1.691015	2.236866	1	3.794799	-3.517438	-0.405487
6	0.924187	0.163504	3.554816	1	4.000961	-1.315719	2.632762
1	1.530830	1.059357	3.391132	1	4.584191	-2.810488	1.884281
1	0.044509	0.466131	4.138459	1	5.167527	-1.253874	1.298305
1	1.480518	-0.569510	4.145203	1	1.535032	-2.102274	2.185592
E (CH ₃ CN) = -1575.196723				1	1.166620	-2.817028	0.599511
NImag = 1 (-269.4)				1	2.364422	-3.568735	1.643713
34. 3c-A-<i>t</i>[‡] (-1574.856377)				1	-2.405623	4.843683	0.424285
6	2.808593	1.798934	-2.276291	1	-3.665931	4.598844	-0.800956
6	2.292617	2.434073	-0.965240	1	-4.132154	4.928143	0.898194
6	3.427210	2.124496	0.025201	1	-1.141507	-1.935525	-2.067871
6	3.707422	0.633603	-0.258654	1	-2.158156	-4.158235	-2.456014
6	3.672001	0.582852	-1.821451	1	-4.230785	-4.810627	-1.241002
6	0.974153	1.836249	-0.474453	1	-5.286590	-3.205007	0.338158
16	1.025588	-0.025481	-0.416330	1	-4.263765	-0.951985	0.692369
6	2.685508	-0.275211	0.484066	8	0.435503	0.907307	2.407379
6	-0.426208	-0.414152	0.596848	6	-1.604903	-0.270773	2.830310
6	-0.421178	0.130514	1.990016	1	-2.465132	0.288310	2.427459
6	3.103545	-1.771416	0.676646	1	-1.840383	-1.336306	2.737104
6	3.546025	-2.472119	-0.621968	1	-1.426565	-0.003515	3.874051
6	4.284727	-1.776563	1.679481	E (CH ₃ CN) = -1575.194018			
6	1.968603	-2.602084	1.312736	NImag = 1 (-261.3)			
6	-2.001506	0.049547	-0.405166	35. 3c-c (-1574.8647868)			
7	-2.796099	0.949854	0.240002	6	3.515143	-0.583916	1.137355
6	-2.623910	2.238755	-0.123669	6	2.915409	0.158460	0.110200
8	-1.861158	2.726955	-0.974651	6	3.431155	0.029723	-1.186977
6	-2.621636	-1.311600	-0.626462	6	4.489715	-0.840667	-1.453317
6	-3.800060	-1.678923	0.034503	6	5.062233	-1.592369	-0.425999
6	-4.370635	-2.934323	-0.181418	6	4.573903	-1.454858	0.874348
6	-3.780663	-3.836263	-1.069139	6	1.779600	1.148700	0.381845
6	-2.615235	-3.471465	-1.747777	7	1.408904	1.842366	-0.800399
6	-2.042743	-2.219206	-1.526067	6	0.600824	2.880735	-0.597196
8	-3.468117	3.051205	0.589164	8	0.351666	3.564843	-1.767171
6	-3.405810	4.431905	0.249821	6	-0.513453	4.684833	-1.639506
1	2.488194	0.144182	1.473331	6	0.440621	0.505325	1.056941
1	4.696330	0.346568	0.109089	6	0.567248	-0.395387	2.253125
1	3.163949	2.328821	1.068357	6	0.996529	0.303112	3.533758
1	4.315124	2.719981	-0.221885	16	-0.611054	-0.137271	-0.331846
1	4.693783	0.672578	-2.204808	6	0.352495	-1.631849	-0.885783
1	3.277875	-0.358939	-2.206876	6	-0.517360	-2.738970	-1.482421
1	2.111557	3.509629	-1.075104	6	-1.572891	-3.205722	-0.467663

6	-2.601208	-2.053313	-0.509731	6	3.738247	3.459810	-0.099499
6	-2.168110	-0.895070	0.433334	6	2.991419	4.284005	-0.944622
6	-2.682144	-1.717402	-2.035887	6	1.909361	3.748469	-1.645179
6	-1.374413	-2.268940	-2.675403	6	1.912654	0.110802	-0.424238
6	-3.263158	0.179451	0.778773	7	2.980546	-0.661452	0.072183
6	-2.695751	1.287064	1.694000	6	2.857266	-1.963332	-0.193655
8	0.311567	-1.594098	2.246908	8	3.938954	-2.674955	0.286463
6	-3.900340	0.860540	-0.447781	6	3.893551	-4.072799	0.038150
6	-4.370247	-0.552407	1.576812	6	0.573626	0.142784	0.588064
8	0.053073	3.259374	0.468363	6	0.563181	-0.766424	1.819320
1	-1.834813	-1.339561	1.373657	6	1.700081	-0.544520	2.778599
1	-3.572497	-2.392519	-0.141155	16	-0.953350	-0.014956	-0.461386
1	-1.164630	-3.387952	0.531386	6	-0.902126	-1.818124	-0.966559
1	-2.041472	-4.133006	-0.819470	6	-2.282060	-2.406516	-1.256385
1	-3.560845	-2.205836	-2.469521	6	-3.217377	-2.256392	-0.046449
1	-2.796009	-0.650260	-2.227006	6	-3.598745	-0.759752	-0.109380
1	0.174756	-3.540671	-1.767303	6	-2.523264	0.106695	0.600715
1	-1.593899	-3.120917	-3.327684	6	-3.787384	-0.506485	-1.642841
1	-0.860783	-1.520347	-3.288035	6	-3.055452	-1.671230	-2.369150
1	0.894623	-1.986087	-0.011028	6	-2.926062	1.580338	0.956847
1	1.055741	-1.214885	-1.608926	6	-1.740806	2.364209	1.560165
1	-0.060215	1.443660	1.326694	8	-0.325348	-1.580114	2.029896
1	2.101327	1.828110	1.193649	6	-3.482052	2.395052	-0.226825
1	-3.151641	1.356224	-1.075257	6	-4.014907	1.485243	2.054602
1	-4.467729	0.159173	-1.066823	8	1.925664	-2.566022	-0.769790
1	-4.600042	1.632061	-0.106606	1	-2.239704	-0.394525	1.527925
1	-3.962631	-1.057502	2.460733	1	-4.534268	-0.578127	0.426737
1	-5.109038	0.178207	1.923741	1	-2.752850	-2.547312	0.900403
1	-4.907209	-1.293823	0.976853	1	-4.113114	-2.872262	-0.192364
1	-2.179135	0.867323	2.565957	1	-4.854311	-0.501972	-1.888068
1	-2.017443	1.969092	1.170533	1	-3.396053	0.461665	-1.957701
1	-3.522840	1.897804	2.073286	1	-2.097150	-3.456089	-1.515025
1	-1.514107	4.391015	-1.300003	1	-3.779888	-2.355944	-2.823007
1	-0.119984	5.422187	-0.931611	1	-2.400326	-1.319762	-3.173636
1	-0.577026	5.124565	-2.638550	1	-0.383562	-2.343144	-0.169530
1	3.174719	-0.477881	2.163548	1	-0.247539	-1.819498	-1.838481
1	5.021182	-2.018944	1.688962	1	0.521971	1.166953	0.957928
1	5.888498	-2.268017	-0.632132	1	1.508702	-0.285499	-1.371383
1	4.875066	-0.922979	-2.466933	1	-2.758173	2.476116	-1.045404
1	2.987854	0.643631	-1.963279	1	-4.408850	1.971955	-0.625224
1	0.103836	0.730299	4.010552	1	-3.706890	3.413572	0.109728
1	1.436552	-0.426198	4.218014	1	-3.654798	0.931921	2.929786
1	1.689114	1.130420	3.354330	1	-4.286466	2.493310	2.386678
				1	-4.931232	1.003735	1.699615
				1	-1.259508	1.815652	2.378066
				1	-0.984642	2.617532	0.809087
				1	-2.103538	3.312558	1.971560
				1	3.018195	-4.539759	0.504520
				1	3.863394	-4.293058	-1.034942
				1	4.809125	-4.481496	0.474641
				1	0.741862	1.988913	-2.057328
				1	1.334301	4.374356	-2.323538
E (CH ₃ CN) = -1575.204611							
NImag = 0							
36. 3c-R[‡] (-1574.8567483)							
6	1.573008	2.401737	-1.488493				
6	2.310187	1.570819	-0.633165				
6	3.402760	2.113863	0.053322				

1	3.258431	5.330659	-1.067075	1	-1.401854	0.368989	-1.289852
1	4.593078	3.865219	0.436646	1	2.732214	-2.139174	-2.078489
1	3.991178	1.448151	0.675440	1	4.419145	-1.859672	-1.601268
1	2.636386	-0.754753	2.239158	1	3.709761	-3.467675	-1.448403
1	1.748828	0.507527	3.087391	1	3.900065	-2.282853	2.117896
1	1.572393	-1.187927	3.651665	1	4.446701	-3.517021	0.972235
E (CH ₃ CN) = -1575.198641				1	5.104051	-1.884958	0.877689
NImag = 1 (-15.2)				1	1.425963	-2.827469	1.409432
37. 3c-t (-1574.8628908)				1	1.078031	-3.004325	-0.329537
6	-2.594005	-2.145533	-1.268064	1	2.219486	-4.085026	0.453385
6	-2.821875	-1.001032	-0.489725	1	-1.631876	4.981987	-0.126294
6	-4.097856	-0.800090	0.044534	1	-3.215288	4.646115	-0.846828
6	-5.115315	-1.731871	-0.174346	1	-3.118500	5.285886	0.824378
6	-4.874886	-2.875091	-0.937485	1	-1.619303	-2.304277	-1.729440
6	-3.608084	-3.077076	-1.490638	1	-3.412600	-3.954549	-2.102405
6	-1.716483	0.052688	-0.278254	1	-5.668006	-3.598254	-1.109537
7	-2.128628	1.163971	0.520997	1	-6.101551	-1.559843	0.250098
6	-2.108941	2.332832	-0.113782	1	-4.266256	0.103794	0.620846
8	-2.644067	3.334459	0.677787	1	-2.415032	-0.211512	2.561337
6	-2.647050	4.626929	0.089542	1	-2.019140	-1.911358	2.272001
6	-0.465317	-0.650846	0.400283	1	-1.373546	-1.085403	3.735760
6	-0.430427	-0.466977	1.927571	E (CH ₃ CN) = -1575.204494			
6	-1.635150	-0.971752	2.681168	NImag = 0			
16	1.065161	-0.040247	-0.475236	38. 3c-E[‡] (-1574.8525933)			
6	1.039256	1.782060	-0.074370	6	-3.244825	0.950506	-2.621480
6	2.409207	2.434873	-0.254788	6	-2.248943	-0.224377	-2.691344
6	3.452528	1.799287	0.678154	6	-3.026868	-1.363560	-2.014020
6	3.738165	0.452673	-0.021996	6	-3.593869	-0.668631	-0.755552
6	2.667584	-0.607833	0.367387	6	-4.029665	0.732059	-1.295523
6	3.799663	0.858915	-1.531743	6	-0.929551	0.038613	-1.962243
6	3.022753	2.204017	-1.652692	16	-1.119555	0.464713	-0.153545
6	3.041512	-2.106020	0.098993	6	-2.535702	-0.663891	0.380679
6	1.865379	-3.048651	0.430463	6	0.644233	-0.298202	0.522203
8	0.532257	0.017952	2.498070	6	0.652350	-1.833638	0.435215
6	3.501958	-2.396684	-1.342052	6	-3.047172	-0.343293	1.828586
6	4.192108	-2.456450	1.075636	6	-3.838254	0.973798	1.945906
8	-1.661227	2.623890	-1.248237	6	-3.963099	-1.516116	2.255769
1	2.446038	-0.505719	1.430456	6	-1.872957	-0.287525	2.827505
1	4.697805	0.041912	0.302636	6	1.840573	0.313470	-0.217738
1	3.105578	1.688790	1.710735	7	2.804049	-0.530496	0.455570
1	4.364278	2.409328	0.691301	6	3.523503	-1.299252	-0.395507
1	4.845532	0.987921	-1.828732	8	3.581593	-1.269865	-1.627820
1	3.383596	0.096028	-2.191527	6	2.013795	1.803544	0.031338
1	2.253972	3.500519	-0.048861	6	2.492055	2.258783	1.268077
1	3.709642	3.022454	-1.892179	6	2.627199	3.623359	1.518286
1	2.262668	2.182654	-2.440444	6	2.293339	4.557237	0.532807
1	0.690322	1.854458	0.954954	6	1.835348	4.114964	-0.708108
1	0.270513	2.184192	-0.748616	6	1.699353	2.746135	-0.954255
1	-0.468632	-1.720405	0.180319	8	4.264677	-2.219457	0.325222

6	5.107443	-3.048499	-0.468748	6	-2.404806	0.637652	1.385752
1	-2.085630	-1.660980	0.414601	6	-1.141056	1.036799	2.092771
1	-4.455945	-1.218380	-0.367140	6	2.785486	-1.841742	1.219127
1	-2.408301	-2.238879	-1.790293	6	3.752526	-2.832560	0.541764
1	-3.850083	-1.687562	-2.662316	6	3.366792	-1.447422	2.596231
1	-5.109443	0.736269	-1.476923	6	1.441164	-2.559269	1.474180
1	-3.830004	1.533461	-0.583929	6	-2.235864	-0.025905	0.006056
1	-1.972826	-0.465706	-3.725058	7	-2.790880	1.290923	0.149527
1	-3.922341	0.906198	-3.480992	6	-2.160057	2.431244	-0.367621
1	-2.746268	1.925243	-2.657164	8	-1.640737	2.495687	-1.460442
1	-0.281134	-0.837933	-1.990238	6	-3.111058	-1.151270	-0.429944
1	-0.407807	0.905752	-2.374463	6	-4.507401	-1.039425	-0.443108
1	0.632579	0.051987	1.553084	6	-5.294623	-2.124824	-0.824484
1	1.792660	0.117819	-1.296314	6	-4.696632	-3.330987	-1.198489
1	-3.247693	1.838040	1.622319	6	-3.305267	-3.444179	-1.196109
1	-4.767480	0.953908	1.368882	6	-2.515347	-2.359284	-0.815074
1	-4.110419	1.139113	2.994655	8	-2.330602	3.466574	0.477146
1	-3.437301	-2.476886	2.203980	6	-1.740095	4.698843	0.037851
1	-4.286050	-1.369268	3.292315	1	1.836453	0.060486	1.006243
1	-4.866627	-1.588395	1.642477	1	4.348747	0.448525	1.001611
1	-1.250464	-1.187297	2.779660	1	2.406990	2.142569	0.282349
1	-1.236103	0.588922	2.665294	1	4.057718	2.509779	-0.254079
1	-2.262473	-0.211941	3.848559	1	5.664906	0.220904	-0.930095
1	4.529991	-3.628674	-1.196327	1	4.579187	-1.109404	-1.318904
1	5.848407	-2.455972	-1.016209	1	2.732244	2.516704	-2.338683
1	5.611213	-3.718412	0.233121	1	4.839452	1.464893	-2.719248
1	1.374136	2.407888	-1.936441	1	3.797501	0.117367	-3.179476
1	1.595689	4.832015	-1.489433	1	0.728564	1.361340	-1.458867
1	2.404160	5.620999	0.727124	1	1.277706	0.625269	-2.969162
1	3.005378	3.961338	2.480086	1	-3.233055	0.306940	2.009530
1	2.788270	1.521838	2.008997	1	-1.199805	-0.079935	-0.328251
8	0.317473	-2.398596	-0.598666	1	3.413046	-3.107182	-0.462340
6	1.021700	-2.631005	1.671525	1	4.764163	-2.422447	0.459645
1	2.043964	-2.998193	1.532160	1	3.819822	-3.751773	1.136941
1	1.013932	-2.031097	2.584487	1	2.720688	-0.725919	3.111834
1	0.348704	-3.490660	1.769008	1	3.451864	-2.335220	3.234334
E (CH ₃ CN) = -1575.196825				1	4.366318	-1.008311	2.516353
NImag = 1 (-70.8)				1	0.711464	-1.881367	1.934339
39. 1c-PC (-1574.9223226)				1	0.999895	-2.946261	0.550603
				1	1.588556	-3.407090	2.154254
6	4.077055	0.770843	-2.346344	1	-0.657932	4.585467	-0.066907
6	2.865384	1.565456	-1.806942	1	-2.164877	5.010273	-0.919856
6	3.240645	1.780115	-0.329892	1	-1.974570	5.426165	0.815921
6	3.743810	0.380208	0.091183	1	-1.430941	-2.439943	-0.824634
6	4.617671	-0.036626	-1.128528	1	-2.832784	-4.375538	-1.496691
6	1.542663	0.793880	-1.919851	1	-5.312260	-4.175203	-1.497435
16	1.600790	-0.902131	-1.184943	1	-6.377091	-2.027538	-0.836361
6	2.525857	-0.534053	0.394627	1	-4.966603	-0.093336	-0.170764
				8	-0.236305	1.604504	1.501872
				6	-1.053266	0.669115	3.558131

1	-1.810190	1.222733	4.128585
1	-1.261553	-0.398437	3.702568
1	-0.060459	0.909367	3.942712

E (CH₃CN) = -1575.24229
NImag = 0

40. **3d-A-*c*[‡]** (-1574.8596597)

6	3.699161	-0.618187	-1.350692
6	3.242492	0.014932	-0.186976
6	4.041750	-0.020747	0.963949
6	5.259615	-0.700583	0.955201
6	5.702518	-1.340647	-0.205933
6	4.921412	-1.291801	-1.362212
6	1.935874	0.759778	-0.192282
7	1.821391	1.726613	0.759510
6	1.005120	2.754729	0.456450
8	1.047012	3.708048	1.439574
6	0.247010	4.860574	1.201342
8	0.276737	2.923205	-0.540356
6	0.644801	-0.623070	0.207634
16	-0.980954	0.150635	-0.017308
6	-2.365890	-1.140645	0.109357
6	-3.558408	-0.572902	-0.715097
6	-3.244272	-0.593159	-2.225881
6	-2.417856	0.690318	-2.399114
6	-1.004572	0.509268	-1.847696
6	-3.232846	1.738767	-1.609802
6	-3.917612	0.929806	-0.467639
6	-2.701802	-1.585102	1.576471
6	-3.416327	-0.506169	2.413190
6	0.836138	-1.940749	-0.450178
6	-3.622740	-2.826532	1.469307
6	-1.440202	-2.026989	2.345769
1	-1.963027	-2.011511	-0.415719
1	-4.416782	-1.211657	-0.490107
1	-2.720637	-1.498424	-2.551441
1	-4.178004	-0.518067	-2.797185
1	-5.005601	1.047610	-0.509491
1	-3.605067	1.284865	0.515259
1	-2.296202	0.973396	-3.451790
1	-3.984951	2.194639	-2.262278
1	-2.594866	2.543424	-1.230464
1	-0.486531	-0.326698	-2.316437
1	-0.426248	1.434817	-1.888227
1	0.841961	-0.634361	1.275894
1	-2.817620	0.407107	2.501982
1	-4.393213	-0.239681	1.999140
1	-3.584279	-0.886211	3.427541
1	-3.149991	-3.627857	0.889122
1	-3.826776	-3.217138	2.472656

1	-4.589126	-2.598547	1.009715
1	-0.854760	-2.763516	1.785390
1	-0.791256	-1.182411	2.595373
1	-1.736654	-2.492020	3.292544
1	1.617487	1.003621	-1.212707
1	0.539115	5.367281	0.275600
1	-0.816233	4.604659	1.130195
1	0.415364	5.518364	2.057480
1	3.697854	0.516452	1.841749
1	5.872432	-0.720646	1.853114
1	6.655711	-1.863099	-0.212595
1	5.265937	-1.771599	-2.274766
1	3.093636	-0.580335	-2.253980
8	0.259389	-2.271167	-1.488101
6	1.797894	-2.907696	0.223250
1	2.525837	-2.412727	0.868673
1	1.210394	-3.603833	0.837993
1	2.314969	-3.492217	-0.541303

E (CH₃CN) = -1575.197629
NImag = 1 (-276.6)

41. **3d-A-*t*[‡]** (-1574.85706212)

6	-2.074644	2.424587	-1.369951
6	-2.381961	1.497599	-0.364706
6	-3.001120	1.957313	0.805789
6	-3.271241	3.313508	0.978570
6	-2.945305	4.232972	-0.023081
6	-2.353677	3.783653	-1.204024
6	-2.099876	0.041055	-0.587793
7	-3.096765	-0.806952	-0.211012
6	-2.937772	-2.073915	-0.659197
8	-4.047916	-2.829691	-0.402850
6	-3.963493	-4.187810	-0.823566
8	-1.939320	-2.577673	-1.204873
6	-0.494496	-0.473217	0.377668
16	0.991166	0.137569	-0.442282
6	2.556010	-0.557592	0.394165
6	3.689599	0.474555	0.149336
6	3.421939	1.775055	0.938254
6	2.464902	2.531833	0.003821
6	1.059173	1.931776	0.064570
6	3.143324	2.374994	-1.373999
6	3.850309	0.988453	-1.319056
6	2.860873	-2.046481	0.009017
6	3.334120	-2.240132	-1.444433
6	-0.531653	-0.341736	1.851893
6	3.977409	-2.531303	0.968137
6	1.637790	-2.960394	0.241860
1	2.291373	-0.536630	1.454847
1	4.614176	0.001151	0.490440

1	3.007246	1.600596	1.936170	16	-0.975430	0.178622	-0.017061
1	4.355643	2.339855	1.050809	6	-2.317615	-1.143527	0.106167
1	4.914614	1.088402	-1.555622	6	-3.536845	-0.577199	-0.683522
1	3.433464	0.298594	-2.054118	6	-3.252976	-0.552725	-2.200284
1	2.351645	3.585972	0.284892	6	-2.458693	0.753100	-2.357348
1	3.877289	3.175502	-1.515301	6	-1.031205	0.592200	-1.839727
1	2.428887	2.447972	-2.201406	6	-3.279017	1.763596	-1.526988
1	0.653450	1.961426	1.074434	6	-3.919932	0.912032	-0.390390
1	0.372573	2.423345	-0.626556	6	-2.626742	-1.624519	1.570020
1	-0.635286	-1.489704	0.009207	6	-3.382724	-0.589861	2.426236
1	2.593588	-1.879507	-2.167056	6	0.876455	-1.920604	-0.597414
1	4.286991	-1.740136	-1.643866	6	-3.493639	-2.902080	1.444263
1	3.480570	-3.308979	-1.637307	6	-1.345434	-2.019061	2.331182
1	3.680279	-2.420830	2.017698	1	-1.919051	-1.999750	-0.446091
1	4.173287	-3.594086	0.788257	1	-4.376546	-1.239468	-0.456788
1	4.923149	-1.999800	0.823161	1	-2.717364	-1.438058	-2.560185
1	1.203355	-2.814942	1.237370	1	-4.200150	-0.485008	-2.749729
1	0.850605	-2.820646	-0.504953	1	-5.010767	1.007100	-0.403381
1	1.954559	-4.007099	0.171998	1	-3.591697	1.249671	0.593285
1	-1.638471	-0.147244	-1.567343	1	-2.362359	1.064353	-3.404576
1	-3.807065	-4.262699	-1.904873	1	-4.055203	2.217967	-2.151444
1	-3.142988	-4.712346	-0.321861	1	-2.648909	2.572005	-1.142470
1	-4.919649	-4.640579	-0.551132	1	-0.503430	-0.214174	-2.346526
1	-3.288707	1.238853	1.566046	1	-0.469936	1.531929	-1.845716
1	-3.747615	3.655058	1.893983	1	0.817833	-0.758108	1.223616
1	-3.164566	5.288940	0.111681	1	-2.818998	0.343118	2.535127
1	-2.119553	4.485992	-2.000221	1	-4.369167	-0.352867	2.017301
1	-1.632619	2.073091	-2.300887	1	-3.535369	-0.997463	3.432124
8	0.246222	0.366751	2.499644	1	-2.982862	-3.678186	0.861715
6	-1.608608	-1.150349	2.543772	1	-3.690158	-3.309649	2.442146
1	-2.559845	-1.076031	2.000604	1	-4.464320	-2.710468	0.977220
1	-1.330307	-2.212995	2.537509	1	-0.730782	-2.725266	1.762965
1	-1.702867	-0.814583	3.579360	1	-0.736209	-1.148089	2.592151
				1	-1.617503	-2.508334	3.272791
				1	1.560546	0.944546	-1.177284
				1	0.677895	5.315202	0.308810
				1	-0.800012	4.636445	1.014407
				1	0.391434	5.454781	2.071906
				1	3.533800	0.429899	1.893922
6	3.710617	-0.563492	-1.337022	1	5.802701	-0.632242	1.920171
6	3.173466	-0.022947	-0.161714	1	6.729616	-1.617069	-0.167690
6	3.942956	-0.045118	1.008233	1	5.391571	-1.542115	-2.264455
6	5.213067	-0.623586	1.006556	1	3.131652	-0.529263	-2.258091
6	5.736615	-1.174720	-0.166506	8	0.321970	-2.158859	-1.661295
6	4.984479	-1.136146	-1.341695	6	1.771532	-2.954817	0.060419
6	1.776069	0.593485	-0.156925	1	2.556694	-2.506749	0.672109
7	1.636001	1.584014	0.846727	1	1.150221	-3.585341	0.712015
6	0.956524	2.666715	0.484714	1	2.209548	-3.592890	-0.710179
8	0.962900	3.614450	1.490555				
6	0.267425	4.815467	1.193115				
8	0.337741	2.919313	-0.579769				
6	0.705829	-0.603147	0.150426				

E (CH₃CN) = -1575.196469
NImag = 1 (-269.0)

42. **3d-c** (-1574.8625574)

E (CH₃CN) = -1575.205601
NImag = 0

43. 3d-R[‡] (-1574.8514649)				1	0.990394	-0.738668	3.484060
				1	2.186372	-1.849776	2.787681
6	4.214393	-0.119937	0.387008	1	2.313932	-0.086354	2.497287
6	3.031793	-0.502387	-0.260679	1	2.052726	-2.121356	-1.303480
6	2.943001	-1.806805	-0.765394	1	3.899649	-3.720159	-1.009041
6	3.991381	-2.714519	-0.606356	1	5.974999	-3.031529	0.182062
6	5.155546	-2.327865	0.059042	1	6.173646	-0.707284	1.052847
6	5.263353	-1.025036	0.550080	1	4.288547	0.907448	0.726552
6	1.906419	0.510980	-0.456908	1	0.901307	4.993898	-1.939670
7	2.328124	1.814355	-0.188111	1	0.155172	5.051824	-0.332371
6	1.476179	2.742201	-0.620565	1	1.647420	5.990856	-0.651540
8	1.968938	4.015155	-0.432272				
6	1.112772	5.061578	-0.866509	E (CH ₃ CN) = -1575.195125			
6	0.547904	0.120306	0.552496	NImag = 1 (-41.8)			
6	0.731524	-1.111395	1.398482	44. 3d-t (-1574.8602557)			
6	1.627417	-0.928249	2.608797				
16	-1.031751	0.162278	-0.417326	6	-1.984954	2.383051	-1.510667
6	-2.431482	-0.601713	0.616269	6	-2.216353	1.545066	-0.412000
6	-3.427269	-1.245802	-0.387793	6	-2.747098	2.111162	0.755213
6	-2.796661	-2.485707	-1.058365	6	-3.003129	3.480029	0.831812
6	-1.982690	-1.855375	-2.198434	6	-2.748073	4.309013	-0.264135
6	-0.713903	-1.196677	-1.652903	6	-2.245920	3.754639	-1.441560
6	-3.844904	-0.366266	-1.613598	6	-1.919688	0.059120	-0.520824
6	-2.979726	-0.851090	-2.813167	6	-3.042551	-0.734824	-0.162224
6	-3.044925	0.413277	1.644877	7	-2.910609	-2.002743	-0.556970
6	-1.948487	1.093335	2.491293	6	-4.036902	-2.744167	-0.273532
6	-3.904968	1.523774	1.009926	8	-3.970343	-4.110773	-0.656389
6	-3.926182	-0.412424	2.613988	6	-1.921011	-2.559335	-1.095152
8	0.208141	-2.192925	1.152200	6	-0.625315	-0.429127	0.349294
8	0.340403	2.585416	-1.125750	16	0.948838	0.166450	-0.451935
1	-1.955383	-1.402015	1.186198	6	2.435955	-0.680117	0.372515
1	-4.307138	-1.528685	0.196838	6	3.618642	0.321849	0.296229
1	-2.193549	-3.091264	-0.374429	6	3.340845	1.566326	1.170309
1	-3.584827	-3.124220	-1.475589	6	2.519729	2.454923	0.224006
1	-4.910007	-0.512640	-1.820222	6	1.081649	1.947204	0.104095
1	-3.707537	0.700008	-1.433526	6	3.317970	2.373159	-1.092858
1	-1.643417	-2.596529	-2.932412	6	3.913518	0.935673	-1.111874
1	-3.601256	-1.361978	-3.556188	6	2.687106	-2.133859	-0.166154
1	-2.478024	-0.024700	-3.327844	6	3.130764	-2.207772	-1.640183
1	-0.088564	-1.926708	-1.141468	6	-0.631627	-0.286469	1.859372
1	-0.148731	-0.696398	-2.442513	6	3.801214	-2.745337	0.720661
1	0.500612	1.010739	1.173194	6	1.433354	-3.020186	0.005048
1	-3.333966	2.126003	0.294898	1	2.132282	-0.765351	1.418415
1	-4.790302	1.127261	0.503678	1	4.492183	-0.217841	0.670387
1	-4.256739	2.200760	1.796867	1	2.823804	1.334536	2.106164
1	-3.344738	-1.193442	3.118089	1	4.287330	2.063256	1.415515
1	-4.338182	0.247371	3.385669	1	4.994152	0.964348	-1.284275
1	-4.773431	-0.889811	2.111763	1	3.487420	0.343121	-1.922011
1	-1.265354	0.364214	2.940605	1	2.436512	3.487416	0.584974
1	-1.364652	1.813922	1.908740	1	4.118272	3.120787	-1.080007
1	-2.414619	1.652360	3.310081	1	2.699520	2.583352	-1.972394
1	1.484034	0.373526	-1.465760				

1	0.565036	1.998344	1.059647	6	3.087584	-4.139564	-0.791746
1	0.514578	2.493919	-0.651401	6	3.857610	-3.239935	-0.052579
1	-0.649246	-1.489472	0.064337	6	3.482731	-1.897857	0.042142
1	2.405078	-1.736961	-2.312527	8	3.860575	2.919087	0.114044
1	4.109834	-1.748320	-1.806016	6	3.818856	4.291290	-0.258803
1	3.210876	-3.259256	-1.937806	6	-3.107655	1.824353	-2.010800
1	3.540536	-2.701274	1.784927	6	-3.850860	2.814811	0.175863
1	3.933038	-3.799939	0.455827	8	-0.249371	0.621750	2.542489
1	4.770045	-2.254981	0.584040	1	-2.284619	0.957044	1.297958
1	1.028455	-2.959722	1.022517	1	-4.638240	0.328654	0.451487
1	0.631518	-2.787605	-0.702506	1	-3.206048	-0.891204	2.360254
1	1.707342	-4.066259	-0.171164	1	-4.576713	-1.768722	1.659921
1	-1.570117	-0.150805	-1.546916	1	-5.001905	-1.308700	-1.178474
1	-3.822133	-4.222468	-1.736296	1	-3.474883	-0.778811	-1.856769
1	-3.154529	-4.637041	-0.146956	1	-2.647309	-3.306799	1.377366
1	-4.930564	-4.546160	-0.366696	1	-4.083209	-3.351706	-0.537244
1	-2.987246	1.469969	1.596946	1	-2.575960	-2.917689	-1.335899
1	-3.414091	3.900357	1.746303	1	-0.890794	-1.614722	1.754305
1	-2.954759	5.374423	-0.204426	1	-0.551973	-2.574126	0.291407
1	-2.067895	4.384095	-2.310059	1	0.542111	1.465053	0.161528
1	-1.611858	1.951561	-2.437819	1	-2.364353	1.228474	-2.552258
8	0.255130	0.302104	2.472536	1	-4.086651	1.348938	-2.128714
6	-1.762240	-0.976674	2.581379	1	-3.157930	2.802508	-2.502237
1	-2.708595	-0.837814	2.043314	1	-3.625871	2.971987	1.237370
1	-1.574630	-2.059410	2.577832	1	-3.943804	3.800755	-0.292185
1	-1.795834	-0.625977	3.615931	1	-4.828856	2.329034	0.099996
E (CH ₃ CN) = -1575.204301				1	-1.089636	2.998111	0.565138
NImag = 0				1	-0.626628	2.509370	-1.077941
45. 3d-E[‡] (-1574.85667654)				1	-1.675036	3.892020	-0.841209
6	-3.933959	-1.200548	-0.962204	1	1.606536	0.349327	-1.529307
6	-3.751166	-0.289998	0.293940	1	3.846926	4.413737	-1.346900
6	-3.601462	-1.320584	1.433232	1	2.914133	4.783320	0.115883
6	-2.678635	-2.374681	0.800133	1	4.704751	4.746791	0.191152
6	-3.308517	-2.579834	-0.594920	1	4.091547	-1.178350	0.578434
6	-1.237644	-1.855358	0.748004	1	4.762871	-3.580828	0.443906
16	-1.038120	-0.328457	-0.286683	1	3.383614	-5.182592	-0.868475
6	-2.540737	0.686049	0.270309	1	1.360432	-4.362943	-2.066488
6	0.729288	0.418499	0.399682	1	0.718686	-1.980523	-1.926942
6	0.748909	0.269549	1.923361	1	2.137751	-1.321849	2.299886
6	1.944620	-0.298719	2.643380	1	2.836780	0.282042	2.398055
6	-2.723725	2.020235	-0.531293	1	1.737445	-0.294685	3.715950
6	-1.449483	2.888267	-0.464204	E (CH ₃ CN) = -1575.195429			
6	1.917274	0.033940	-0.519376	NImag = 1 (-77.6)			
7	2.934237	0.880324	0.037806	46. 3d-PC (-1574.91875214)			
6	2.821880	2.157264	-0.367321	6	3.819250	-2.049796	-0.762407
8	1.927907	2.680552	-1.062937	6	3.837249	-0.685335	-0.443556
6	2.323400	-1.433039	-0.590218	6	4.999608	-0.124322	0.097426
6	1.577772	-2.337982	-1.361496	6	6.125455	-0.918593	0.323402
6	1.947954	-3.681320	-1.455990	6	6.099930	-2.278214	0.009410

6	4.943563	-2.842300	-0.534946	6	2.297151	0.002142	2.647137
6	2.631393	0.154243	-0.730000	1	3.327583	-0.220171	2.347850
7	2.421129	1.370572	0.014654	1	2.250556	1.081370	2.831640
6	2.123394	2.575276	-0.630225	1	2.044996	-0.551449	3.553575
8	1.170987	3.241753	0.054911	E (CH ₃ CN) = -1575.242375			
6	0.845421	4.538064	-0.474755	NImag = 0			
8	2.688398	2.986582	-1.620092	<u>System 4 (R = COMe; X = Me, Y = CO₂Me)</u>			
6	1.436442	0.314445	0.211971	47. <u>4-<i>si</i>,<i>si</i>-c[‡]</u> (-1383.1095943)			
16	-2.163688	-0.339082	-1.316229	6	-0.550402	-3.081621	0.102539
6	-2.969573	-0.000380	0.334363	6	-0.717000	-2.486187	1.522549
6	-3.913840	-1.175608	0.708003	6	-2.230002	-2.254106	1.617420
6	-3.074914	-2.435329	1.021008	6	-2.529435	-1.569479	0.268872
6	-2.743404	-2.964928	-0.385475	6	-1.712986	-2.450487	-0.729772
6	-1.658623	-2.095624	-1.039241	6	0.034638	-1.162928	1.679196
6	-4.107744	-2.873194	-1.106078	16	-0.256991	-0.034491	0.235704
6	-4.849859	-1.681151	-0.430234	6	-2.170386	-0.046382	0.315008
6	-3.562064	1.448145	0.400266	6	0.557697	1.456604	0.852623
6	-4.811795	1.652512	-0.478047	6	0.577789	2.556898	-0.132113
6	1.334316	-0.376276	1.547774	6	1.028612	3.910713	0.398663
6	-3.934219	1.753975	1.869538	6	-2.924702	0.881186	-0.702307
6	-2.487159	2.471483	-0.028551	6	-2.417200	0.754460	-2.151753
1	-2.147954	-0.012978	1.061452	8	0.310362	2.401764	-1.319902
1	-4.496005	-0.873533	1.585349	6	-4.432164	0.517188	-0.671232
1	-2.185517	-2.230127	1.626763	6	-2.830719	2.350744	-0.237062
1	-3.689169	-3.168640	1.560065	6	2.418826	0.958770	1.034812
1	-5.799153	-2.016037	0.004366	7	2.643841	-0.333593	0.663408
1	-5.083155	-0.900206	-1.154035	6	3.087875	-0.494096	-0.614033
1	-2.363943	-3.994875	-0.356959	8	3.433532	0.350249	-1.438227
1	-4.665002	-3.806583	-0.964230	6	2.677240	1.257903	2.503955
1	-3.991596	-2.724652	-2.184929	8	3.129114	-1.840590	-0.920722
1	-0.754667	-2.103987	-0.422064	6	3.643699	-2.133506	-2.216822
1	-1.405955	-2.469847	-2.037629	1	0.214851	1.721302	1.853000
1	0.473616	0.411399	-0.291725	1	-2.405665	0.322330	1.320414
1	-4.613587	1.410564	-1.527577	1	-3.594260	-1.627392	0.043394
1	-5.654206	1.040838	-0.139150	1	-2.532454	-1.659814	2.488138
1	-5.129482	2.701595	-0.431315	1	-2.761027	-3.212963	1.669221
1	-3.070093	1.632907	2.534300	1	-2.369041	-3.233453	-1.124050
1	-4.281904	2.790122	1.958941	1	-1.343249	-1.887799	-1.589690
1	-4.738182	1.109375	2.239579	1	-0.336865	-3.159281	2.299819
1	-1.555322	2.340650	0.534021	1	-0.656021	-4.170666	0.142620
1	-2.247168	2.389070	-1.093500	1	0.438052	-2.864314	-0.315226
1	-2.850783	3.490891	0.151672	1	-0.268887	-0.625007	2.584544
1	2.345668	0.193452	-1.782648	1	1.125238	-1.278147	1.637907
1	1.722278	5.190465	-0.453487	1	2.842750	1.715185	0.363887
1	0.486279	4.453863	-1.503371	1	-1.370155	1.055138	-2.242944
1	0.060803	4.926439	0.174565	1	-2.531766	-0.266089	-2.532422
1	5.013676	0.935346	0.333650	1	-3.007918	1.411292	-2.801110
1	7.024066	-0.472310	0.740977	1	-4.825416	0.466504	0.352101
1	6.976508	-2.895716	0.185617				
1	4.916672	-3.900306	-0.781306				
1	2.919853	-2.491260	-1.185472				
8	0.459554	-1.214556	1.700357				

1	-4.993013	1.295304	-1.199681	1	-2.320196	-2.073477	-2.535265
1	-4.650473	-0.430507	-1.172385	1	0.577096	-1.934591	-0.154206
1	-3.200560	2.466346	0.790003	1	0.157279	-1.876763	-1.880264
1	-1.816722	2.739863	-0.295414	1	2.001463	-0.930233	-1.495212
1	-3.451834	2.980722	-0.883532	1	-2.277732	2.315747	-0.879664
1	3.027653	-1.684472	-3.003204	1	-3.832479	1.450353	-0.797123
1	4.667146	-1.761959	-2.332623	1	-3.615330	2.970640	0.067787
1	3.629302	-3.223132	-2.302913	1	-3.592510	0.505520	2.865690
1	0.377864	4.247281	1.215298	1	-4.256617	2.032976	2.279155
1	2.049865	3.859185	0.793523	1	-4.664124	0.533308	1.446447
1	0.998973	4.635843	-0.416912	1	-1.318303	1.760773	2.747313
1	2.181763	0.528590	3.153365	1	-0.812512	2.539551	1.232440
1	3.755801	1.175470	2.684182	1	-2.203134	3.155610	2.111579
1	2.358683	2.266218	2.793111	1	4.080406	-1.347597	2.974356
E (CH ₃ CN) = -1383.407475				1	4.757375	-2.571369	1.881136
NImag = 1 (-284.9)				1	5.837770	-1.346536	2.620058
48. 4- <i>si</i> , <i>si</i> - <i>t</i> [‡] (-1383.11782309)				1	2.897588	2.415821	0.012411
6	-2.614750	-2.490138	-1.565794	1	2.021722	3.967963	-0.303651
6	-1.394259	-2.773634	-0.657272	1	1.751343	3.046757	1.197740
6	-1.975531	-2.621357	0.753305	1	2.750037	1.904207	-2.489876
6	-2.805058	-1.327865	0.626702	1	3.162641	0.408215	-3.329043
6	-3.515767	-1.514458	-0.747428	1	1.456417	0.882615	-3.160611
6	-0.242603	-1.789986	-0.866260	E (CH ₃ CN) = -1383.413008			
16	-0.755366	-0.004623	-0.762763	NImag = 1 (-273.7)			
6	-1.908004	-0.066662	0.766873	49. 4- <i>si</i> , <i>re</i> - <i>c</i> [‡] (-1383.1123653)			
6	0.815984	0.758729	-0.330258	6	2.652208	1.287473	2.689307
6	0.816831	2.213495	-0.549372	6	2.378830	0.365389	1.513646
6	1.952356	2.963622	0.120987	7	3.343408	0.324249	0.570622
6	-2.631653	1.309679	1.045372	6	3.220049	-0.716284	-0.285313
6	-3.110737	2.042537	-0.225176	8	4.273435	-0.774324	-1.149101
8	-0.004898	2.789101	-1.266390	6	4.211227	-1.820821	-2.112794
6	-3.856329	1.064838	1.959532	8	2.299102	-1.552557	-0.356883
6	-1.675124	2.238749	1.826606	6	0.657870	1.086720	0.768131
6	2.399936	0.078686	-1.370186	6	1.086494	1.998345	-0.321668
7	3.474182	0.207027	-0.562304	16	-0.410276	-0.194044	0.081186
6	3.517723	-0.697877	0.447194	6	-0.274223	-1.569765	1.308270
8	2.635016	-1.494656	0.812893	6	-1.373455	-2.621381	1.129187
6	2.429178	0.872821	-2.657996	6	-2.749468	-2.024515	1.451365
8	4.706511	-0.627480	1.115500	6	-3.011698	-1.137233	0.217562
6	4.842518	-1.529940	2.208955	6	-2.257256	0.222522	0.339255
1	1.162564	0.378682	0.627730	6	-2.566642	-2.066893	-0.955196
1	-1.219303	-0.249072	1.599970	6	-1.528322	-3.060887	-0.346929
1	-3.535816	-1.272271	1.435229	6	-2.788746	1.408281	-0.546714
1	-1.211806	-2.580240	1.538080	6	-2.421457	1.289488	-2.039790
1	-2.641329	-3.463470	0.979227	6	-4.331920	1.465775	-0.418300
1	-4.504960	-1.955029	-0.585547	6	-2.258434	2.752942	0.000723
1	-3.676512	-0.570359	-1.271841	1	0.212331	1.559203	1.643348
1	-0.977193	-3.772194	-0.834021	1	-2.329476	0.549965	1.383950
1	-3.148568	-3.423907	-1.770418	1	-4.074017	-0.901934	0.138998

1	-2.781051	-1.475889	2.400629	7	2.809584	-0.172422	0.765565
1	-3.504196	-2.819332	1.502960	6	2.980500	-1.036442	-0.274451
1	-3.440656	-2.609160	-1.330892	8	2.814950	-0.823781	-1.482409
1	-2.151458	-1.514009	-1.799927	6	2.757463	2.146414	1.490740
1	-1.111852	-3.462310	1.782368	8	3.341014	-2.274301	0.180606
1	-1.907752	-4.087034	-0.390095	6	3.525534	-3.256082	-0.835506
1	-0.571106	-3.044467	-0.877546	1	-2.080910	1.159851	-0.342537
1	-0.286282	-1.142498	2.316246	1	-3.788907	-0.608602	0.367999
1	0.714476	-1.970952	1.075914	1	-2.720657	1.356630	1.867242
1	-1.338905	1.274246	-2.197823	1	-3.574559	0.035575	2.690965
1	-2.857093	0.394758	-2.496168	1	-3.195303	-2.609607	1.422556
1	-2.822744	2.155377	-2.579641	1	-1.697420	-2.502745	0.523240
1	-4.659040	1.450146	0.629138	1	-1.335377	0.095081	3.761455
1	-4.691502	2.401076	-0.860851	1	-2.105439	-2.148646	3.433783
1	-4.830746	0.648467	-0.947551	1	-0.562395	-2.248755	2.590126
1	-2.494308	2.872274	1.065862	1	-0.202878	1.447747	2.039279
1	-1.182139	2.861932	-0.128999	1	0.750754	-0.037877	2.377000
1	-2.732467	3.581136	-0.537705	1	1.223258	1.000528	-1.432725
1	1.951947	-0.586061	1.839984	1	3.150609	1.427632	-0.542204
1	4.186032	-2.805537	-1.633674	1	-1.180404	-2.397987	-1.666616
1	3.324965	-1.723151	-2.748471	1	-2.935432	-2.442205	-1.388197
1	5.117379	-1.720678	-2.714783	1	-2.298955	-2.223308	-3.019029
8	0.932342	1.725291	-1.508318	1	-3.577028	1.201060	-2.188537
6	1.848592	3.246258	0.077879	1	-3.742039	-0.184322	-3.278566
1	1.513993	3.673685	1.028110	1	-4.349015	-0.293871	-1.626710
1	2.902583	2.955624	0.173910	1	-1.039729	1.236819	-2.737062
1	1.761856	3.986513	-0.720990	1	-0.112749	-0.279759	-2.655605
1	3.478813	0.851840	3.264131	1	-1.412647	-0.101971	-3.830525
1	1.788894	1.380392	3.357939	1	2.602256	-3.424086	-1.400719
1	2.973173	2.281573	2.370997	1	4.308323	-2.958326	-1.540627
E (CH ₃ CN) = -1383.408478				1	3.817825	-4.170142	-0.313490
NImag = 1 (-292.8)				8	-0.690715	2.951980	0.365634
50. 4- <i>re</i> , <i>si</i> -c [‡] (-1383.1235435)				6	0.902172	3.698987	-1.262417
6	-1.538587	-1.752303	2.584444	1	1.933186	3.452180	-1.534635
6	-1.419080	-0.219835	2.713956	1	0.325177	3.793107	-2.191942
6	-2.715367	0.278034	2.053413	1	0.870503	4.665551	-0.752160
6	-2.768794	-0.567110	0.760653	1	3.807040	2.198425	1.808117
6	-2.314634	-1.980906	1.254837	1	2.169112	1.867332	2.367827
6	-0.196089	0.359290	2.002105	1	2.455023	3.143737	1.157782
16	-0.100831	-0.071982	0.194798	E (CH ₃ CN) = -1383.414651			
6	-1.900627	0.081437	-0.353202	NImag = 1 (-269.3)			
6	0.832590	1.311247	-0.469048	51. 4- <i>re</i> , <i>si</i> -t [‡] (-1383.1182696)			
6	0.249782	2.640124	-0.378877	6	-1.588333	3.015643	1.039941
6	-2.147861	-0.428483	-1.818301	6	-0.784400	2.699833	-0.241731
6	-2.139869	-1.962411	-1.966345	6	-1.890152	2.369005	-1.257491
6	-3.537121	0.106911	-2.242245	6	-2.796942	1.417536	-0.449165
6	-1.110415	0.146127	-2.806624	6	-2.867735	2.130016	0.940927
6	2.660900	1.114737	0.388225	6	0.171183	1.516941	-0.085293
				16	-0.669168	0.023440	0.648178

6	-2.224915	-0.029484	-0.453814	52. $4-re, re-c^{\ddagger}$ (-1383.11989221)			
6	0.518714	-1.285667	0.299755				
6	0.814240	-1.553262	-1.134219	6	-3.034594	2.695067	-0.602913
6	-3.234809	-1.171716	-0.101021	6	-2.525303	1.275692	-0.438903
6	-3.999819	-0.946455	1.217107	7	-3.108670	0.596470	0.577052
6	-4.252663	-1.243299	-1.267278	6	-3.128932	-0.748991	0.450084
6	-2.536582	-2.545996	-0.030894	8	-3.848399	-1.314801	1.467752
6	2.140636	-0.949134	1.361880	6	-3.963139	-2.732522	1.414846
7	3.266550	-0.889870	0.610253	8	-2.609304	-1.472433	-0.419286
6	3.647877	0.355401	0.233699	6	-0.619729	1.538719	0.002475
8	3.130626	1.453368	0.491852	16	0.122757	-0.109594	-0.029896
6	2.095824	-2.131360	2.319192	6	2.010335	0.009229	0.113042
8	4.789430	0.292205	-0.521220	6	2.576521	-1.267880	-0.574768
6	5.308818	1.550656	-0.936415	6	2.370238	-1.204271	-2.103143
1	-1.808953	-0.245784	-1.440852	6	0.918264	-1.683042	-2.252065
1	-3.793368	1.356632	-0.895441	6	-0.063274	-0.594324	-1.822353
1	-1.511501	1.927794	-2.185365	6	0.864276	-2.923902	-1.333513
1	-2.446685	3.278175	-1.517936	6	1.887987	-2.621584	-0.198302
1	-3.768254	2.751996	0.977740	6	2.530032	0.288716	1.567192
1	-2.940585	1.429205	1.774337	6	2.396598	-0.911945	2.524019
1	-0.164261	3.547586	-0.555523	6	0.094384	2.587275	-0.751341
1	-1.856825	4.077016	1.057373	6	4.028042	0.663412	1.442562
1	-1.010273	2.817288	1.948860	6	1.818190	1.495642	2.213675
1	0.558060	1.183042	-1.047585	1	2.265745	0.875985	-0.502853
1	1.020854	1.711212	0.573750	1	3.641641	-1.301750	-0.329647
1	0.172671	-2.172546	0.823130	1	2.547753	-0.209403	-2.525208
1	1.815494	-0.013135	1.836212	1	3.050455	-1.909017	-2.597734
1	-3.322419	-0.864943	2.074823	1	2.649294	-3.407050	-0.145338
1	-4.623260	-0.047655	1.186185	1	1.403144	-2.593166	0.778358
1	-4.663447	-1.798496	1.404817	1	0.660767	-1.929358	-3.289444
1	-3.750635	-1.429663	-2.223715	1	1.163498	-3.816155	-1.893683
1	-4.952090	-2.068162	-1.090988	1	-0.146170	-3.099280	-0.950853
1	-4.848040	-0.330629	-1.367125	1	0.073696	0.326090	-2.389224
1	-1.897068	-2.724085	-0.901935	1	-1.097882	-0.942128	-1.840530
1	-1.930029	-2.653028	0.873664	1	-0.812660	1.783774	1.042562
1	-3.292327	-3.339002	-0.002521	1	1.355017	-1.231532	2.639070
1	4.592260	2.092981	-1.562961	1	2.986909	-1.771985	2.194213
1	5.560474	2.183142	-0.078436	1	2.762140	-0.626461	3.517283
1	6.209987	1.323030	-1.510909	1	4.170040	1.533003	0.790048
8	0.419891	-0.836190	-2.053883	1	4.424006	0.920051	2.431584
6	1.732537	-2.724080	-1.381033	1	4.638373	-0.157135	1.053146
1	2.721376	-2.432182	-0.989832	1	1.834963	2.377952	1.565110
1	1.414579	-3.620633	-0.836207	1	0.778360	1.274230	2.472153
1	1.787513	-2.931304	-2.451844	1	2.329765	1.760431	3.145855
1	2.281242	-3.073286	1.792510	1	-2.398130	0.761636	-1.399142
1	2.900720	-2.005684	3.052723	1	-4.450278	-3.061174	0.490735
1	1.145163	-2.197369	2.861575	1	-2.982244	-3.217032	1.475303
				1	-4.571528	-3.011516	2.278470
				8	0.792111	2.366416	-1.745414
				6	-0.056690	4.022319	-0.256483
				1	-0.839239	4.150112	0.493807
				1	0.899768	4.332418	0.184048

E (CH₃CN) = -1383.411094
NImag = 1 (-265.6)

1	-0.248085	4.682997	-1.107300
1	-3.015914	3.235207	0.348353
1	-4.084205	2.630960	-0.914355
1	-2.486905	3.258389	-1.364888

E (CH₃CN) = -1383.412099

NImag = 1 (-279.7)

53. **4-*re, re*-t[‡]** (-1383.1202312)

6	2.070902	-2.991394	-0.079591
6	2.238612	-1.544372	-0.498853
7	3.445526	-1.017492	-0.199939
6	3.676177	0.216700	-0.710314
8	4.992401	0.562046	-0.584276
6	5.322115	1.864267	-1.058151
8	2.854138	1.010121	-1.198265
6	0.855107	-0.475646	0.464259
16	-0.641121	-0.297108	-0.511114
6	-1.953867	0.692938	0.446937
6	-3.343330	0.196732	-0.032384
6	-3.588517	-1.256337	0.431354
6	-2.875346	-2.070899	-0.659945
6	-1.358010	-2.015664	-0.469976
6	-3.360124	-1.392472	-1.958042
6	-3.545099	0.106246	-1.581224
6	-1.701462	2.240108	0.407682
6	-2.012733	2.898972	-0.950062
6	0.702248	-0.882782	1.865678
6	-2.620806	2.863607	1.487349
6	-0.246124	2.589900	0.787637
1	-1.802507	0.358217	1.476470
1	-4.080435	0.872578	0.410440
1	-3.214048	-1.459501	1.439582
1	-4.662924	-1.476793	0.414296
1	-4.551731	0.449488	-1.840908
1	-2.850218	0.741909	-2.131102
1	-3.143738	-3.134131	-0.631016
1	-4.314588	-1.833017	-2.265351
1	-2.661659	-1.532308	-2.790618
1	-1.066659	-2.425456	0.496566
1	-0.832424	-2.533000	-1.277244
1	1.435050	0.421630	0.267749
1	-1.400771	2.482135	-1.757619
1	-3.067369	2.804526	-1.226878
1	-1.785171	3.969423	-0.891246
1	-2.422475	2.437235	2.477666
1	-2.434686	3.941842	1.545652
1	-3.684637	2.730843	1.265289
1	0.058979	2.105283	1.721544
1	0.471287	2.320667	0.005806
1	-0.163911	3.672832	0.934721

1	1.817264	-1.306144	-1.486114
1	5.089232	1.973408	-2.122571
1	4.778646	2.639684	-0.507286
1	6.396894	1.973517	-0.895918
8	-0.331164	-1.375766	2.336612
6	1.942930	-0.692803	2.718391
1	2.853620	-0.912126	2.146327
1	2.009366	0.357505	3.033654
1	1.869534	-1.319152	3.611112
1	2.357872	-3.131460	0.966426
1	1.053186	-3.363594	-0.222693
1	2.749225	-3.603677	-0.686384

E (CH₃CN) = -1383.414682

NImag = 1 (-267.4)

Addition of Semistabilized ylide (R = Ph)

System 5 (R = Ph; X = Ph; Y = SO₂Me)

54. **5-*si, si*-c[‡]** (-2013.2720646)

6	3.624133	-1.973669	-0.026995
6	2.542631	-3.078665	-0.241728
6	1.790063	-2.650184	-1.523801
6	2.871840	-1.915574	-2.324347
6	3.506417	-1.009612	-1.249503
6	2.666154	0.284745	-1.030419
16	1.058651	-0.295954	-0.135119
6	0.615765	-1.712787	-1.240838
6	-0.429324	0.697713	-0.387924
1	-0.589311	0.815172	-1.461305
6	3.387831	1.498790	-0.335131
6	2.710017	2.811409	-0.781006
6	3.399661	1.427903	1.205380
6	4.856764	1.572796	-0.820744
6	-2.027416	-0.395109	0.302624
7	-1.807747	-1.699002	0.615175
1	2.321700	0.627797	-2.012983
1	4.493830	-0.679198	-1.575839
1	2.485165	-1.363399	-3.189821
1	3.621055	-2.627495	-2.693066
1	4.627312	-2.412661	-0.012669
1	3.491735	-1.463047	0.929294
1	1.374913	-3.510898	-2.061869
1	3.020498	-4.050167	-0.408144
1	1.867864	-3.179339	0.612394
1	0.219183	-1.274796	-2.163624
1	-0.197963	-2.196275	-0.692779
1	-2.168635	0.302206	1.131123
1	2.394646	1.488170	1.633045
1	3.875559	0.513953	1.573213

1	3.969468	2.276833	1.600696	6	-3.682515	1.122407	1.448161
1	4.931988	1.551551	-1.914858	6	-2.709680	0.692163	2.555994
1	5.291876	2.519281	-0.481840	6	-1.292970	0.611936	1.980667
1	5.476104	0.766562	-0.415320	6	-3.956856	-1.264764	1.734944
1	2.768304	2.932458	-1.870377	6	-3.280918	-0.670345	3.007777
1	1.660890	2.861693	-0.488397	6	-2.859638	-1.347074	-1.555908
1	3.218716	3.668721	-0.325566	6	-4.085270	-0.836417	-2.356236
16	-1.232911	-2.027586	2.113733	6	-1.661667	-1.333815	-2.530951
8	0.024098	-2.805183	2.003209	6	-3.120396	-2.800439	-1.116407
8	-1.220429	-0.847153	3.014354	6	1.544807	1.418213	0.331703
6	-2.473543	-3.173918	2.751641	7	1.412427	2.241785	-0.729539
1	-2.121441	-3.533689	3.721250	16	-0.028409	2.994453	-0.867946
1	-3.421618	-2.644076	2.859145	6	0.450247	4.488240	-1.746052
1	-2.573040	-4.002627	2.048931	6	2.901768	0.886449	0.602657
6	-0.498983	1.981830	0.353772	8	-0.954489	2.244624	-1.765133
6	-0.880811	3.156229	-0.322831	8	-0.620032	3.399068	0.439003
6	-1.048140	4.360078	0.362477	1	0.148145	0.143076	-1.115539
6	-0.828467	4.420640	1.739469	1	-2.395692	0.628756	-0.809497
6	-0.461969	3.260090	2.426044	1	-4.729569	-0.140093	0.013967
6	-0.311241	2.050507	1.749648	1	-3.322026	1.978144	0.868482
1	-1.044846	3.121163	-1.397287	1	-4.653370	1.390335	1.883861
1	-1.343265	5.252391	-0.183905	1	-5.017974	-1.461015	1.922131
1	-0.951569	5.358757	2.273816	1	-3.508562	-2.217489	1.449310
1	-0.311784	3.288916	3.502075	1	-2.666259	1.414341	3.380025
1	-0.095475	1.143846	2.308308	1	-4.020413	-0.516782	3.800876
6	-2.958196	-0.163614	-0.848190	1	-2.507616	-1.330804	3.415923
6	-3.181676	-1.154573	-1.816198	1	-1.024032	1.566199	1.521612
6	-4.051311	-0.923923	-2.880558	1	-0.554287	0.341690	2.742372
6	-4.721876	0.297298	-2.992473	1	0.975874	1.625296	1.236206
6	-4.521143	1.282753	-2.024815	1	-2.299041	-3.197820	-0.508998
6	-3.647103	1.053661	-0.960985	1	-4.051279	-2.903592	-0.549964
1	-2.683938	-2.112388	-1.705750	1	-3.207008	-3.438537	-2.003552
1	-4.216130	-1.703488	-3.620466	1	-3.964254	0.213314	-2.647700
1	-5.404069	0.473403	-3.820163	1	-4.184114	-1.426895	-3.273715
1	-5.051939	2.229123	-2.091356	1	-5.026390	-0.936980	-1.806768
1	-3.503203	1.821004	-0.205877	1	-1.387825	-0.312630	-2.816825
				1	-0.779955	-1.827696	-2.115855
				1	-1.935796	-1.878910	-3.441896
				1	-0.465004	5.042212	-1.965126
				1	1.114128	5.072798	-1.107409
				1	0.956188	4.199296	-2.668251
				1	1.808673	-0.970836	-2.389142
6	1.473931	-2.529707	0.609966	1	3.330307	-2.876636	-2.768823
6	1.258308	-1.557342	-0.386986	1	3.660410	-4.593896	-0.992909
6	1.951503	-1.710453	-1.605514	1	2.460808	-4.350875	1.176154
6	2.810864	-2.786835	-1.817912	1	0.970679	-2.438029	1.569606
6	2.996748	-3.750136	-0.825044	6	3.203839	0.361990	1.867460
6	2.320839	-3.613207	0.389665	6	4.486160	-0.095734	2.162648
6	0.425388	-0.350485	-0.191729	6	5.487097	-0.040191	1.190099
16	-1.105112	-0.725583	0.700486	6	5.195183	0.477163	-0.074171
6	-2.637434	-0.344412	-0.369157	6	3.913041	0.937398	-0.367375
6	-3.824305	-0.174540	0.623769	1	2.426473	0.321413	2.628064

E (CH₃CN) = -2013.641421
NImag = 1 (-207.0)

55. **5**-*si*,*si*-*t*[‡] (-2013.2718475)

1	4.705891	-0.492342	3.150508
1	6.488725	-0.395850	1.417307
1	5.971769	0.525664	-0.833304
1	3.679471	1.360821	-1.338377

E (CH₃CN) = -2013.635492

NImag = 1 (-222.8)

56. **5-si, re-c[‡]** (-2013.2726994)

6	-1.439703	1.526738	-1.348050
6	-2.863901	2.084350	-1.445066
6	-3.818670	1.036237	-2.030101
6	-3.986784	0.060832	-0.848986
6	-2.773190	-0.913034	-0.758321
16	-1.304975	0.153722	-0.118231
6	-4.182734	1.034564	0.354374
6	-3.475797	2.366689	-0.050493
6	-2.982380	-2.256267	0.027702
6	-4.373301	-2.838238	-0.327643
6	0.328952	-0.513855	-0.422860
6	0.837001	-1.348211	0.689635
6	-1.937289	-3.289377	-0.445608
6	-2.898359	-2.110093	1.560465
6	1.798495	1.022471	-0.616602
7	2.084966	1.599303	0.564371
16	1.120613	2.845851	1.008832
6	2.266592	3.808820	2.005668
6	2.859870	0.164006	-1.212057
8	0.694412	3.691429	-0.140122
8	0.021245	2.405495	1.909328
1	0.368213	-0.991030	-1.403145
1	-2.488517	-1.185274	-1.782094
1	-4.874381	-0.558045	-0.991068
1	-3.443720	0.558432	-2.943414
1	-4.785292	1.496967	-2.269879
1	-5.254569	1.200658	0.505905
1	-3.789620	0.635296	1.291632
1	-2.801290	2.992046	-2.056218
1	-4.204680	3.180376	-0.124891
1	-2.715050	2.674979	0.673414
1	-1.086192	1.145531	-2.312686
1	-0.752920	2.295333	-0.984122
1	-1.910280	-1.779505	1.894338
1	-3.645718	-1.410722	1.948346
1	-3.088941	-3.083574	2.027097
1	-4.536673	-2.882612	-1.411635
1	-4.438049	-3.862543	0.055514
1	-5.194877	-2.271817	0.122099
1	-2.014165	-3.459869	-1.527250
1	-0.916122	-2.984887	-0.214820
1	-2.110585	-4.249532	0.053746

1	1.240035	1.589434	-1.363439
1	2.655556	3.170208	2.799995
1	3.075261	4.166122	1.366381
1	1.704199	4.646311	2.424023
6	1.513369	-2.552217	0.411106
6	2.073845	-3.317417	1.432953
6	1.972904	-2.899296	2.760842
6	1.322762	-1.697454	3.050455
6	0.770304	-0.920777	2.032197
1	1.602109	-2.886056	-0.620036
1	2.587017	-4.244180	1.188454
1	2.402165	-3.498548	3.559494
1	1.254496	-1.350871	4.078708
1	0.304186	0.030070	2.271502
6	2.831618	-0.134373	-2.582606
6	3.831893	-0.910524	-3.165725
6	4.879178	-1.401030	-2.381532
6	4.917241	-1.106726	-1.016691
6	3.916485	-0.330067	-0.434265
1	2.022890	0.256642	-3.197626
1	3.799911	-1.124929	-4.230937
1	5.662734	-2.003942	-2.833279
1	5.731440	-1.483005	-0.402615
1	3.940780	-0.085658	0.621913

E (CH₃CN) = -2013.639350

NImag = 1 (-203.0)

57. **5-re, si-c[‡]** (-2013.2677823)

6	-3.613689	-1.193138	1.457181
6	-2.537933	-1.938224	2.301015
6	-1.562011	-0.832632	2.763857
6	-2.468599	0.404246	2.869035
6	-3.275972	0.331136	1.555491
6	-2.471316	0.934561	0.365300
16	-1.054267	-0.281207	0.038958
6	-0.434612	-0.595418	1.758738
6	0.359852	0.401071	-0.837510
6	0.742517	1.822002	-0.718503
6	-3.308472	1.302070	-0.910810
6	-2.407532	1.792759	-2.062591
6	-4.182105	0.149700	-1.444703
6	-4.226721	2.486567	-0.517748
6	1.856346	-1.030538	-0.635685
6	2.891373	-0.410731	0.246439
7	1.362989	-2.222941	-0.218927
16	0.533018	-3.110818	-1.322170
6	1.576325	-4.571313	-1.539341
8	-0.720905	-3.590781	-0.701646
8	0.439754	-2.438662	-2.643775
1	-1.983756	1.855862	0.702485

1	-4.192998	0.921467	1.633341	6	3.941989	0.555694	-0.017997
1	-1.919143	1.345308	2.993613	6	4.136949	1.127862	-1.461991
1	-3.146138	0.300852	3.725680	6	1.252224	1.847574	-0.176844
1	-4.614775	-1.363413	1.867572	16	1.279905	0.085614	-0.760154
1	-3.628042	-1.559509	0.431050	6	2.855021	-0.544621	0.136754
1	-1.079605	-1.082995	3.716571	6	-0.274296	-0.623417	-0.181761
1	-2.994215	-2.417559	3.173673	6	-1.973775	0.473717	-0.852504
1	-2.031309	-2.716502	1.721528	7	-2.502845	1.243229	0.112893
1	0.206566	0.236131	2.053858	16	-2.044934	2.816753	0.161637
1	0.183496	-1.483230	1.602262	8	-1.257366	3.114123	1.384624
1	0.155995	0.118119	-1.868982	6	3.302046	-1.993204	-0.269183
1	2.061569	-0.898140	-1.701091	6	3.950662	-2.083459	-1.664352
1	-3.585072	-0.729503	-1.709934	6	-2.761058	-0.737263	-1.231340
1	-4.951875	-0.156352	-0.729725	6	-2.592066	-1.315422	-2.498153
1	-4.695891	0.481933	-2.354159	6	-3.336387	-2.431813	-2.877239
1	-3.644718	3.342537	-0.155379	6	-4.260095	-2.989328	-1.989726
1	-4.789964	2.817211	-1.397459	6	-4.436069	-2.418081	-0.727077
1	-4.957740	2.219953	0.251896	6	-3.695526	-1.298314	-0.349525
1	-1.718084	2.579849	-1.743983	6	-0.485776	-0.972567	1.244037
1	-1.821048	0.978861	-2.498683	6	-0.814224	-2.306707	1.568277
1	-3.036266	2.199729	-2.862659	6	-1.097057	-2.691218	2.877125
1	1.045093	-5.262822	-2.197718	6	-1.059560	-1.749410	3.907396
1	2.523983	-4.267615	-1.988246	6	-0.771620	-0.419097	3.602021
1	1.741500	-5.026207	-0.561331	6	-0.505644	-0.026903	2.288977
6	1.173824	2.481302	-1.891334	6	4.334597	-2.455798	0.790177
6	1.626035	3.798059	-1.865326	6	2.131356	-2.993945	-0.218985
6	1.646432	4.514420	-0.666306	8	-1.464551	3.294824	-1.123046
6	1.216884	3.885855	0.503074	6	-3.637391	3.631383	0.373452
6	0.779978	2.561705	0.480736	1	2.540896	-0.586223	1.185716
1	1.146436	1.944234	-2.836808	1	4.875803	0.117492	0.345749
1	1.950638	4.270572	-2.789085	1	3.145451	1.594547	1.775786
1	1.989881	5.544777	-0.644478	1	4.476819	2.425477	0.955387
1	1.228981	4.425561	1.446711	1	5.204100	1.288273	-1.648384
1	0.473531	2.105291	1.415641	1	3.786747	0.443480	-2.235258
6	3.121238	-0.880910	1.548853	1	2.411221	3.572604	0.153251
6	4.118622	-0.318277	2.343525	1	4.054415	3.319249	-1.581788
6	4.914516	0.717738	1.848212	1	2.678281	2.542037	-2.358163
6	4.709504	1.179505	0.547097	1	0.806453	1.858941	0.815168
6	3.709718	0.617262	-0.245770	1	0.555378	2.342233	-0.857584
1	2.531081	-1.714954	1.912897	1	-0.384442	-1.491082	-0.828613
1	4.286014	-0.699748	3.347916	1	-1.470395	0.954056	-1.695571
1	5.695660	1.152270	2.466720	1	3.267849	-1.753164	-2.455146
1	5.331138	1.975234	0.145100	1	4.871664	-1.497427	-1.736236
1	3.562129	0.978653	-1.259067	1	4.211097	-3.127468	-1.873988
				1	3.905922	-2.438270	1.799038
E (CH ₃ CN) = -2013.635958				1	4.639243	-3.486634	0.576802
NImag = 1 (-217.0)				1	5.242819	-1.844917	0.794451
58. 5-re,si-t[‡] (-2013.2689355)				1	1.597536	-2.950716	0.733986
				1	1.409950	-2.823834	-1.024300
				1	2.518633	-4.011736	-0.343809
6	3.360018	2.475849	-1.503688	1	-3.441031	4.697748	0.505872
6	2.614394	2.540691	-0.155559	1	-4.244594	3.457647	-0.516383
6	3.579070	1.815848	0.793918	1	-4.121438	3.216527	1.258758

1	-0.854243	-3.048264	0.774500	1	-0.841021	1.721607	-1.645911
1	-1.344253	-3.728136	3.091040	1	0.745306	-0.371205	1.271505
1	-1.272340	-2.045773	4.931191	1	-2.807159	0.079164	2.781257
1	-0.779659	0.333629	4.386175	1	-4.400293	-0.577060	2.352001
1	-0.385555	1.029361	2.084031	1	-3.440484	-1.340152	3.620665
1	-3.835514	-0.835584	0.621295	1	-3.149961	-3.770115	0.767397
1	-5.157217	-2.844342	-0.034154	1	-3.719180	-3.550379	2.427985
1	-4.842502	-3.859003	-2.282971	1	-4.606114	-2.810535	1.097583
1	-3.201160	-2.861899	-3.866462	1	-0.812626	-2.911394	1.550040
1	-1.876909	-0.879164	-3.193240	1	-0.733762	-1.440188	2.535687
E (CH ₃ CN) = -2013.635909				1	-1.578771	-2.859127	3.145467
NImag = 1 (-191.4)				1	1.512180	1.319741	-1.244089
59. 5-<i>re</i>,<i>re</i>-c[‡] (-2013.268747)				1	1.494537	4.800073	1.756665
6	-3.623333	1.851345	-1.065039	1	2.297090	4.931060	0.156010
6	-2.838874	0.948603	-2.043088	1	0.714779	5.735576	0.437842
6	-3.601347	-0.383118	-1.967955	1	2.121663	-2.195415	1.356919
6	-3.788047	-0.565341	-0.447130	1	2.921814	-4.363391	0.522120
6	-4.177152	0.877752	0.016218	1	2.150382	-5.225466	-1.689950
6	-1.377240	0.768075	-1.628061	1	0.570839	-3.851642	-3.040696
16	-1.175571	0.178154	0.126325	1	-0.209830	-1.694529	-2.231525
6	-2.513279	-1.174726	0.205902	6	3.712205	-0.137713	-0.988012
6	0.512104	-0.433031	0.210663	6	4.953074	-0.742004	-0.784283
6	1.757355	1.213476	-0.184376	6	5.556114	-0.694538	0.473333
6	3.059871	0.527293	0.058533	6	4.912485	-0.033636	1.523951
6	-2.709539	-1.795260	1.634690	6	3.677134	0.577307	1.317763
6	-3.380548	-0.844203	2.644914	1	3.244259	-0.180020	-1.968438
6	0.882147	-1.753039	-0.353919	1	5.448160	-1.248457	-1.608709
6	0.468872	-2.259716	-1.603592	1	6.523596	-1.163506	0.633523
6	0.916188	-3.495044	-2.073345	1	5.381636	0.015341	2.503584
6	1.801217	-4.265644	-1.319739	1	3.183065	1.121443	2.116407
6	2.231021	-3.781330	-0.082473	E (CH ₃ CN) = -2013.636235			
6	1.775166	-2.554777	0.391997	NImag = 1 (-207.9)			
7	1.462327	2.223669	0.661119	60. 5-<i>re</i>,<i>re</i>-t[‡] (-2013.2637168)			
16	0.460986	3.401537	0.127474	6	4.130068	0.789347	-1.717599
8	0.379125	3.463250	-1.359846	6	3.386019	2.084756	-2.153126
8	-0.837264	3.393961	0.843863	6	2.607680	2.538317	-0.899959
6	1.341181	4.873739	0.679012	6	3.535319	2.094070	0.241741
6	-3.601737	-3.050033	1.460166	6	3.907327	0.654492	-0.175196
6	-1.374865	-2.275879	2.240194	6	2.809984	-0.347477	0.271877
1	-2.133879	-1.974492	-0.439224	16	1.239845	0.027246	-0.755541
1	-4.602145	-1.265691	-0.239886	6	1.227405	1.887251	-0.781435
1	-3.081007	-1.220986	-2.447923	6	-0.304932	-0.428808	0.052802
1	-4.580902	-0.281487	-2.451557	6	-0.446378	-0.334627	1.527976
1	-5.268098	0.949400	0.082262	6	3.192489	-1.869557	0.265827
1	-3.786334	1.125988	1.002725	6	1.997182	-2.754539	0.681741
1	-2.816294	1.366515	-3.056692	6	3.729250	-2.380356	-1.085030
1	-4.443655	2.344676	-1.597272	6	4.292591	-2.055721	1.341336
1	-2.991088	2.631933	-0.631594	6	-1.959174	0.174347	-0.941703
1	-0.865566	0.062957	-2.282882	6	-2.260710	1.573979	-0.510172

7	-2.909477	-0.736952	-0.621217
16	-2.786173	-2.165055	-1.427329
6	-4.497989	-2.716909	-1.360754
8	-2.404860	-2.004747	-2.850780
8	-1.986794	-3.153699	-0.648307
1	2.512054	-0.102223	1.296471
1	4.830538	0.338449	0.318336
1	3.077040	2.155395	1.235470
1	4.433322	2.723829	0.253578
1	5.201425	0.867850	-1.928688
1	3.767940	-0.078871	-2.268125
1	2.432242	3.621033	-0.900751
1	4.101665	2.863239	-2.438230
1	2.730462	1.921723	-3.015413
1	0.694809	2.228581	0.105118
1	0.604332	2.123349	-1.645874
1	-0.440577	-1.455310	-0.278762
1	3.006134	-2.233835	-1.894925
1	4.671631	-1.900577	-1.367176
1	3.919932	-3.457035	-1.012677
1	3.952426	-1.716873	2.327056
1	4.539507	-3.119723	1.424686
1	5.220107	-1.527489	1.097572
1	1.519742	-2.397121	1.599203
1	1.231536	-2.823284	-0.096190
1	2.352927	-3.774616	0.865074
1	-1.515381	0.120093	-1.942519
1	-4.816056	-2.742122	-0.317561
1	-5.113877	-2.022830	-1.934600
1	-4.531714	-3.716909	-1.798588
6	-1.227919	-1.335379	2.148088
6	-1.494901	-1.292737	3.515573
6	-0.976677	-0.269228	4.311857
6	-0.191017	0.719039	3.718255
6	0.062211	0.692579	2.346608
1	-1.620460	-2.143233	1.538505
1	-2.103381	-2.074970	3.962498
1	-1.178324	-0.243886	5.379333
1	0.222904	1.523455	4.321379
1	0.665118	1.489931	1.925824
6	-2.038912	2.638168	-1.395630
6	-2.353719	3.949699	-1.035920
6	-2.900228	4.214040	0.220937
6	-3.143507	3.157900	1.103543
6	-2.834889	1.847703	0.740298
1	-1.644230	2.431208	-2.389024
1	-2.186159	4.759950	-1.741269
1	-3.148383	5.233329	0.505736
1	-3.583070	3.355429	2.077957
1	-3.044815	1.023129	1.412101

E (CH₃CN) = -2013.636442
NImag = 1 (-240.3)

System 6 (R = Ph; X = Me; Y = SO₂Me)

61. **6-*si*,*si*-c[‡]** (-1821.5332115)

6	-2.417520	-2.459585	-0.990772
6	-1.343397	-3.376940	-0.331023
6	-1.297916	-2.920492	1.143935
6	-2.747916	-2.493752	1.407232
6	-3.050419	-1.623483	0.170908
6	-2.499146	-0.178716	0.355308
16	-0.571974	-0.337079	0.189539
6	-0.343758	-1.746517	1.373259
6	0.440706	0.852944	1.061226
1	0.113437	0.900974	2.102600
6	-3.168341	0.920190	-0.532150
6	-2.591102	2.312962	-0.218123
6	-3.035768	0.655419	-2.044203
6	-4.673514	0.969116	-0.161088
6	2.441403	0.098778	1.119556
6	2.717756	0.445666	2.566514
7	2.649325	-1.189173	0.797551
1	-2.638910	0.122079	1.400802
1	-4.128611	-1.527000	0.023523
1	-2.890453	-1.966032	2.358311
1	-3.404399	-3.373065	1.413890
1	-3.199708	-3.059000	-1.468550
1	-1.982234	-1.834559	-1.772495
1	-0.963766	-3.723403	1.812325
1	-1.657330	-4.425608	-0.376695
1	-0.366447	-3.297492	-0.814311
1	-0.475422	-1.318407	2.373679
1	0.706742	-2.017655	1.237800
1	2.731209	0.862674	0.395693
1	2.391733	1.460741	2.810646
1	2.236577	-0.267451	3.243159
1	3.800397	0.383872	2.738901
1	-1.987859	0.587466	-2.356313
1	-3.544608	-0.264549	-2.348597
1	-3.490766	1.482392	-2.601641
1	-4.817537	1.124005	0.915332
1	-5.144201	1.810528	-0.681484
1	-5.218711	0.066432	-0.452431
1	-2.572909	2.512563	0.859836
1	-1.577816	2.438314	-0.600793
1	-3.213571	3.083205	-0.687764
16	2.818917	-1.531547	-0.810690
8	1.783629	-2.510867	-1.213996
8	2.981374	-0.326798	-1.659603
6	4.388766	-2.421817	-0.824346
1	4.544328	-2.791987	-1.840318
1	5.188463	-1.736045	-0.539126
1	4.321942	-3.252133	-0.119794

6	0.634863	2.185644	0.448967	1	2.669339	-0.297016	3.190003
6	0.503304	3.341282	1.241759	1	2.437326	-1.930568	3.828263
6	0.769088	4.608111	0.722245	1	3.658455	-1.646393	2.591764
6	1.161906	4.753624	-0.609052	1	0.058911	-0.347973	2.776718
6	1.307433	3.615028	-1.406401	1	-0.640314	-1.744574	1.933921
6	1.062549	2.345280	-0.886243	1	0.165217	-1.970774	3.482996
1	0.178827	3.242536	2.275753	16	-0.289166	3.176562	0.523962
1	0.658445	5.483175	1.357997	8	0.293581	2.314867	1.588812
1	1.361591	5.740242	-1.018186	8	0.608291	3.453920	-0.630208
1	1.633865	3.711845	-2.438673	6	-0.715301	4.745939	1.290079
1	1.237437	1.468427	-1.503771	1	0.206403	5.166603	1.697568
E (CH ₃ CN) = -1821.857444				1	-1.138808	5.405104	0.530668
NImag = 1 (-192.3)				1	-1.438125	4.556487	2.084730
62. 6-si,si-t[‡] (-1821.53378667)				6	-2.163250	-1.164397	-0.197665
6	3.373938	-1.832512	-1.102079	6	-3.143974	-1.112471	0.817173
6	3.117960	-1.153357	-2.481576	6	-4.234428	-1.980865	0.816967
6	2.695089	0.293341	-2.141458	6	-4.375853	-2.942128	-0.185587
6	3.453229	0.571744	-0.834826	6	-3.413481	-3.011991	-1.196289
6	3.183640	-0.715410	-0.026557	6	-2.332478	-2.133604	-1.209286
6	1.791133	-0.662057	0.667575	1	-3.042033	-0.373792	1.608435
6	0.493859	-0.801298	-0.722184	1	-4.971892	-1.911573	1.613101
6	1.192401	0.458158	-1.899263	1	-5.221332	-3.624390	-0.181596
6	-1.091255	-0.150265	-0.200207	1	-3.509602	-3.751225	-1.988105
1	-0.954238	0.356856	0.747084	1	-1.607526	-2.198255	-2.017673
6	1.564446	-1.658961	1.858228	E (CH ₃ CN) = -1821.851919			
6	0.202076	-1.408480	2.542608	NImag = 1 (-205.0)			
6	1.650516	-3.145406	1.461744	63. 6-si,re-c[‡] (-1821.5331615)			
6	2.654369	-1.359171	2.918975	6	-0.549869	-1.925676	1.112775
6	-1.807664	1.826544	-0.976423	6	-1.587097	-2.964334	0.671196
6	-3.165981	1.461699	-1.508791	6	-3.003920	-2.514427	1.048454
7	-1.781267	2.633375	0.086169	6	-3.273122	-1.402602	0.015164
1	1.626412	0.348247	1.057738	6	-2.593295	-0.069418	0.450295
1	3.921281	-0.824777	0.771315	16	-0.704239	-0.336545	0.183851
1	3.122524	1.486234	-0.331965	6	-2.744283	-2.047671	-1.303827
1	4.528150	0.663280	-1.035814	6	-1.664760	-3.089414	-0.870957
1	4.398829	-2.214866	-1.048136	6	-3.143240	1.259259	-0.178914
1	2.712769	-2.686328	-0.945789	6	-4.691233	1.212598	-0.183406
1	2.960010	0.998119	-2.938681	6	0.377487	0.760929	1.063856
1	4.035307	-1.138827	-3.079833	6	0.768799	1.965847	0.303003
1	2.360214	-1.680668	-3.071886	6	-2.738938	2.453843	0.711966
1	0.985299	1.452766	-1.498020	6	-2.661664	1.516457	-1.621077
1	0.608994	0.301224	-2.812541	6	2.338776	-0.180492	1.478036
1	-1.021545	1.893953	-1.726844	7	3.068398	-0.329739	0.373046
1	-3.111441	0.632177	-2.217699	16	2.813906	-1.718791	-0.480163
1	-3.851112	1.194348	-0.700565	6	4.446428	-1.962304	-1.194681
1	-3.578623	2.338053	-2.027508	6	2.823950	0.877976	2.438466
1	0.927025	-3.402765	0.679707	8	2.516533	-2.890308	0.387021
1	2.649863	-3.425863	1.114215	8	1.868943	-1.497086	-1.604316
1	1.422278	-3.769063	2.333923	1	0.003269	0.955025	2.070992

1	-2.706317	0.022193	1.537798	6	-1.301257	2.024337	0.001117
1	-4.343816	-1.202171	-0.056761	6	-2.142861	-1.743650	-1.530375
1	-3.098554	-2.177958	2.088147	6	-2.402747	-0.379845	-2.206437
1	-3.713767	-3.337926	0.899811	6	-1.215307	-2.572409	-2.440318
1	-3.575555	-2.546699	-1.813240	6	-3.512351	-2.459604	-1.425380
1	-2.341496	-1.312037	-2.003043	6	1.737579	2.026689	0.332258
1	-1.301269	-3.910712	1.144555	6	1.338408	2.879513	1.513675
1	-1.977873	-4.102384	-1.144357	7	2.674833	1.098315	0.594156
1	-0.694076	-2.908294	-1.342955	16	3.401386	0.393643	-0.712550
1	-0.633173	-1.694649	2.180934	6	5.140257	0.803970	-0.446105
1	0.459437	-2.281829	0.894169	8	3.299627	-1.076828	-0.583070
1	-1.574798	1.630074	-1.682504	8	2.989007	1.004183	-1.999830
1	-2.963544	0.715698	-2.303537	1	-2.357446	-0.970734	0.469805
1	-3.106767	2.447129	-1.992035	1	-2.142126	-3.534788	0.533077
1	-5.096931	0.937815	0.798295	1	-1.960689	-1.851002	2.609877
1	-5.077253	2.207651	-0.430757	1	-1.334948	-3.493837	2.813570
1	-5.090305	0.516801	-0.928052	1	-0.086592	-4.642146	0.494983
1	-3.102701	2.321176	1.739066	1	0.444113	-3.336732	-0.550912
1	-1.659334	2.603972	0.743633	1	0.573999	-2.024571	3.429771
1	-3.183751	3.375899	0.320264	1	1.347722	-3.916974	2.183834
1	1.888313	-1.053410	1.953036	1	1.948719	-2.636205	1.122921
1	3.752255	0.516683	2.900333	1	-0.296972	0.059641	2.369066
1	3.049576	1.810989	1.916651	1	1.390403	-0.253883	1.882350
1	2.100628	1.072020	3.236010	1	0.166311	1.276882	-1.370188
1	4.713693	-1.068298	-1.759705	1	1.780714	2.555507	-0.623224
1	5.161194	-2.138502	-0.389366	1	0.451632	3.481610	1.307174
1	4.382652	-2.831659	-1.852604	1	1.163723	2.270817	2.405737
6	0.821719	3.219534	0.945724	1	2.171984	3.557700	1.740195
6	1.275741	4.357072	0.278639	1	-0.212432	-2.137642	-2.512654
6	1.679759	4.276076	-1.054930	1	-1.117770	-3.607596	-2.099594
6	1.642171	3.039161	-1.703193	1	-1.634207	-2.601018	-3.452925
6	1.207694	1.894463	-1.036672	1	-4.206726	-1.908533	-0.779418
1	0.498988	3.299240	1.981976	1	-3.965051	-2.520245	-2.421177
1	1.302967	5.310023	0.801643	1	-3.430387	-3.482879	-1.045858
1	2.024989	5.162737	-1.579831	1	-3.001210	0.283294	-1.573733
1	1.971163	2.958187	-2.736339	1	-1.474963	0.139365	-2.459956
1	1.228253	0.934663	-1.543713	1	-2.951030	-0.538257	-3.142092
E (CH ₃ CN) = -1821.855294				1	5.720821	0.286556	-1.213502
NImag = 1 (-190.0)				1	5.268800	1.884515	-0.532539
64. 6-re,si-c[‡] (-1821.5308982)				1	5.428257	0.458888	0.548155
				6	-1.568783	3.134383	-0.832576
				6	-2.610985	4.016535	-0.561934
				6	-3.441550	3.815381	0.543501
6	0.055268	-3.557314	0.443284	6	-3.204150	2.718772	1.372835
6	1.042712	-3.078095	1.549115	6	-2.151779	1.841404	1.111643
6	0.237517	-2.056643	2.386355	1	-0.941370	3.299633	-1.705555
6	-1.207696	-2.562176	2.248413	1	-2.782287	4.860018	-1.226163
6	-1.310899	-2.854347	0.735840	1	-4.260283	4.498182	0.751560
6	-1.603397	-1.553610	-0.070114	1	-3.840920	2.542162	2.236364
16	-0.003589	-0.532498	0.028057	1	-1.998802	1.005372	1.786121
6	0.364170	-0.632072	1.843658	E (CH ₃ CN) = -1821.854068			
6	-0.118589	1.207367	-0.321633	NImag = 1 (-207.0)			

65. **6-re,si-t[‡]** (-1821.52900225)

6	3.057386	-2.658251	0.150166
6	1.769867	-3.499558	-0.092221
6	0.948366	-2.677758	-1.107288
6	2.039088	-1.994234	-1.944155
6	2.991450	-1.460380	-0.854785
6	2.480474	-0.110870	-0.275762
16	0.893103	-0.499254	0.739449
6	0.039303	-1.638605	-0.449615
6	-0.246950	0.852991	0.985669
6	-0.488653	1.888279	-0.047306
6	3.552990	0.741663	0.486929
6	2.937579	2.004620	1.120938
6	4.302954	-0.034321	1.587622
6	4.580246	1.227359	-0.567202
6	-2.227490	0.182435	1.700026
6	-2.358786	1.301632	2.710184
7	-3.145137	0.184313	0.736025
16	-3.410780	-1.238820	-0.058742
6	-5.211224	-1.296711	-0.045890
8	-3.001936	-1.137476	-1.480321
8	-2.917020	-2.426647	0.688132
1	2.104694	0.506476	-1.099656
1	3.983151	-1.263083	-1.272214
1	1.656338	-1.213750	-2.611564
1	2.559877	-2.736166	-2.562583
1	3.953619	-3.253289	-0.055196
1	3.131393	-2.333039	1.188529
1	0.285921	-3.310401	-1.709344
1	2.021568	-4.474607	-0.523191
1	1.213184	-3.691312	0.831284
1	-0.444365	-1.022306	-1.204781
1	-0.742496	-2.109009	0.150763
1	0.104147	1.289713	1.919668
1	-1.860628	-0.768921	2.093122
1	-1.546972	1.291227	3.443074
1	-2.392176	2.275942	2.214051
1	-3.307237	1.170380	3.246495
1	3.621318	-0.419285	2.354575
1	4.879442	-0.873884	1.187470
1	5.009692	0.638746	2.086918
1	4.094963	1.815428	-1.355216
1	5.323189	1.871066	-0.082509
1	5.125844	0.405819	-1.041624
1	2.345997	2.576108	0.400567
1	2.296714	1.765141	1.974728
1	3.739984	2.653552	1.490781
1	-5.510309	-2.167641	-0.633573
1	-5.556515	-1.390093	0.985101
1	-5.587743	-0.378519	-0.498812
6	-0.236120	3.239929	0.274113

6	-0.514264	4.270390	-0.621761
6	-1.049318	3.980804	-1.877716
6	-1.334273	2.654741	-2.203618
6	-1.078443	1.622134	-1.300171
1	0.189524	3.481873	1.246783
1	-0.305680	5.299283	-0.339316
1	-1.260588	4.779964	-2.583336
1	-1.792629	2.415453	-3.160938
1	-1.407869	0.623382	-1.554977

E (CH₃CN) = -1821.851174

NImag = 1 (-168.2)

66. **6-re,re-c[‡]** (-1821.52973804)

6	-1.838982	1.925919	1.486636
6	-1.372274	1.982333	0.156174
6	-2.029701	2.891039	-0.705468
6	-3.079480	3.693422	-0.267177
6	-3.530831	3.609116	1.051993
6	-2.902398	2.717300	1.921328
6	-0.211149	1.235898	-0.377135
6	1.735695	2.142174	-0.084456
7	2.638729	1.600033	-0.909955
16	3.546877	0.356927	-0.324223
8	3.195652	-0.929159	-0.970354
16	-0.013343	-0.518827	-0.128377
6	-1.625242	-1.539157	-0.046640
6	-1.253967	-2.868574	0.674294
6	-0.967303	-2.629173	2.170994
6	0.489377	-2.142868	2.145211
6	0.573248	-0.705292	1.626794
6	0.059782	-3.568635	0.192119
6	1.173534	-3.153784	1.198792
6	-2.360716	-1.700573	-1.422916
6	-3.750309	-2.318252	-1.124996
6	-2.616952	-0.338006	-2.098900
6	-1.618051	-2.605111	-2.425614
6	1.325140	3.554444	-0.429496
6	5.175333	0.817061	-0.941829
8	3.620224	0.341287	1.163696
1	-2.286953	-0.956692	0.604580
1	-2.110044	-3.537009	0.548899
1	-1.662354	-1.923272	2.641772
1	-1.036313	-3.577916	2.717609
1	-0.089044	-4.653757	0.202182
1	0.332384	-3.297964	-0.828067
1	0.951305	-2.135498	3.139759
1	1.516755	-4.020842	1.773282
1	2.044089	-2.721915	0.696331
1	-0.012074	-0.031993	2.253250
1	1.610163	-0.358531	1.593563

1	-0.112094	1.350213	-1.455450	1	1.266579	-3.550648	-1.934098
1	-0.613861	-2.229002	-2.649872	1	2.971971	-3.914328	-0.289986
1	-1.527620	-3.635329	-2.068576	1	1.818754	-3.013904	0.692526
1	-2.176207	-2.633811	-3.368741	1	0.029802	-1.352585	-2.143116
1	-4.320150	-1.701002	-0.420020	1	-0.306069	-2.199532	-0.596977
1	-4.327497	-2.378460	-2.054446	1	-2.170038	0.173215	1.391132
1	-3.688416	-3.332504	-0.718422	1	2.284943	1.680242	1.381322
1	-3.100881	0.372324	-1.422348	1	3.836963	0.829313	1.257450
1	-1.693948	0.117087	-2.468499	1	3.779115	2.591927	1.176795
1	-3.275121	-0.481927	-2.963629	1	4.523017	1.681316	-2.363242
1	1.793075	1.932779	0.986728	1	4.925782	2.780544	-1.039762
1	2.176582	4.211822	-0.208755	1	5.243679	1.055302	-0.863340
1	1.106416	3.651567	-1.497393	1	2.269977	2.927922	-2.217912
1	0.467395	3.894789	0.152955	1	1.292937	2.877927	-0.739758
1	5.112749	0.932261	-2.024850	1	2.796531	3.796147	-0.768279
1	5.484646	1.751407	-0.470742	6	-0.749736	1.966444	0.325174
1	5.859598	0.006969	-0.679653	6	-1.254431	3.069631	-0.390232
1	-1.702660	2.961411	-1.740023	6	-1.440067	4.305923	0.229584
1	-3.553899	4.380326	-0.963695	6	-1.112812	4.472023	1.576140
1	-4.354192	4.228601	1.395939	6	-0.622493	3.382339	2.301113
1	-3.232050	2.641422	2.954675	6	-0.456843	2.138436	1.694187
1	-1.362959	1.271899	2.207953	1	-1.499656	2.953192	-1.443483
E (CH ₃ CN) = -1821.852453				1	-1.833240	5.141065	-0.344737
NImag = 1 (-195.2)				1	-1.250247	5.435800	2.058956
System 7 (R = Ph; X = Ph; Y = CO₂Me)				1	-0.388964	3.493419	3.356928
67. 7- <i>si,si</i> -c [‡] (-1653.2553275)				1	-0.152202	1.277894	2.284864
6	3.518309	-1.795842	-0.084602	6	-0.862504	-1.782187	2.186816
6	2.468289	-2.947516	-0.186033	8	-0.616548	-0.845262	2.953711
6	1.664961	-2.639434	-1.472383	8	-0.418451	-3.054033	2.477910
6	2.700433	-1.930134	-2.353453	6	0.229274	-3.183915	3.741005
6	3.327069	-0.923776	-1.366210	1	1.115482	-2.543763	3.805711
6	2.435384	0.346923	-1.214861	1	-0.444584	-2.917866	4.562003
16	0.908597	-0.240454	-0.194091	1	0.516571	-4.235309	3.819108
6	0.468915	-1.724448	-1.210878	6	-3.090944	-0.605564	-0.427468
6	-0.653301	0.645078	-0.341559	6	-3.350557	-1.763360	-1.176178
1	-0.943232	0.672922	-1.393190	6	-4.351054	-1.772059	-2.147212
6	3.120140	1.646704	-0.658275	6	-5.117655	-0.627643	-2.381301
6	2.314170	2.877894	-1.122409	6	-4.882407	0.523769	-1.626798
6	3.256466	1.676021	0.877576	6	-3.879977	0.533230	-0.657007
6	4.535468	1.783504	-1.271146	1	-2.776706	-2.657491	-0.957044
6	-2.018595	-0.581982	0.615849	1	-4.542982	-2.679396	-2.715092
7	-1.528310	-1.784338	1.004164	1	-5.901337	-0.637664	-3.134607
1	2.030954	0.590235	-2.204278	1	-5.486702	1.413338	-1.786645
1	4.292130	-0.579473	-1.742098	1	-3.708795	1.429067	-0.066045
1	2.271434	-1.458756	-3.245907	E (CH ₃ CN) = -1653.607610			
1	3.465818	-2.641228	-2.689200	NImag = 1 (-229.7)			
1	4.534405	-2.203994	-0.079676				
1	3.405506	-1.223223	0.838362				

68. 7-*si,si*- $t^{\ddagger}$ (-1653.25319353)

6	-4.011490	-0.674856	1.864561
6	-3.298580	0.177687	2.960092
6	-2.780570	1.434589	2.220307
6	-3.804480	1.605978	1.090598
6	-3.936830	0.166200	0.554371
6	-2.767257	-0.174221	-0.411683
16	-1.172103	-0.293715	0.651389
6	-1.374709	1.261146	1.640993
6	0.311333	0.062734	-0.306440
1	0.035510	0.797695	-1.057418
6	-2.955453	-1.395201	-1.386939
6	-2.058814	-1.195823	-2.629214
6	-2.638449	-2.765215	-0.753303
6	-4.418259	-1.422413	-1.892985
6	1.730111	1.311434	0.520381
7	2.150684	2.049400	-0.528199
1	-2.585613	0.710695	-1.032736
1	-4.857424	0.061942	-0.022552
1	-3.496828	2.332126	0.330193
1	-4.766646	1.936733	1.501328
1	-5.060984	-0.837447	2.130994
1	-3.558361	-1.662766	1.757435
1	-2.735301	2.308129	2.881503
1	-4.010128	0.473181	3.738150
1	-2.491897	-0.371409	3.458032
1	-1.075000	2.089016	0.988264
1	-0.635882	1.153480	2.439821
1	1.058438	1.784542	1.238350
1	-1.587213	-2.851905	-0.461620
1	-3.260768	-2.971814	0.123523
1	-2.835428	-3.556176	-1.486102
1	-4.732258	-0.452113	-2.296780
1	-4.498010	-2.154615	-2.703886
1	-5.129240	-1.719789	-1.115359
1	-2.296927	-0.254395	-3.139846
1	-0.995835	-1.192748	-2.383671
1	-2.226280	-2.011174	-3.342379
6	1.000200	-1.135591	-0.835767
6	1.652727	-1.031295	-2.080508
6	2.403541	-2.090467	-2.589701
6	2.515592	-3.285286	-1.877621
6	1.882828	-3.400594	-0.637600
6	1.145093	-2.339054	-0.117786
1	1.581394	-0.100800	-2.636207
1	2.898220	-1.980004	-3.551470
1	3.092841	-4.113762	-2.278947
1	1.974093	-4.319045	-0.063138
1	0.690677	-2.440150	0.864134
6	1.281268	3.008684	-0.920166
8	0.102257	3.187859	-0.561689

8	1.845007	3.822383	-1.863856
6	1.003177	4.862919	-2.348383
1	0.106712	4.460049	-2.832592
1	0.685194	5.530163	-1.540188
1	1.604530	5.414636	-3.074681
6	2.722759	0.401387	1.156412
6	3.918339	0.071441	0.503571
6	4.846830	-0.770624	1.113508
6	4.600168	-1.290536	2.386362
6	3.416288	-0.959846	3.049973
6	2.487367	-0.120685	2.435971
1	4.102840	0.504015	-0.473401
1	5.770481	-1.018121	0.596287
1	5.328137	-1.942962	2.862024
1	3.221187	-1.349175	4.046259
1	1.570132	0.140737	2.962170

E (CH₃CN) = -1653.603815

NImag = 1 (-252.0)

69. 7-*si, re*- $c^{\ddagger}$ (-1653.2563371)

6	-1.397525	1.291033	-1.665621
6	-2.833797	1.732372	-1.961082
6	-3.708451	0.523764	-2.316545
6	-3.904860	-0.146028	-0.941261
6	-2.659526	-1.000063	-0.554116
16	-1.268393	0.259208	-0.140401
6	-4.212070	1.077711	-0.023707
6	-3.538518	2.308841	-0.708421
6	-2.860691	-2.112077	0.538704
6	-4.211153	-2.828458	0.292992
6	0.388659	-0.423803	-0.230828
6	0.901698	-0.887308	1.076159
6	-1.757512	-3.182520	0.387142
6	-2.851700	-1.580916	1.986879
6	1.831639	0.961197	-0.873356
7	2.290544	1.698314	0.151215
1	0.437672	-1.168969	-1.024935
1	-2.311330	-1.507167	-1.462465
1	-4.757283	-0.826758	-0.971609
1	-3.260320	-0.139221	-3.066452
1	-4.677942	0.858220	-2.707046
1	-5.296774	1.218195	0.031858
1	-3.860081	0.938241	1.000558
1	-2.775979	2.467264	-2.772820
1	-4.295096	3.040060	-1.011768
1	-2.833439	2.824598	-0.048966
1	-0.970452	0.719139	-2.496366
1	-0.756656	2.138203	-1.414946
1	-1.892447	-1.128943	2.258205
1	-3.642977	-0.844677	2.161125

1	-3.023423	-2.414168	2.678197	6	-1.336811	-3.324345	-2.754634
1	-4.319184	-3.155928	-0.748517	6	-1.362543	-4.294875	-1.748718
1	-4.260149	-3.722352	0.924410	6	-1.012136	-3.926959	-0.449630
1	-5.072667	-2.203778	0.549419	6	-0.651697	-2.612476	-0.152533
1	-1.764959	-3.617545	-0.620451	16	0.876044	0.393108	0.232131
1	-0.761060	-2.786243	0.585686	6	2.336176	-0.797944	0.429858
1	-1.930593	-3.997007	1.099965	6	2.892209	-0.616925	1.869436
1	1.170018	1.426736	-1.607621	6	1.871247	-1.107889	2.920175
6	1.666031	-2.068771	1.144244	6	0.949122	0.111692	3.078079
6	2.249726	-2.481122	2.341268	6	0.015747	0.256823	1.874787
6	2.083025	-1.726539	3.503713	6	3.163747	0.857195	2.319814
6	1.339457	-0.545992	3.449703	6	1.956456	1.272669	3.208456
6	0.766203	-0.122163	2.251863	6	3.381380	-0.697881	-0.740225
1	1.804759	-2.664375	0.245537	6	4.266945	-1.964830	-0.648987
1	2.832789	-3.398428	2.364062	6	2.695573	-0.714156	-2.123463
1	2.532903	-2.050152	4.438409	6	4.287988	0.546385	-0.673992
1	1.216752	0.060948	4.343095	7	-1.452518	2.360442	-0.505559
1	0.211844	0.810868	2.223254	6	-0.773641	2.936851	-1.531804
6	1.472868	2.678707	0.582940	8	-0.480820	4.242020	-1.238873
8	0.273947	2.872168	0.301778	6	0.241834	4.935246	-2.251578
8	2.111884	3.501279	1.466255	8	-0.402391	2.427553	-2.597450
6	1.323225	4.565453	1.987980	1	1.884073	-1.792294	0.357384
1	0.957041	5.221073	1.190637	1	3.811474	-1.207886	1.919421
1	0.458941	4.188424	2.545727	1	1.347873	-2.024515	2.624643
1	1.984762	5.121974	2.655794	1	2.382183	-1.311995	3.869189
6	2.792983	-0.003487	-1.482953	1	4.098682	0.900923	2.888029
6	3.949239	-0.395689	-0.793034	1	3.282134	1.535722	1.475130
6	4.847741	-1.290511	-1.373485	1	0.300437	0.036448	3.959350
6	4.609073	-1.804454	-2.650388	1	2.264456	1.372595	4.254891
6	3.463880	-1.413722	-3.349365	1	1.525605	2.233149	2.907115
6	2.565229	-0.521098	-2.767033	1	-0.686731	-0.573335	1.808707
1	4.129115	0.033665	0.186371	1	-0.560988	1.183404	1.906756
1	5.742106	-1.583814	-0.829301	1	-0.056249	0.327882	-1.867170
1	5.313771	-2.498047	-3.102169	1	-2.183885	0.874735	-1.805489
1	3.276494	-1.798001	-4.349025	1	3.711456	1.476561	-0.723661
1	1.678465	-0.211285	-3.318557	1	4.906152	0.567037	0.228722
E (CH ₃ CN) = -1653.605939				1	4.967119	0.540174	-1.534266
NImag = 1 (-222.0)				1	3.668123	-2.878312	-0.743138
70. 7- <i>re</i> , <i>si</i> -c [‡] (-1653.2527306)				1	4.996037	-1.960167	-1.466839
				1	4.831549	-2.020764	0.287706
				1	1.990292	-1.544604	-2.224629
				1	2.162165	0.219036	-2.331048
6	-3.237573	1.295189	1.385124	1	3.460081	-0.826027	-2.901051
6	-2.907025	0.569479	0.228276	1	-0.931154	-1.276735	-3.262072
6	-3.534501	-0.667403	0.011252	1	-1.600483	-3.590375	-3.775308
6	-4.444430	-1.177701	0.937671	1	-1.648478	-5.318108	-1.974930
6	-4.750129	-0.456931	2.093913	1	-1.027122	-4.666096	0.347743
6	-4.147596	0.785474	2.309655	1	-0.408921	-2.367816	0.875886
6	-1.948036	1.137198	-0.768023	1	1.214027	4.466926	-2.441045
6	-0.325887	-0.189753	-0.949111	1	-0.314658	4.959273	-3.194239
6	-0.612157	-1.616354	-1.152241	1	0.382016	5.950347	-1.872437
6	-0.958773	-2.016586	-2.465589	1	-3.315337	-1.229949	-0.890701

1	-4.919401	-2.137608	0.751457
1	-5.463691	-0.852337	2.812543
1	-4.399249	1.365345	3.194605
1	-2.785912	2.272785	1.518348

E (CH₃CN) = -1653.602213

NImag = 1 (-230.9)

71. $7-re,si-t^{\ddagger}$ (-1653.2504854)

6	-4.058176	0.276857	-1.825164
6	-3.368185	-0.455371	-3.006541
6	-2.338181	-1.381933	-2.334932
6	-3.103588	-1.850081	-1.088636
6	-3.671576	-0.523038	-0.534488
6	-2.635478	0.153877	0.394414
16	-1.112096	0.645135	-0.649367
6	-1.025130	-0.681120	-1.971253
6	0.421270	0.469627	0.292168
6	0.499299	-0.517409	1.392934
6	-3.151563	1.323616	1.304201
6	-1.996793	1.988122	2.083542
6	-3.916415	2.429052	0.550841
6	-4.100981	0.685471	2.348775
6	2.087173	0.268772	-0.932210
7	2.844804	-0.752108	-0.497219
1	-2.227623	-0.609524	1.064902
1	-4.557408	-0.711714	0.079076
1	-2.483663	-2.389436	-0.365014
1	-3.922166	-2.516121	-1.386974
1	-5.145395	0.300785	-1.950769
1	-3.731675	1.316512	-1.772862
1	-2.052077	-2.214192	-2.989420
1	-4.093557	-1.062708	-3.559909
1	-2.912980	0.235607	-3.724276
1	-0.242367	-1.382530	-1.664632
1	-0.636491	-0.133174	-2.835365
1	0.595144	1.480493	0.653447
1	1.539760	0.149014	-1.873438
1	-3.296093	2.906043	-0.216134
1	-4.830301	2.058602	0.076704
1	-4.211555	3.209460	1.261687
1	-3.588710	-0.085018	2.936753
1	-4.449843	1.456758	3.044611
1	-4.988696	0.234515	1.893203
1	-1.387929	1.255452	2.621039
1	-1.339108	2.567669	1.427205
1	-2.412107	2.686337	2.819266
6	1.016346	-0.087221	2.631792
6	1.183917	-0.970072	3.696357
6	0.827311	-2.312777	3.558938
6	0.325787	-2.760823	2.336566

6	0.175253	-1.881336	1.263999
1	1.296567	0.956413	2.752415
1	1.589605	-0.605801	4.636753
1	0.951231	-3.002907	4.388960
1	0.066561	-3.808502	2.206043
1	-0.149480	-2.273767	0.307604
6	2.520533	-1.975270	-0.972038
8	1.542419	-2.323709	-1.657899
8	3.458064	-2.897834	-0.598917
6	3.212582	-4.226558	-1.043683
1	2.276490	-4.619707	-0.631188
1	3.155175	-4.280719	-2.135990
1	4.056454	-4.819189	-0.682431
6	2.654314	1.640917	-0.746796
6	2.149729	2.725443	-1.478261
6	2.672879	4.007359	-1.309185
6	3.710744	4.223154	-0.399564
6	4.224295	3.146693	0.328886
6	3.704481	1.864513	0.155147
1	1.343995	2.560476	-2.192084
1	2.275815	4.835831	-1.890767
1	4.121806	5.220701	-0.266518
1	5.040529	3.306511	1.029367
1	4.107042	1.010003	0.688808

E (CH₃CN) = -1653.602204

NImag = 1 (-235.1)

72. $7-re,re-c^{\ddagger}$ (-1653.2538035)

6	0.805943	-2.281937	-1.181693
6	1.119275	-1.514626	-0.040789
6	2.085320	-2.050097	0.840114
6	2.706365	-3.270482	0.591585
6	2.374707	-4.016097	-0.541834
6	1.418709	-3.511986	-1.423067
6	0.579165	-0.172044	0.281754
6	1.629645	1.527531	-0.283550
7	1.298997	2.505522	0.584701
16	-1.153474	0.219376	-0.004831
6	-2.327955	-1.262744	0.215567
6	-3.588058	-0.966470	-0.646406
6	-3.254361	-1.021016	-2.152316
6	-2.672664	0.378338	-2.407866
6	-1.258633	0.507272	-1.842435
6	-4.210401	0.461034	-0.492645
6	-3.675291	1.305368	-1.686674
6	-2.594903	-1.644538	1.715126
6	-3.268005	-3.039834	1.707015
6	-1.282032	-1.780760	2.514907
6	-3.509833	-0.656322	2.464662
1	-1.791302	-2.106133	-0.231057

1	-4.324471	-1.732684	-0.387492	6	-1.867237	-1.614861	3.200915
1	-2.574232	-1.839068	-2.418467	6	-1.335705	-0.724807	4.135995
1	-4.175657	-1.154839	-2.732822	6	-0.458098	0.267978	3.700033
1	-5.302108	0.383075	-0.531171	6	-0.418424	-0.451467	-0.073798
1	-3.964522	0.925396	0.462285	6	-2.004135	0.230328	-1.107408
1	-2.596530	0.613460	-3.476572	7	-2.984205	-0.670465	-0.866315
1	-4.491264	1.570419	-2.367479	16	1.156257	0.081628	-0.747094
1	-3.200263	2.236659	-1.362982	6	2.670411	-0.469303	0.285293
1	-0.565032	-0.176639	-2.331308	6	3.810039	0.551503	0.030080
1	-0.884993	1.532624	-1.909075	6	3.450619	1.930847	0.623977
1	0.732043	0.083406	1.327643	6	2.586007	2.551141	-0.484969
1	-3.091936	0.356320	2.481598	6	1.187384	1.929606	-0.516864
1	-4.515097	-0.608910	2.035060	6	4.107154	0.888280	-1.468001
1	-3.615047	-0.982624	3.505836	6	3.410508	2.249855	-1.754090
1	-2.632852	-3.786574	1.215688	6	3.022603	-1.985992	0.092383
1	-3.433551	-3.371627	2.738183	6	4.023559	-2.354182	1.216038
1	-4.242403	-3.038379	1.207739	6	1.781203	-2.886781	0.275981
1	-0.552055	-2.418085	2.007257	6	3.658786	-2.322051	-1.270320
1	-0.815668	-0.809260	2.705488	1	2.329083	-0.357119	1.319231
1	-1.500078	-2.228605	3.491196	1	4.702820	0.145429	0.514425
1	1.263182	1.583864	-1.313748	1	2.947645	1.869046	1.595667
1	2.359500	-1.483773	1.725579	1	4.360301	2.528302	0.760422
1	3.449862	-3.642531	1.291749	1	5.188534	0.966569	-1.619725
1	2.853460	-4.972006	-0.734747	1	3.753313	0.111749	-2.146256
1	1.146346	-4.075414	-2.312257	1	2.434893	3.628507	-0.345368
1	0.076019	-1.929460	-1.901529	1	4.154597	3.039932	-1.901671
6	0.258862	3.292102	0.236891	1	2.790828	2.222468	-2.656908
8	-0.505918	3.211264	-0.741839	1	0.620009	2.161034	0.383390
8	0.094144	4.298235	1.150389	1	0.609090	2.299316	-1.365148
6	-0.960532	5.210492	0.866324	1	-0.556506	-1.413245	-0.564731
1	-0.813942	5.704764	-0.099820	1	3.003441	-2.051763	-2.105647
1	-1.933498	4.706579	0.849043	1	4.627551	-1.833179	-1.414725
1	-0.937066	5.948332	1.671832	1	3.828371	-3.403200	-1.329711
6	3.020520	0.996834	-0.184472	1	3.598279	-2.164781	2.208702
6	3.787873	1.210714	0.970486	1	4.260938	-3.422081	1.155754
6	5.095375	0.734030	1.047894	1	4.969568	-1.808424	1.138646
6	5.660310	0.045427	-0.029389	1	1.222919	-2.642383	1.185120
6	4.907724	-0.162372	-1.186817	1	1.094630	-2.830515	-0.574442
6	3.597477	0.309201	-1.260877	1	2.105831	-3.930792	0.352563
1	3.343554	1.779438	1.780764	1	-1.490555	0.178284	-2.076743
1	5.681571	0.910813	1.946557	1	-1.936896	-2.227362	1.145733
1	6.682730	-0.319311	0.029956	1	-2.550756	-2.397526	3.519829
1	5.341387	-0.689650	-2.032729	1	-1.598246	-0.805642	5.187184
1	3.013098	0.143643	-2.163207	1	-0.031966	0.971027	4.411612
				1	0.547523	1.174819	2.056629
E (CH ₃ CN) = -1653.603647				6	-2.819975	-1.857273	-1.499899
NImag = 1 (-231.0)				8	-1.818907	-2.283736	-2.097789
				8	-3.940940	-2.634797	-1.374027
73. 7-re, re- [‡] (-1653.2464825)				6	-3.862992	-3.906935	-2.008603
				1	-3.697974	-3.806801	-3.086721
6	-0.126670	0.377953	2.349675	1	-3.050011	-4.513273	-1.594286
6	-0.645705	-0.513455	1.388747	1	-4.824652	-4.390320	-1.820375
6	-1.519957	-1.521512	1.854772	6	-2.289322	1.627071	-0.658885

6	-2.931790	1.880754	0.562323
6	-3.212023	3.188727	0.954482
6	-2.874471	4.264428	0.127292
6	-2.262268	4.021582	-1.103256
6	-1.973946	2.711095	-1.489984
1	-3.222544	1.038945	1.180798
1	-3.706298	3.370679	1.905595
1	-3.102486	5.282420	0.433131
1	-2.022600	4.848411	-1.767567
1	-1.523903	2.521769	-2.463626

E (CH₃CN) = -1653.601541

NImag = 1 (-263.4)

System 8 (R = Ph; X = Me; Y = CO₂Me)

74. **8-*si,si-c***[‡] (-1461.51560961)

6	-3.061673	1.138929	-0.898056
6	-3.509873	-0.146639	-0.132704
6	-3.081788	0.096336	1.333552
6	-3.199939	1.620419	1.465801
6	-2.491875	2.110620	0.185849
6	-0.943481	2.105501	0.372515
16	-0.446172	0.238964	0.332296
6	-1.646472	-0.360158	1.605819
6	1.055067	-0.305093	1.115134
1	1.057622	0.007681	2.161704
6	-0.098615	3.017513	-0.581721
6	1.292780	3.255829	0.041786
6	0.072007	2.446911	-2.003866
6	-0.781473	4.403448	-0.689566
6	0.870828	-2.458722	1.102956
6	1.264089	-2.699414	2.540916
7	-0.327654	-2.928635	0.727960
1	-0.728080	2.426814	1.398666
1	-2.777985	3.140462	-0.036279
1	-2.760838	2.019130	2.388221
1	-4.255201	1.920783	1.443528
1	-3.919591	1.611733	-1.387515
1	-2.336908	0.912495	-1.682664
1	-3.722614	-0.442215	2.041702
1	-4.598001	-0.260352	-0.183348
1	-3.070586	-1.063309	-0.538687
1	-1.283567	0.004693	2.573802
1	-1.530409	-1.449834	1.552810
1	1.689497	-2.503024	0.380736
1	2.162971	-2.141397	2.821399
1	0.447066	-2.448109	3.225027
1	1.475982	-3.769826	2.668349
1	0.615925	1.497056	-2.006034
1	-0.889136	2.293680	-2.504894

1	0.649480	3.152647	-2.612116
1	-1.020787	4.819585	0.296958
1	-0.096359	5.101566	-1.183127
1	-1.700042	4.377324	-1.284233
1	1.205467	3.717905	1.033582
1	1.870641	2.336597	0.144742
1	1.872422	3.937929	-0.590764
6	2.338735	-0.061832	0.423244
6	3.436119	0.436208	1.152664
6	4.686865	0.597478	0.556105
6	4.869638	0.279426	-0.790258
6	3.792743	-0.225723	-1.524650
6	2.546985	-0.411279	-0.928529
1	3.300592	0.706316	2.198021
1	5.516419	0.981946	1.144495
1	5.841069	0.411588	-1.258934
1	3.928542	-0.501455	-2.567444
1	1.740018	-0.877603	-1.487701
6	-0.513165	-3.023586	-0.623397
8	0.234815	-2.691652	-1.544924
8	-1.750898	-3.559742	-0.885372
6	-2.028529	-3.771921	-2.268310
1	-1.993624	-2.833765	-2.831860
1	-1.309126	-4.466172	-2.714473
1	-3.033693	-4.198207	-2.305453

E (CH₃CN) = -1461.821630

NImag = 1 (-210.0)

75. **8-*si,si-t***[‡] (-1461.51431123)

6	-3.935280	-0.200120	-1.037292
6	-3.403877	-1.080223	-2.211583
6	-2.429942	-2.085538	-1.552191
6	-3.025486	-2.256368	-0.148488
6	-3.310095	-0.796765	0.261508
6	-2.013552	-0.107724	0.775207
16	-0.873613	0.139101	-0.744475
6	-0.992777	-1.566851	-1.459499
6	0.853731	0.264578	-0.301763
1	1.008658	-0.312908	0.604064
6	-2.173133	1.186916	1.652332
6	-0.882504	1.424545	2.467891
6	-2.496387	2.460542	0.845427
6	-3.311765	0.955385	2.675990
6	2.269200	-0.946599	-1.334272
6	2.884014	-0.008174	-2.339905
7	3.071336	-1.406339	-0.366843
1	-1.466783	-0.839990	1.381099
1	-4.028587	-0.768097	1.083005
1	-2.362577	-2.786066	0.544389
1	-3.968191	-2.815076	-0.205200

1	-5.026710	-0.263249	-0.976071	6	-4.168541	2.086347	-0.518123
1	-3.688927	0.854471	-1.177451	6	0.560482	0.522966	1.095854
1	-2.383171	-3.031443	-2.105058	6	1.270613	1.556090	0.315705
1	-4.228158	-1.621688	-2.687616	6	-2.037565	2.898624	0.460146
1	-2.919000	-0.485549	-2.993621	6	-2.035896	1.808203	-1.803832
1	-0.347973	-2.206211	-0.846576	6	2.174860	-0.778961	1.727196
1	-0.549086	-1.457144	-2.453354	7	3.048439	-0.986560	0.742585
1	1.519710	-1.623627	-1.747844	6	2.669703	0.069207	2.875444
1	2.128577	0.472712	-2.969536	1	0.169338	0.867601	2.054785
1	3.483594	0.760925	-1.847133	1	-2.591318	0.600119	1.423205
1	3.553783	-0.589570	-2.987783	1	-4.443405	-0.299096	-0.137817
1	-1.695504	2.720752	0.145799	1	-3.514905	-1.398319	2.105308
1	-3.432070	2.369070	0.284568	1	-4.386516	-2.447235	0.975951
1	-2.610769	3.305957	1.533673	1	-4.008714	-1.911047	-1.778112
1	-3.187356	0.011427	3.220654	1	-2.501807	-1.040637	-2.006599
1	-3.296494	1.764552	3.414157	1	-2.202474	-3.589494	1.335276
1	-4.303339	0.958467	2.212415	1	-2.867033	-3.764854	-0.959584
1	-0.629603	0.546179	3.074410	1	-1.319536	-2.949233	-1.186735
1	-0.024707	1.663822	1.837958	1	-1.001717	-1.562439	2.253548
1	-1.030118	2.268178	3.151980	1	-0.065885	-2.432296	0.990174
6	1.375250	1.647525	-0.257605	1	-0.949142	1.680488	-1.779545
6	2.431528	1.932110	0.633813	1	-2.460252	1.043344	-2.461981
6	3.036648	3.187901	0.656897	1	-2.236927	2.782980	-2.263384
6	2.599530	4.203959	-0.195123	1	-4.688076	1.994480	0.443900
6	1.557412	3.938269	-1.086292	1	-4.290421	3.120682	-0.858200
6	0.961212	2.679240	-1.125773	1	-4.675173	1.444021	-1.245503
1	2.790804	1.145151	1.290832	1	-2.491688	2.933008	1.458804
1	3.852430	3.372654	1.351434	1	-0.958597	2.787816	0.574253
1	3.065139	5.185233	-0.168692	1	-2.216616	3.868650	-0.017849
1	1.210025	4.714097	-1.764473	1	1.492807	-1.582777	2.016221
1	0.167981	2.493087	-1.845772	1	3.466879	-0.480623	3.392207
6	2.537245	-2.398677	0.391691	1	3.103089	1.004402	2.509444
8	1.357086	-2.784037	0.452028	1	1.881321	0.289015	3.603100
8	3.488798	-2.960746	1.193638	6	1.613104	2.781419	0.922356
6	3.026185	-4.003016	2.046752	6	2.373402	3.735779	0.247636
1	2.260808	-3.640275	2.741509	6	2.804826	3.497941	-1.058246
1	2.601661	-4.832406	1.471183	6	2.479404	2.286675	-1.672432
1	3.904391	-4.341899	2.600904	6	1.735748	1.322475	-0.994787
E (CH ₃ CN) = -1461.818887				1	1.273467	2.984793	1.935782
NImag = 1 (-242.0)				1	2.620449	4.671691	0.742842
76. 8-si, re-c[‡] (-1461.51509640)				1	3.391726	4.243118	-1.588156
				1	2.823092	2.080549	-2.682925
				1	1.515752	0.376341	-1.479672
				6	2.685632	-1.898485	-0.191608
6	-0.972724	-1.862715	1.200398	8	1.567282	-2.402808	-0.393070
6	-2.230090	-2.636889	0.792881	8	3.740463	-2.218249	-0.995282
6	-3.493421	-1.820384	1.093233	6	3.458412	-3.162177	-2.023888
6	-3.457452	-0.752068	-0.017823	1	3.108550	-4.113359	-1.608772
6	-2.474417	0.399024	0.350915	1	2.694098	-2.786357	-2.712683
16	-0.703701	-0.343569	0.190659	1	4.401417	-3.309115	-2.555113
6	-3.087423	-1.600126	-1.274173	E (CH ₃ CN) = -1461.820279			
6	-2.313120	-2.846249	-0.739399	NImag = 1 (-221.2)			
6	-2.657804	1.770850	-0.393119				

77. 8-re,si-c[‡] (-1461.51402975)				1	4.607112	-0.261741	1.969682
				1	2.215737	0.096694	1.646254
6	-1.908646	2.932347	0.622287	6	-2.519707	-2.289499	-0.573086
6	-2.436546	2.045678	1.789578	8	-2.092989	-2.299143	-1.730651
6	-1.167721	1.519602	2.497778	8	-3.850393	-2.093719	-0.310744
6	-0.160096	2.658747	2.272663	6	-4.671198	-1.951463	-1.466396
6	-0.353005	2.979936	0.774612	1	-4.366208	-1.089566	-2.069814
6	0.456624	1.993315	-0.116190	1	-4.626619	-2.843607	-2.099722
16	-0.395543	0.302629	0.056562	1	-5.687570	-1.808013	-1.091912
6	-0.655707	0.211611	1.894100	E (CH ₃ CN) = -1461.819442			
6	0.589376	-1.118621	-0.331984	NImag = 1 (-227.6)			
6	2.034557	-1.201383	-0.085437	78. 8-re,si-t[‡] (-1461.50950085)			
6	0.697607	2.427235	-1.604366	6	3.578050	-2.010564	-0.196395
6	1.493740	1.351637	-2.374856	6	2.652212	-3.256639	-0.203659
6	-0.594289	2.733408	-2.386525	6	1.326248	-2.748250	-0.798141
6	1.575756	3.702874	-1.570867	6	1.818574	-1.769699	-1.873733
6	-0.536972	-2.762329	0.434323	6	2.877526	-0.945061	-1.106872
6	0.212497	-3.193538	1.670475	6	2.205531	0.236867	-0.367035
7	-1.823123	-2.417519	0.594758	16	1.039965	-0.463593	0.978218
1	1.446881	1.858866	0.330619	6	0.415152	-2.061894	0.223847
1	0.022163	3.980874	0.544940	6	-0.424700	0.543571	1.207384
1	0.871535	2.393015	2.532859	6	-0.930266	1.386394	0.102652
1	-0.438870	3.530652	2.877448	6	3.154316	1.362293	0.177246
1	-2.307549	3.949256	0.700207	6	2.375963	2.416873	0.993341
1	-2.225201	2.545829	-0.346749	6	4.317704	0.848889	1.047759
1	-1.347594	1.322139	3.561507	6	3.742920	2.085677	-1.059761
1	-3.028756	2.644190	2.489799	6	-2.078495	-0.561685	2.015846
1	-3.077706	1.230435	1.438738	6	-2.038905	0.006521	3.417262
1	0.284609	-0.098780	2.352083	7	-3.176226	-0.291463	1.309566
1	-1.379389	-0.607671	1.967159	1	1.510312	0.721803	-1.060080
1	0.300335	-1.366926	-1.350702	1	3.597090	-0.503695	-1.803052
1	-0.256303	-3.305160	-0.474581	1	1.024983	-1.154933	-2.310986
1	1.294553	-3.205666	1.518981	1	2.294289	-2.327333	-2.689636
1	-0.030713	-2.565925	2.532446	1	4.572868	-2.251385	-0.584900
1	-0.106462	-4.215535	1.917650	1	3.724582	-1.643839	0.820360
1	-1.275449	1.875474	-2.404881	1	0.729265	-3.567080	-1.217905
1	-1.131609	3.594671	-1.977626	1	3.063488	-4.038279	-0.852680
1	-0.340250	2.970715	-3.426042	1	2.529452	-3.697441	0.791643
1	2.511808	3.531920	-1.025749	1	-0.581756	-1.852451	-0.175029
1	1.836855	3.990042	-2.595417	1	0.277094	-2.703127	1.100099
1	1.066168	4.558537	-1.116611	1	-0.180261	1.140299	2.084586
1	2.387493	1.034156	-1.828665	1	-1.613417	-1.547265	1.909510
1	0.891831	0.463285	-2.583750	1	-1.059397	-0.120963	3.891005
1	1.814416	1.760553	-3.339850	1	-2.310699	1.066734	3.414184
6	2.785051	-2.053194	-0.929943	1	-2.785168	-0.518386	4.028247
6	4.145245	-2.266849	-0.729021	1	3.959460	0.309433	1.931656
6	4.819504	-1.625206	0.313707	1	4.997345	0.194220	0.493993
6	4.102241	-0.772464	1.153086	1	4.905050	1.703461	1.403537
6	2.735717	-0.566959	0.962939	1	2.951449	2.494518	-1.698652
1	2.280122	-2.551874	-1.753957				
1	4.685160	-2.931313	-1.399210				
1	5.882906	-1.785385	0.466475				

1	4.369914	2.921915	-0.730342	1	-1.267729	2.221070	-2.496765
1	4.372129	1.430658	-1.671337	1	-0.264483	3.661615	-2.720023
1	1.508660	2.801496	0.448996	1	1.310589	4.432689	-0.403913
1	2.029722	2.018976	1.953018	1	1.522457	3.002043	0.585545
1	3.038023	3.261843	1.215556	1	1.204646	1.774605	-3.399576
6	-1.258452	2.728606	0.384100	1	2.434167	3.434306	-2.186524
6	-1.799701	3.566958	-0.587524	1	2.776473	2.025194	-1.178039
6	-2.019395	3.093592	-1.882361	1	-0.051377	-0.070299	-2.346510
6	-1.712236	1.765441	-2.179087	1	1.664115	-0.107737	-1.837990
6	-1.188031	0.919646	-1.200858	1	-0.132124	-1.470100	1.294377
1	-1.086332	3.114798	1.386269	1	0.657928	2.171261	2.547252
1	-2.045035	4.594909	-0.332577	1	0.049517	3.779276	2.100447
1	-2.436085	3.746347	-2.644461	1	-0.605849	2.942812	3.508567
1	-1.899166	1.373739	-3.175948	1	-3.378091	2.663012	0.983016
1	-1.026106	-0.123943	-1.444863	1	-2.932534	3.290175	2.576274
6	-3.378761	-1.065407	0.210682	1	-2.303204	4.067898	1.125860
8	-2.620592	-1.890373	-0.324363	1	-2.576224	0.317168	1.810910
8	-4.619407	-0.834540	-0.309789	1	-0.996980	0.187117	2.602441
6	-4.938056	-1.587219	-1.474939	1	-2.268901	1.158631	3.338222
1	-4.250886	-1.358425	-2.296973	1	1.313036	-2.216705	-1.349803
1	-4.894711	-2.664192	-1.281075	1	0.933378	-4.718791	-0.723401
1	-5.955200	-1.294834	-1.745922	1	0.005034	-4.162359	0.669774
E (CH ₃ CN) = -1461.815272				1	-0.573589	-3.814873	-0.984394
NImag = 1 (-221.6)				1	-2.028288	-2.681337	1.718592
79. 8-re, re-c[‡] (-1461.51410928)				1	-4.327275	-3.395020	1.216425
6	-2.411029	-1.149460	-1.283944	1	-5.443204	-2.661927	-0.892254
6	-1.756397	-1.546889	-0.098558	1	-4.190020	-1.211142	-2.484031
6	-2.494805	-2.362788	0.789724	1	-1.899096	-0.529775	-2.011667
6	-3.796861	-2.765157	0.506550	6	3.123208	-1.694325	0.305803
6	-4.424941	-2.354544	-0.671813	8	3.196034	-0.819723	-0.573277
6	-3.721053	-1.541207	-1.560208	8	4.132860	-1.838852	1.214636
6	-0.353448	-1.242155	0.254074	6	5.234621	-0.952731	1.045944
6	1.151479	-2.644208	-0.354485	1	5.699895	-1.075734	0.062301
7	2.138946	-2.597025	0.546594	1	4.926270	0.093258	1.151374
16	0.335702	0.387759	0.008356	1	5.946040	-1.213963	1.832706
6	-0.917502	1.819396	0.162329	E (CH ₃ CN) = -1461.818758			
6	-0.332160	3.013542	-0.644996	NImag = 1 (-218.1)			
6	-0.352061	2.722001	-2.160252	80. 8-re, re-t[‡] (-1461.5085348)			
6	0.920264	1.881236	-2.345484	6	0.032433	2.733307	-0.120156
6	0.732445	0.462555	-1.807522	6	-0.932437	1.741972	0.148792
6	1.175106	3.345960	-0.388902	6	-2.150156	2.170497	0.728067
6	1.975501	2.675111	-1.544038	6	-2.383705	3.512641	1.011857
6	-1.344808	2.135669	1.639768	6	-1.408993	4.478819	0.746154
6	-2.556802	3.097900	1.564913	6	-0.200934	4.076894	0.178867
6	-1.822626	0.869177	2.379888	6	-0.835497	0.303867	-0.171537
6	-0.239353	2.796808	2.485800	6	-2.208080	-0.309422	-1.617430
6	0.309806	-3.896768	-0.347007	7	-3.345439	-0.579492	-0.961689
1	-1.813540	1.456343	-0.352994	16	0.700922	-0.536356	-0.449925
1	-0.957543	3.880186	-0.412426	6	2.173657	-0.036923	0.669293

6	3.474355	-0.375175	-0.105543
6	3.643026	0.555276	-1.326514
6	2.759691	-0.125282	-2.385063
6	1.273635	0.109929	-2.096799
6	3.537595	-1.796717	-0.754654
6	3.169544	-1.608379	-2.255603
6	2.049238	-0.607004	2.124434
6	3.089087	0.148032	2.988793
6	0.655037	-0.318172	2.724511
6	2.314027	-2.120813	2.234869
6	-2.274908	0.847528	-2.586715
1	2.091805	1.050442	0.755526
1	4.301513	-0.240571	0.598022
1	3.368275	1.597080	-1.124090
1	4.688221	0.549012	-1.659363
1	4.551481	-2.197533	-0.653997
1	2.870818	-2.508846	-0.268533
1	2.944172	0.261400	-3.394781
1	4.037696	-1.804889	-2.893638
1	2.374283	-2.288703	-2.578710
1	1.019492	1.169215	-2.148739
1	0.640304	-0.426633	-2.808635
1	-1.336172	-0.343966	0.540084
1	1.615219	-2.703227	1.624559
1	3.336178	-2.387995	1.948321
1	2.174093	-2.434802	3.275654
1	2.907934	1.229462	2.978280
1	3.014732	-0.190479	4.028276
1	4.119799	-0.029041	2.663998
1	0.352913	0.725112	2.585566
1	-0.118475	-0.961338	2.294037
1	0.678092	-0.521124	3.801375
1	-1.592443	-1.158435	-1.944514
1	-2.924856	0.562691	-3.424123
1	-2.717894	1.724520	-2.107664
1	-1.294550	1.118935	-2.990178
1	-2.924404	1.433006	0.917871
1	-3.334712	3.804983	1.450066
1	-1.588991	5.524754	0.978237
1	0.572191	4.811003	-0.035600
1	0.988509	2.468716	-0.559813
6	-3.320274	-1.709047	-0.207317
8	-2.333695	-2.355076	0.173708
8	-4.584439	-2.067862	0.173481
6	-4.655959	-3.217959	1.009986
1	-4.239214	-4.100826	0.513646
1	-4.111341	-3.064347	1.948038
1	-5.718566	-3.369127	1.214179

E (CH₃CN) = -1461.816459
 NImag = 1 (-251.1)

Addition of Nonstabilized ylide (R = Me)

System 9 (R = Me; X = Ph; Y = SO₂Me)

81. **9-*si,si*-c[‡]** (-1821.5265852)

6	0.301857	-0.088567	1.525840
6	1.296968	0.347261	2.601036
6	2.475913	-0.631007	2.679239
6	3.261543	-0.282420	1.399058
6	2.650538	-0.986659	0.154139
16	0.961920	-0.091193	-0.206770
6	3.214587	1.282691	1.393016
6	1.986169	1.686571	2.260835
6	3.615662	-1.119993	-1.068519
6	4.729608	-2.120613	-0.670564
6	-0.382028	-0.997981	-0.941855
6	-0.380050	-1.122342	-2.450897
6	2.894306	-1.713857	-2.290966
6	4.265522	0.211101	-1.494465
6	-2.218491	0.161296	-0.623139
7	-2.121630	1.282841	0.106830
16	-1.513966	2.607752	-0.672958
6	-2.802668	3.830815	-0.356252
6	-3.033121	-0.942416	-0.039510
8	-0.306434	3.079566	0.041677
8	-1.416521	2.424183	-2.139654
1	-0.537439	-1.940639	-0.411547
1	2.340836	-2.001209	0.433820
1	4.296466	-0.628471	1.474928
1	2.175042	-1.684320	2.734457
1	3.088121	-0.413225	3.563503
1	4.142331	1.671189	1.826646
1	3.141584	1.699106	0.387701
1	0.731420	0.403023	3.539575
1	2.312953	2.175774	3.185141
1	1.314609	2.371977	1.736350
1	-0.066961	-1.103399	1.709438
1	-0.550028	0.592713	1.450940
1	-2.269366	0.252608	-1.708796
1	3.514633	0.960822	-1.766437
1	4.902678	0.632005	-0.710818
1	4.896395	0.043260	-2.375217
1	4.310107	-3.095166	-0.392807
1	5.400233	-2.278592	-1.522858
1	5.344143	-1.765906	0.162571
1	2.330649	-2.617954	-2.032839
1	2.208139	-0.993862	-2.742097
1	3.628034	-1.985793	-3.058517
1	-1.386873	-1.415553	-2.771973
1	-0.164100	-0.159862	-2.928836
1	0.299196	-1.880668	-2.855078

1	-2.448366	4.786727	-0.748989	1	4.523961	2.376601	-1.961857
1	-3.717748	3.522100	-0.864647	1	4.350777	-1.336389	-2.548653
1	-2.962156	3.894681	0.721182	1	5.173331	0.161770	-3.007493
6	-3.591389	-1.925841	-0.870975	1	5.483514	-0.556582	-1.428443
6	-4.363652	-2.959035	-0.339778	1	2.077334	-0.159714	-3.132616
6	-4.598054	-3.023045	1.034585	1	1.808727	1.485975	-2.527340
6	-4.064575	-2.037552	1.869993	1	3.138534	1.165137	-3.636844
6	-3.295079	-1.004964	1.338481	1	-1.741358	0.723142	-2.259524
1	-3.434445	-1.872172	-1.945085	1	-0.550537	1.943852	-1.784365
1	-4.790446	-3.708120	-1.001820	1	-0.122304	0.657439	-2.936975
1	-5.201451	-3.825840	1.450108	1	-4.338503	-4.172398	-0.312088
1	-4.258351	-2.069302	2.939361	1	-4.945738	-2.722832	0.558129
1	-2.903440	-0.221418	1.978469	1	-4.901782	-2.741137	-1.237585
E (CH ₃ CN) = -1821.851097				6	-1.974628	2.237140	1.317353
NImag = 1 (-163.4)				6	-2.294507	3.589269	1.417858
82. 9-si,si-t[‡] (-1821.5248595)				6	-3.243582	4.147885	0.557416
6	0.793691	-0.834992	1.493920	6	-3.872065	3.341931	-0.394193
6	1.997258	-1.182483	2.369740	6	-3.552916	1.987925	-0.491502
6	3.110775	-1.844154	1.548179	1	-1.238153	1.806761	1.992687
6	3.680911	-0.647538	0.760513	1	-1.808374	4.206588	2.168932
6	2.829529	-0.362573	-0.502929	1	-3.495668	5.202368	0.634086
16	1.097398	0.351623	0.089007	1	-4.618675	3.768394	-1.059327
6	3.710983	0.489990	1.834636	1	-4.050503	1.347098	-1.211754
6	2.701994	0.065249	2.940643	E (CH ₃ CN) = -1821.850286			
6	3.531053	0.480066	-1.614796	NImag = 1 (-165.9)			
6	4.702504	-0.368599	-2.171822	83. 9-si,re-c[‡] (-1821.5264271)			
6	-0.358570	-0.015496	-0.851545	6	3.714151	1.322821	0.739260
6	-0.682613	0.881739	-2.022057	6	2.740780	1.993126	1.753940
6	2.575841	0.754324	-2.790544	6	2.057627	0.810573	2.474715
6	4.086647	1.829420	-1.118549	6	3.151367	-0.263799	2.479205
6	-2.258795	-0.024907	0.284986	6	3.645246	-0.215041	1.020633
7	-3.034648	-0.807697	-0.464933	6	2.709948	-1.034352	0.088499
16	-2.734393	-2.432303	-0.300670	16	1.053317	-0.021528	-0.080203
6	-4.413329	-3.082733	-0.323814	6	0.812227	0.332878	1.726374
6	-2.592888	1.419840	0.358886	6	-0.456418	-0.893758	-0.417236
8	-2.046658	-2.948031	-1.503350	1	-0.517361	-1.814948	0.167710
8	-2.129405	-2.770438	1.013242	6	3.361249	-1.495282	-1.254922
1	-0.390380	-1.078576	-1.096043	6	2.336157	-2.176887	-2.178110
1	2.540417	-1.318004	-0.956654	6	4.028699	-0.350998	-2.042554
1	4.696086	-0.865059	0.415256	6	4.433927	-2.557776	-0.904257
1	2.758185	-2.660593	0.907941	6	-2.231085	0.287314	0.270318
1	3.876479	-2.254339	2.218578	7	-2.546050	1.195445	-0.654143
1	4.721586	0.580806	2.246288	1	2.387883	-1.940299	0.616602
1	3.456927	1.464458	1.415441	1	4.641678	-0.658091	0.934695
1	1.614583	-1.836772	3.162528	1	2.796376	-1.254809	2.786846
1	3.229555	-0.199614	3.863345	1	3.960948	0.026035	3.160970
1	1.995731	0.863885	3.193545	1	4.739915	1.672056	0.897990
1	0.333434	-1.725923	1.056591	1	3.453198	1.573469	-0.289694
1	0.030251	-0.330739	2.089952	1	1.726394	1.082015	3.484740
1	-1.800357	-0.437055	1.181547	1	3.295584	2.598558	2.478810
1	3.298947	2.460704	-0.691869	1	2.010819	2.648858	1.269110
1	4.873182	1.705457	-0.367679	1	0.396467	-0.578440	2.170477

1	0.059419	1.123197	1.714565	1	4.380606	1.701278	1.341292
6	-0.816012	-1.024720	-1.880707	1	3.212447	1.620484	0.035065
1	3.312194	0.437041	-2.298267	1	1.159548	0.723951	3.552420
1	4.858865	0.103519	-1.493006	1	2.737838	2.383381	2.854068
1	4.434378	-0.743843	-2.982245	1	1.586771	2.493708	1.513536
1	3.992719	-3.411419	-0.375246	1	0.087854	-0.903763	2.013810
1	4.887337	-2.937461	-1.827155	1	-0.356450	0.769649	1.591277
1	5.244929	-2.158832	-0.286718	6	-0.585230	-2.532831	-0.120960
1	1.735923	-2.924841	-1.646823	1	0.271285	-3.211540	-0.259945
1	1.659014	-1.449459	-2.629869	1	-0.821845	-2.508512	0.949250
1	2.857440	-2.686437	-2.996783	1	-1.444801	-3.000779	-0.611693
1	-1.744721	0.598201	1.191732	1	-0.306866	-1.143005	-1.791629
1	-1.890653	-1.226361	-1.951316	6	-2.178319	0.265572	-0.651106
1	-0.638971	-0.084166	-2.412975	1	-2.085285	0.280817	-1.737503
1	-0.309366	-1.838778	-2.410529	7	-1.990222	1.397586	0.030280
16	-1.628609	2.567322	-0.643336	6	3.395714	-1.312808	-1.221672
8	-0.989324	2.819836	0.678204	6	3.807477	-0.026338	-1.964728
8	-0.745301	2.606652	-1.826660	1	2.947582	0.616675	-2.180938
6	-2.892484	3.829331	-0.880065	1	4.538786	0.559243	-1.399418
1	-3.446024	3.595452	-1.790660	1	4.271164	-0.290713	-2.922446
1	-3.556363	3.835553	-0.014020	6	4.670200	-2.132643	-0.901314
1	-2.377782	4.787650	-0.979276	1	4.432241	-3.047654	-0.344735
6	-3.143599	-0.874639	0.423015	1	5.156878	-2.431507	-1.836584
6	-4.143415	-1.141879	-0.524650	1	5.404420	-1.563080	-0.323397
6	-5.010499	-2.220683	-0.353230	6	2.535735	-2.175367	-2.171275
6	-4.898477	-3.043907	0.769115	1	2.182224	-3.089408	-1.679842
6	-3.914029	-2.779055	1.725430	1	1.665752	-1.633987	-2.550447
6	-3.045546	-1.703926	1.551357	1	3.134650	-2.476071	-3.038517
1	-4.237043	-0.478747	-1.378333	16	-1.257903	2.636392	-0.794458
1	-5.781120	-2.415196	-1.094859	8	-0.091296	3.107843	-0.017671
1	-5.577020	-3.882369	0.902762	8	-1.060026	2.338306	-2.230328
1	-3.827397	-3.408021	2.607756	6	-2.508229	3.932399	-0.669072
1	-2.282533	-1.497842	2.299479	1	-2.080867	4.839405	-1.103106
E (CH ₃ CN) = -1821.850494				1	-3.396224	3.623497	-1.223439
NImag = 1 (-165.5)				1	-2.744354	4.086234	0.384886
84. 9-re,si-c [‡] (-1821.52917048)				6	-3.153986	-0.711045	-0.110197
				6	-3.539635	-0.695806	1.239150
16	0.953908	-0.168121	-0.111672	6	-4.485093	-1.602081	1.715093
6	0.470603	0.057953	1.661993	6	-5.071487	-2.530770	0.850523
6	1.603338	0.557709	2.562899	6	-4.706734	-2.543894	-0.497349
6	2.291060	1.829569	2.020709	6	-3.755384	-1.641200	-0.971894
6	2.756905	-0.455642	2.600285	1	-3.100745	0.046645	1.897834
6	3.411050	-0.255091	1.216233	1	-4.773755	-1.578920	2.763021
6	2.641087	-1.052804	0.126595	1	-5.812765	-3.232862	1.223006
6	3.399868	1.302059	1.061270	1	-5.167453	-3.252673	-1.180644
6	-0.385446	-1.149849	-0.704423	1	-3.478835	-1.648274	-2.024178
1	2.385058	-2.035775	0.540402	E (CH ₃ CN) = -1821.852429			
1	4.437076	-0.633411	1.218421	NImag = 1 (-129.8)			
1	2.435576	-1.488068	2.785552				
1	3.467569	-0.182135	3.390192				

85. 9-re,si-t[‡] (-1821.5320346)				6	-4.273861	3.078811	-0.415869
				6	-3.955737	3.887071	0.678302
16	1.155478	0.154854	0.317897	6	-3.090289	3.406137	1.664700
6	1.029532	-1.692294	0.254232	6	-2.543684	2.129790	1.550785
6	2.314142	-2.417857	0.661002	1	-3.989110	1.154188	-1.361315
6	2.886775	-1.922950	2.008767	1	-4.952597	3.444751	-1.182136
6	3.454850	-2.106474	-0.318054	1	-4.382847	4.882683	0.765290
6	3.841011	-0.665689	0.077385	1	-2.845149	4.024958	2.524069
6	2.868444	0.358224	-0.568488	1	-1.868127	1.756782	2.317846
6	3.826813	-0.735436	1.637950	E (CH ₃ CN) = -1821.853930 NImag = 1 (-109.9)			
6	-0.277840	0.685495	-0.540733				
1	2.676745	0.035771	-1.598810				
1	4.844597	-0.426719	-0.285091				
1	3.168794	-2.209102	-1.371220	86. 9-re,re-c[‡] (-1821.53101045)			
1	4.301098	-2.781132	-0.136165	16	0.954180	0.008576	-0.099354
1	4.843213	-0.923025	2.000433	6	0.265028	-1.269678	1.048606
1	3.497149	0.197241	2.098616	6	1.203208	-1.618322	2.206142
1	2.064580	-3.484837	0.689927	6	1.748335	-0.368206	2.935437
1	3.455011	-2.727413	2.487833	6	2.486055	-2.285493	1.687394
1	2.097152	-1.628287	2.708165	6	3.254046	-1.092024	1.081116
1	0.713204	-1.971522	-0.753166	6	2.717674	-0.759836	-0.338990
1	0.204543	-1.928751	0.929655	6	3.052080	0.012408	2.167999
6	-0.456318	0.337044	-1.998460	6	-0.176433	-0.030584	-1.422747
1	0.360235	0.678289	-2.652644	1	2.535287	-1.707288	-0.860315
1	-0.601983	-0.738265	-2.149043	1	4.315842	-1.333157	0.977647
1	-1.374104	0.820523	-2.351527	1	2.299404	-3.094990	0.972370
1	-0.398706	1.738993	-0.296570	1	3.055606	-2.707270	2.525379
6	-2.290918	-0.056297	0.369843	1	3.911000	0.008890	2.847687
1	-1.803671	-0.419045	1.275043	1	2.990838	1.015614	1.743359
7	-2.845081	-0.908058	-0.481027	1	0.636847	-2.271479	2.880631
6	3.344914	1.848701	-0.642790	1	1.974475	-0.614682	3.978434
6	3.494403	2.528461	0.733169	1	1.020127	0.449965	2.947852
1	2.562501	2.501820	1.308265	1	0.003270	-2.151411	0.460425
1	4.281452	2.066188	1.336857	1	-0.674278	-0.827683	1.388661
1	3.766548	3.581511	0.594984	6	-0.335813	-1.282175	-2.256917
6	4.716204	1.887305	-1.362282	1	0.541835	-1.520102	-2.878959
1	4.684016	1.356439	-2.321841	1	-0.571710	-2.161493	-1.649219
1	4.990167	2.927990	-1.570045	1	-1.188092	-1.152621	-2.933752
1	5.521386	1.455646	-0.759682	1	-0.033966	0.889782	-1.989130
6	2.367289	2.678988	-1.503942	6	-2.300603	0.584152	-0.555679
1	2.232101	2.234103	-2.496532	7	-2.782570	-0.280986	0.319098
1	1.382189	2.775091	-1.042163	6	3.640279	0.096422	-1.268585
1	2.766402	3.690027	-1.645249	6	3.889769	1.528307	-0.752964
16	-2.437651	-2.505271	-0.294259	1	2.955769	2.080365	-0.600757
8	-1.599998	-2.960780	-1.426167	1	4.446484	1.534770	0.189373
8	-1.950239	-2.816090	1.072988	1	4.485849	2.084103	-1.486369
6	-4.052987	-3.276993	-0.488860	6	5.003932	-0.624455	-1.404925
1	-3.897832	-4.357915	-0.463474	1	4.877961	-1.668335	-1.717745
1	-4.697757	-2.960461	0.332604	1	5.609096	-0.121499	-2.168052
1	-4.469205	-2.970357	-1.449489	1	5.582311	-0.613902	-0.475980
6	-2.853968	1.312405	0.452656	6	3.034008	0.176380	-2.687232
6	-3.732068	1.799204	-0.527479				

1	2.844945	-0.822707	-3.096780	8	2.983844	-2.272496	1.483705
1	2.092861	0.731201	-2.706573	8	3.295015	-2.805923	-0.970764
1	3.732866	0.685076	-3.361350	1	-2.627405	-0.920124	-1.532434
1	-2.556292	0.498504	-1.612879	1	-4.855744	-0.317423	-0.361715
16	-3.397545	-1.695210	-0.316686	1	-3.526982	1.094261	-2.200250
8	-3.778539	-1.566454	-1.738624	1	-4.720327	1.950064	-1.212199
8	-2.520701	-2.821820	0.069138	1	-4.931949	1.093224	1.504901
6	-4.910632	-1.848679	0.650156	1	-3.431600	0.308984	1.967130
1	-4.652334	-1.831933	1.709897	1	-2.625775	3.253392	-0.923228
1	-5.576576	-1.021368	0.399285	1	-3.830093	3.109180	1.138511
1	-5.366370	-2.804120	0.380568	1	-2.311471	2.391663	1.666835
6	-1.930990	1.937783	-0.079619	1	-1.086685	1.439059	-1.739513
6	-1.861333	2.235014	1.290640	1	-0.518435	2.224023	-0.254634
6	-1.538738	3.520942	1.720140	1	-0.076800	-1.519724	-2.376437
6	-1.291953	4.534143	0.790121	1	0.493029	0.163550	-2.456759
6	-1.376845	4.253101	-0.575794	1	1.620678	-1.143770	-2.077413
6	-1.694988	2.966263	-1.005374	1	0.603637	-1.537274	0.141807
1	-2.081783	1.449219	2.005876	1	-1.968158	-2.025792	2.041991
1	-1.489215	3.736968	2.784455	1	-3.729538	-1.827595	2.119949
1	-1.044582	5.537419	1.126859	1	-3.025254	-3.435030	1.938622
1	-1.200582	5.038443	-1.306229	1	-4.485125	-2.674523	-1.458672
1	-1.767661	2.752188	-2.069370	1	-4.442373	-3.868456	-0.154865
E (CH ₃ CN) = -1821.851911				1	-5.192776	-2.298716	0.126208
NImag = 1 (-98.1)				1	-1.924169	-3.188723	-1.599936
87. 9-re, re-<i>t</i>[‡] (-1821.5258814)				1	-0.902671	-2.996860	-0.167144
6	2.493855	2.362693	-0.919304	1	-2.127951	-4.261509	-0.208464
6	2.078342	1.709013	0.250707	1	1.964855	-0.144673	1.400841
6	1.536469	2.472142	1.296399	1	5.785433	-1.439073	-0.564936
6	1.388665	3.854465	1.168607	1	5.593590	-1.164700	1.200133
6	1.781819	4.492935	-0.010156	1	5.710702	-2.837585	0.557534
6	2.337666	3.741450	-1.050360	1	1.235275	1.976055	2.216804
6	2.245257	0.243489	0.419665	1	0.976057	4.432981	1.991414
6	0.408273	-0.626473	-0.424496	1	1.668444	5.569004	-0.112781
6	0.599236	-0.784779	-1.915749	1	2.658779	4.235560	-1.963986
16	-1.128920	-0.017574	0.185809	1	2.945966	1.772829	-1.709981
6	-1.308190	1.605151	-0.682443	E (CH ₃ CN) = -1821.853933			
6	-2.690067	2.243524	-0.500813	NImag = 1 (-150.5)			
6	-3.775783	1.392728	-1.175014	<u>System 10 (R = Me; X = Me; Y = SO₂Me)</u>			
6	-3.907023	0.201760	-0.202972	88. 10-si, si-<i>c</i>[‡] (-1629.78743570)			
6	-2.772641	-0.830801	-0.449182	6	1.915234	2.235335	-0.760272
6	-3.899634	0.912314	1.187314	6	0.692279	2.858367	-0.022588
6	-3.151518	2.265158	0.975673	6	0.743643	2.248360	1.395242
6	-2.978376	-2.283168	0.100690	6	2.250340	2.076730	1.631272
6	-1.915207	-3.227997	-0.504115	6	2.702971	1.414440	0.314768
7	3.224551	-0.340409	-0.266874	6	2.422661	-0.113407	0.339134
16	3.565718	-1.908645	0.170027	16	0.488666	-0.335431	0.184296
6	5.356939	-1.822627	0.362197	6	0.019842	0.902298	1.481265
6	-2.920593	-2.386101	1.638380	6	-0.301556	-1.725573	0.894873
6	-4.358598	-2.798636	-0.376047				

1	0.019997	-1.882390	1.928544	6	-2.293579	2.034714	-1.512310
6	3.270547	-0.964213	-0.657819	6	-3.107938	0.944646	-0.786965
6	2.833838	-2.440805	-0.639159	6	-2.258009	-0.338218	-0.598397
6	3.206070	-0.458766	-2.112566	16	-0.873654	0.036349	0.738711
6	4.742643	-0.918883	-0.177013	6	-0.348423	1.688268	0.064897
6	-2.601375	-1.217843	1.007815	6	0.664252	-0.792717	0.637267
6	-2.744778	-1.633299	2.449639	1	1.009605	-0.862741	-0.395328
7	-2.972755	0.012555	0.703598	6	-3.058919	-1.654077	-0.347150
1	2.632248	-0.496765	1.346027	6	-2.112025	-2.834768	-0.059613
1	3.780520	1.538315	0.169298	6	-4.069968	-1.552939	0.811736
1	2.495838	1.487486	2.523225	6	-3.824603	-1.989647	-1.651474
1	2.726506	3.059535	1.739867	6	2.536934	0.400716	1.307964
1	2.565451	3.018413	-1.164887	6	2.359144	0.406829	2.802171
1	1.597255	1.623784	-1.605944	7	3.516122	-0.325093	0.807936
1	0.272286	2.901869	2.140035	1	-1.658073	-0.498109	-1.502823
1	0.799179	3.946917	0.044224	1	-3.987860	0.664024	-1.374404
1	-0.253241	2.644444	-0.528030	1	-1.682259	1.647579	-2.335296
1	0.210227	0.410608	2.442312	1	-2.966004	2.796269	-1.927258
1	-1.059041	1.007336	1.344100	1	-4.564287	2.059480	0.406169
6	-0.411365	-2.986178	0.066703	1	-3.572926	0.996036	1.385607
1	-2.677453	-2.002782	0.255246	1	-0.990192	3.579864	-0.642377
1	-2.223773	-2.570969	2.659482	1	-3.027985	3.801392	0.605929
1	-2.378862	-0.854176	3.123974	1	-2.098379	2.829586	1.743188
1	-3.812489	-1.781119	2.666345	1	0.346484	1.479601	-0.755139
1	2.180824	-0.457963	-2.498180	1	0.223523	2.122283	0.888378
1	3.611906	0.552120	-2.218871	6	0.827350	-2.071098	1.427875
1	3.799105	-1.119332	-2.756211	1	2.195601	1.284615	0.772500
1	4.841242	-1.304818	0.844990	1	1.387626	0.819063	3.089720
1	5.362108	-1.544958	-0.829729	1	2.462024	-0.598457	3.217925
1	5.165720	0.090342	-0.199955	1	3.145124	1.031862	3.248750
1	2.750742	-2.828306	0.383157	1	-3.579324	-1.300430	1.758501
1	1.873176	-2.583628	-1.138660	1	-4.850681	-0.809620	0.620484
1	3.570458	-3.053986	-1.171334	1	-4.567133	-2.520425	0.948990
1	-1.227915	-3.600545	0.472495	1	-3.136698	-2.111931	-2.496457
1	-0.679183	-2.758509	-0.972152	1	-4.367932	-2.933445	-1.526273
1	0.478419	-3.629406	0.061130	1	-4.561134	-1.225622	-1.920462
16	-3.112510	0.341544	-0.932008	1	-1.297406	-2.894395	-0.790229
8	-2.159749	1.415606	-1.280569	1	-1.669028	-2.764513	0.936546
8	-3.125603	-0.877175	-1.768770	1	-2.671399	-3.776681	-0.101328
6	-4.762266	1.068286	-0.982645	1	1.905352	-2.233529	1.556529
1	-4.926253	1.423680	-2.002536	1	0.372799	-2.004855	2.424874
1	-5.495953	0.303863	-0.720852	1	0.436669	-2.972626	0.938642
1	-4.797811	1.898707	-0.276089	16	3.775938	-0.081584	-0.832488
E (CH ₃ CN) = -1630.064208				8	3.316135	-1.265200	-1.584006
NImag = 1 (-117.5)				8	3.303056	1.246805	-1.290721
				6	5.576207	-0.079276	-0.874746
89. 10- <i>si</i> , <i>si</i> - <i>t</i> [‡] (-1629.78504757)				1	5.873572	-0.020245	-1.924111
				1	5.945052	0.785933	-0.321265
				1	5.932143	-1.007686	-0.425864
6	-3.548526	1.668531	0.526918	E (CH ₃ CN) = -1630.064370			
6	-2.535363	2.832052	0.738427	NImag = 1 (-131.6)			
6	-1.471502	2.634365	-0.363505				

90. **10-si, re-c[‡]** (-1629.7848547)

6	2.408340	2.079934	-0.937642
6	1.258535	2.934535	-0.325042
6	1.142983	2.444705	1.135511
6	2.586588	2.052438	1.474328
6	2.988161	1.225665	0.237366
6	2.451250	-0.227799	0.347087
16	0.522038	-0.157143	0.096878
6	0.196534	1.248979	1.263919
6	-0.457903	-1.422127	0.809347
1	-0.076096	-1.726041	1.787608
6	3.199217	-1.281914	-0.530936
6	2.515772	-2.660582	-0.463408
6	3.316392	-0.875950	-2.013347
6	4.621989	-1.450005	0.059012
6	-2.622460	-0.693827	1.382806
6	-2.792705	-1.668747	2.518584
7	-3.402856	-0.852406	0.332784
1	2.544911	-0.559174	1.389269
1	4.077022	1.159294	0.152256
1	2.685075	1.501895	2.417749
1	3.213144	2.950623	1.546499
1	3.197728	2.725498	-1.337408
1	2.054510	1.467882	-1.768534
1	0.750828	3.225817	1.798598
1	1.519069	3.998370	-0.339372
1	0.314372	2.823092	-0.867616
1	0.213899	0.825817	2.274661
1	-0.822962	1.543433	1.005242
6	-0.846574	-2.544056	-0.131996
1	2.332307	-0.726973	-2.470920
1	3.901308	0.039351	-2.148752
1	3.820900	-1.672768	-2.572437
1	4.582357	-1.787051	1.102040
1	5.170336	-2.206840	-0.513703
1	5.210371	-0.527697	0.022847
1	2.292822	-2.959204	0.567538
1	1.583563	-2.677085	-1.030941
1	3.175565	-3.420619	-0.898202
1	-2.249911	0.291900	1.648952
1	-3.755790	-1.470699	3.008746
1	-2.817938	-2.701631	2.159290
1	-2.001163	-1.562406	3.264855
1	-1.831666	-2.932491	0.154204
1	-0.971112	-2.173020	-1.154726
1	-0.152568	-3.394547	-0.148254
16	-3.293709	0.364914	-0.805220
8	-2.764051	1.632028	-0.236296
8	-2.647058	-0.151531	-2.025627
6	-5.035472	0.624457	-1.185186
1	-5.464836	-0.328878	-1.496620

1	-5.541730	1.006719	-0.297177
1	-5.082585	1.351736	-1.998745

E (CH₃CN) = -1630.063277
NImag = 1 (-131.7)

91. **10-re, si-c[‡]** (-1629.78851042)

16	-0.429567	0.343081	0.155719
6	-0.063986	-0.486388	1.767462
6	-0.818799	-1.802803	1.974207
6	-0.668998	-2.769066	0.776811
6	-2.334381	-1.557358	2.021769
6	-2.668901	-1.290358	0.538300
6	-2.345603	0.182752	0.159574
6	-1.828645	-2.387365	-0.193095
6	0.277841	1.923370	0.403239
1	-2.682008	0.824400	0.983353
1	-3.736906	-1.438644	0.356455
1	-2.629908	-0.738966	2.690124
1	-2.850120	-2.464758	2.360571
1	-2.466830	-3.254612	-0.394387
1	-1.439654	-2.051240	-1.155259
1	-0.435854	-2.241436	2.904022
1	-0.784458	-3.801864	1.124017
1	0.310239	-2.683733	0.297971
1	-0.295832	0.229489	2.561806
1	1.018814	-0.633184	1.717543
6	-0.325877	2.853382	1.437435
1	-1.372942	3.137645	1.243684
1	-0.283437	2.441582	2.453675
1	0.247500	3.787992	1.454944
1	0.376883	2.372280	-0.585932
6	2.600363	1.452404	0.573676
1	2.658446	2.037142	-0.344624
7	2.909851	0.167582	0.553178
6	2.834253	2.181961	1.869695
1	2.387160	3.177562	1.866203
1	2.450667	1.613390	2.721394
1	3.918502	2.294875	2.012775
6	-3.005467	0.744254	-1.145634
6	-2.514921	0.064325	-2.440129
1	-1.428042	0.129393	-2.557188
1	-2.797936	-0.991703	-2.481212
1	-2.970766	0.557669	-3.306781
6	-4.538613	0.556077	-1.038711
1	-4.932303	0.964919	-0.099655
1	-5.029415	1.087389	-1.862191
1	-4.840493	-0.493649	-1.106903
6	-2.749350	2.263772	-1.254640
1	-3.101286	2.792150	-0.360474
1	-1.691022	2.497745	-1.393001

1	-3.292971	2.670950	-2.114761
16	2.999097	-0.543027	-0.958400
8	2.088378	-1.705277	-0.989635
8	2.920028	0.437260	-2.062378
6	4.677987	-1.203910	-0.922155
1	4.812763	-1.790736	-1.833772
1	5.387708	-0.375209	-0.892574
1	4.783413	-1.836929	-0.039901

E (CH₃CN) = -1630.064409

NImag = 1 (-109.0)

92. **10-re,si-t[‡]** (-1629.79040956)

16	-0.805930	-0.277187	0.518348
6	0.067593	1.257198	-0.043372
6	-0.796647	2.520606	-0.007047
6	-1.525677	2.709676	1.343547
6	-1.963656	2.420319	-0.999966
6	-2.910624	1.431210	-0.289798
6	-2.439530	-0.030539	-0.515640
6	-2.874429	1.943352	1.185827
6	0.289370	-1.547315	0.081423
1	-2.111941	-0.121470	-1.558506
1	-3.923351	1.513476	-0.694873
1	-1.660802	2.092124	-2.001120
1	-2.453434	3.397042	-1.104099
1	-3.720431	2.618391	1.354789
1	-2.967330	1.135880	1.914213
1	-0.126328	3.358787	-0.230651
1	-1.707216	3.775152	1.521449
1	-0.931296	2.340688	2.186232
1	0.459865	1.071271	-1.045990
1	0.922815	1.340859	0.630219
6	0.637746	-1.802833	-1.367080
1	-0.215525	-2.095384	-1.999656
1	1.133972	-0.944039	-1.831803
1	1.365071	-2.622204	-1.409642
1	-0.015023	-2.427786	0.647726
6	2.583908	-1.347207	1.067139
1	2.234540	-0.527786	1.695166
7	3.414533	-1.136238	0.079594
6	2.514418	-2.733858	1.645862
1	1.641137	-2.856560	2.289760
1	2.502094	-3.492375	0.858172
1	3.415577	-2.903662	2.252583
6	-3.492210	-1.163699	-0.275014
6	-3.946338	-1.290772	1.193437
1	-3.102748	-1.465504	1.870145
1	-4.479469	-0.398718	1.537039
1	-4.632656	-2.139836	1.295583

6	-4.736447	-0.878110	-1.151608
1	-4.461054	-0.716385	-2.201059
1	-5.414731	-1.738736	-1.116854
1	-5.303246	-0.006693	-0.809409
6	-2.923990	-2.523357	-0.739558
1	-2.595134	-2.480898	-1.784513
1	-2.074708	-2.847981	-0.134085
1	-3.699853	-3.294482	-0.666889
16	3.665122	0.474386	-0.330118
8	3.090028	0.741996	-1.662899
8	3.315460	1.403094	0.770209
6	5.457104	0.473849	-0.505466
1	5.743735	1.467027	-0.858311
1	5.908968	0.265583	0.465819
1	5.732261	-0.289135	-1.234870

E (CH₃CN) = -1630.065590

NImag = 1 (-69.1)

93. **10-re,re-c[‡]** (-1629.7897678)

16	-0.817042	-0.236962	0.520168
6	0.059366	1.248598	-0.152385
6	-0.815363	2.502098	-0.239377
6	-1.575846	2.798658	1.074486
6	-1.960038	2.305221	-1.244391
6	-2.918432	1.374489	-0.472246
6	-2.433796	-0.098156	-0.558990
6	-2.918629	2.014486	0.952962
6	0.307199	-1.514633	0.228698
1	-2.085594	-0.277550	-1.583799
1	-3.921824	1.414559	-0.906305
1	-1.632088	1.893387	-2.205793
1	-2.452680	3.265474	-1.444438
1	-3.770029	2.697915	1.042370
1	-3.025700	1.273865	1.747359
1	-0.150629	3.327611	-0.520909
1	-1.765614	3.874218	1.159319
1	-0.999643	2.504314	1.958515
1	0.480847	0.983219	-1.124164
1	0.901129	1.379295	0.532108
6	0.681478	-1.918033	-1.181292
1	-0.117498	-2.439395	-1.733527
1	1.006592	-1.063901	-1.784700
1	1.541021	-2.597885	-1.144661
1	0.043113	-2.339305	0.893137
6	2.501658	-0.946914	1.390074
7	3.039168	0.152315	0.936731
6	-3.476736	-1.218771	-0.236268
6	-3.929667	-1.245557	1.237818
1	-3.085892	-1.372166	1.924831

1	-4.464994	-0.333573	1.520180
1	-4.614013	-2.087340	1.397651
6	-4.724736	-1.012544	-1.128943
1	-4.451958	-0.917758	-2.187216
1	-5.390066	-1.878939	-1.035565
1	-5.304821	-0.128422	-0.845921
6	-2.888597	-2.600041	-0.601357
1	-2.574090	-2.632037	-1.651109
1	-2.024529	-2.858067	0.015684
1	-3.647261	-3.378442	-0.458053
1	2.725651	-1.911614	0.932668
6	1.963994	-0.950122	2.793664
1	2.804167	-1.090319	3.489593
1	1.489125	0.003761	3.037499
1	1.253527	-1.764107	2.950406
16	3.815510	0.021483	-0.557764
8	4.186955	-1.368033	-0.888561
8	3.055488	0.805057	-1.550739
6	5.327559	0.932293	-0.196509
1	5.059356	1.926834	0.162467
1	5.899198	0.386928	0.556401
1	5.889528	0.998277	-1.130864

E (CH₃CN) = -1630.064703

NImag = 1 (-61.2)

94. **10-*re, re*-t[‡]** (-1629.7843444)

16	-0.746035	-0.363773	-0.050628
6	-1.303287	-2.094609	0.294538
6	-2.696835	-2.429391	-0.247970
6	-2.866169	-2.040708	-1.735542
6	-3.769183	-1.574707	0.443628
6	-3.560334	-0.192717	-0.210447
6	-2.377386	0.555527	0.460619
6	-3.370970	-0.565621	-1.714968
6	0.683620	-0.214013	0.941811
1	-2.450233	0.398693	1.543760
1	-4.450893	0.428419	-0.079944
1	-3.681989	-1.558829	1.536494
1	-4.767154	-1.957726	0.196246
1	-4.332844	-0.484219	-2.232106
1	-2.678957	0.101917	-2.230034
1	-2.850539	-3.503539	-0.087166
1	-3.607071	-2.695771	-2.205994
1	-1.934269	-2.153006	-2.299962
1	-1.250756	-2.253556	1.375730
1	-0.533838	-2.708673	-0.180800
6	0.580973	-0.273284	2.450033
1	0.046503	0.574586	2.904316
1	0.111451	-1.195755	2.815424
1	1.602852	-0.251790	2.848301

1	1.205692	0.667616	0.574935
6	2.496749	-1.456131	0.282956
7	3.512765	-0.658379	0.552190
6	-2.279320	2.102789	0.235888
6	-1.983665	2.508346	-1.222339
1	-1.055508	2.062983	-1.596001
1	-2.797056	2.230055	-1.899952
1	-1.869556	3.596821	-1.282222
6	-3.622737	2.742765	0.663698
1	-3.911643	2.438999	1.677692
1	-3.523025	3.834130	0.662383
1	-4.444320	2.493431	-0.015327
6	-1.184632	2.699567	1.148698
1	-1.352206	2.430894	2.198652
1	-0.179953	2.374584	0.869017
1	-1.203891	3.793109	1.080796
1	2.109654	-1.532875	-0.735120
6	2.352186	-2.679100	1.151478
1	3.106043	-3.416696	0.842930
1	2.538214	-2.438438	2.201411
1	1.366325	-3.140188	1.055022
16	3.796794	0.523503	-0.596923
8	3.531102	0.056566	-1.974863
8	3.169238	1.795415	-0.173598
6	5.575627	0.715580	-0.400619
1	5.786066	0.957997	0.641917
1	6.067398	-0.214742	-0.689600
1	5.883458	1.532938	-1.056404

E (CH₃CN) = -1630.065263

NImag = 1 (-135.2)

System 11 (R = Me; X = Ph; Y = CO₂Me)

95. **11-*si, si*-c[‡]** (-1461.5098157)

6	-3.678015	-1.691501	-0.810615
6	-3.179315	-0.572050	-0.124820
6	-3.618419	-0.341818	1.188157
6	-4.505715	-1.222706	1.805211
6	-4.979567	-2.343728	1.119378
6	-4.566354	-2.571762	-0.195619
6	-2.245329	0.370106	-0.801049
7	-1.981851	1.531681	-0.192078
6	-1.334664	2.449108	-0.972054
8	-1.163556	3.617380	-0.273149
6	-0.540080	4.666436	-1.011302
8	-0.908205	2.329350	-2.121095
6	-0.491447	-0.964649	-1.001134
6	-0.334808	-1.029757	-2.510518
16	0.810796	-0.137089	-0.152229
6	2.407413	-1.092286	0.372778

6	3.060041	-0.230446	1.493723	6	-4.493221	-3.321310	0.087891
6	2.244479	-0.341309	2.798344	6	-3.430749	-3.249882	-0.817527
6	1.087646	0.633633	2.537672	6	-2.314694	0.347794	-0.399276
6	0.089223	0.044437	1.535790	7	-2.793312	1.450056	0.170375
6	3.084245	1.311954	1.254952	6	-2.168727	2.604259	-0.205111
6	1.818427	1.878068	1.975518	8	-2.854441	3.687631	0.259090
6	3.296401	-1.530239	-0.841263	6	-2.282437	4.951136	-0.068511
6	4.727964	-1.863175	-0.359151	8	-1.117774	2.743114	-0.843968
6	2.706266	-2.834979	-1.422522	6	-0.445545	-0.013504	0.764889
6	3.403153	-0.463198	-1.950216	6	-0.851993	-0.848711	1.962343
1	-0.761174	-1.903640	-0.513036	16	0.986875	-0.609605	-0.078049
1	2.032043	-2.009796	0.841489	6	2.663230	0.230688	0.380395
1	4.072857	-0.611497	1.643245	6	3.633683	0.031837	-0.816113
1	1.916851	-1.363518	3.022975	6	3.189029	0.890792	-2.017974
1	2.849447	0.007147	3.645197	6	2.065401	0.040185	-2.622961
1	3.993878	1.727551	1.701411	6	0.798294	0.128600	-1.768139
1	3.104008	1.576567	0.195045	6	3.678745	-1.400314	-1.429167
1	0.521864	0.869154	3.446821	6	2.688363	-1.378160	-2.635503
1	2.112264	2.536968	2.799469	6	3.164392	-0.165479	1.816110
1	1.174085	2.461942	1.310228	6	4.665550	0.176851	1.964019
1	-0.274036	-0.941097	1.846628	6	2.407003	0.693165	2.854424
1	-0.760925	0.712309	1.361974	6	2.981700	-1.660337	2.152617
1	-2.276662	0.349349	-1.892282	1	-0.351892	1.055697	0.940879
1	2.435489	-0.231951	-2.405253	1	2.408146	1.296436	0.416101
1	3.828852	0.473030	-1.574899	1	4.626636	0.338171	-0.479371
1	4.061404	-0.827631	-2.747392	1	2.870871	1.901951	-1.740282
1	4.723944	-2.557281	0.490127	1	4.016470	0.985342	-2.732655
1	5.278373	-2.346016	-1.174755	1	4.695442	-1.615317	-1.774694
1	5.290074	-0.968958	-0.071283	1	3.421570	-2.176729	-0.704833
1	2.794737	-3.655647	-0.699845	1	1.787221	0.370903	-3.630902
1	1.649789	-2.732448	-1.678417	1	3.227128	-1.537444	-3.575551
1	3.246610	-3.130333	-2.329166	1	1.927977	-2.163616	-2.565513
1	0.459160	4.375876	-1.351789	1	0.434250	1.152591	-1.632055
1	-1.134469	4.940430	-1.889020	1	-0.006056	-0.464115	-2.211896
1	-0.474446	5.512816	-0.323750	1	-1.764848	0.427154	-1.336690
1	-3.273025	0.552289	1.696227	1	1.929782	-1.962324	2.158808
1	-4.839498	-1.027240	2.821458	1	3.514718	-2.307286	1.448236
1	-5.675494	-3.026576	1.599930	1	3.384881	-1.861610	3.151946
1	-4.943009	-3.431236	-0.744497	1	4.880459	1.210814	1.668514
1	-3.370541	-1.868043	-1.838790	1	4.955387	0.069158	3.015498
1	0.437972	-1.715323	-2.884079	1	5.307890	-0.489545	1.379066
1	-1.283407	-1.379250	-2.937211	1	2.639498	1.756967	2.722939
1	-0.151981	-0.030981	-2.920158	1	1.324225	0.579664	2.778151
E (CH ₃ CN) = -1461.815881				1	2.705100	0.410864	3.870901
NImag = 1 (-177.6)				1	-1.278135	5.054861	0.356011
96. 11-si _i si _i -t [‡] (-1461.5095453)				1	-2.213473	5.087674	-1.152713
				1	-2.951780	5.698379	0.363157
				1	-4.400780	-0.109134	1.237583
				1	-5.672467	-2.240581	1.533884
6	-2.720615	-2.060166	-0.964253	1	-5.050332	-4.247572	0.202971
6	-3.055358	-0.923785	-0.212680	1	-3.160161	-4.119769	-1.410781
6	-4.129945	-1.003419	0.686057	1	-1.895184	-2.009248	-1.671981
6	-4.839945	-2.193962	0.836234	1	-0.190774	-0.784281	2.838854

1	-1.839245	-0.500539	2.286779
1	-0.954596	-1.907847	1.698232

E (CH₃CN) = -1461.814051
NImag = 1 (-175.7)

97. **11-si, re-c[‡]** (-1461.5131177)

6	-3.159067	-1.540879	1.565727
6	-3.250106	-0.662766	0.474064
6	-4.246750	-0.885110	-0.489701
6	-5.116198	-1.968083	-0.369571
6	-5.011114	-2.840511	0.716721
6	-4.030723	-2.620727	1.688349
6	-2.339515	0.500599	0.371904
7	-2.597863	1.434946	-0.528135
6	-1.829998	2.562405	-0.440566
8	-2.282135	3.508681	-1.307590
6	-1.553749	4.734685	-1.302318
8	-0.842164	2.772465	0.273122
6	-0.510638	-0.736934	-0.383319
6	-0.884009	-0.775204	-1.850091
16	1.021945	0.049499	-0.065370
6	0.895499	0.590895	1.694983
6	2.220960	1.120781	2.254400
6	3.267019	0.002160	2.349504
6	3.655041	-0.203082	0.870931
6	2.585197	-1.069272	0.145491
6	3.805265	1.266017	0.367722
6	2.893671	2.132619	1.293262
6	3.005261	-1.801325	-1.176014
6	2.999605	-0.890121	-2.420687
6	4.427986	-2.389139	-1.017785
6	2.053505	-2.997621	-1.404253
1	-0.627426	-1.667316	0.174091
1	2.262773	-1.848602	0.847491
1	4.607209	-0.733718	0.797189
1	2.895722	-0.908868	2.834170
1	4.139329	0.349208	2.918006
1	4.851911	1.573121	0.467313
1	3.541236	1.381037	-0.685978
1	1.996794	1.571893	3.228553
1	3.497539	2.843485	1.867317
1	2.152023	2.711828	0.734356
1	0.510925	-0.252684	2.279469
1	0.147564	1.384145	1.635932
1	2.006455	-0.484623	-2.636797
1	3.691253	-0.048561	-2.311925
1	3.318074	-1.464713	-3.298373
1	4.527869	-2.974684	-0.095575
1	4.635394	-3.061613	-1.858055
1	5.204327	-1.617309	-1.020220

1	2.140100	-3.724812	-0.587122
1	1.007604	-2.692589	-1.467795
1	2.310790	-3.514706	-2.336101
1	-1.799423	0.745045	1.286761
1	-1.573449	5.203549	-0.313224
1	-0.508940	4.575966	-1.589111
1	-2.051480	5.375314	-2.033140
1	-4.331122	-0.180233	-1.310245
1	-5.884947	-2.127971	-1.121466
1	-5.692818	-3.681904	0.810679
1	-3.949858	-3.288636	2.542264
1	-2.397534	-1.369609	2.324308
1	-0.223256	-1.359381	-2.506722
1	-1.883881	-1.215207	-1.933383
1	-0.955304	0.241032	-2.256578

E (CH₃CN) = -1461.816131
NImag = 1 (-129.5)

98. **11-re, si-c[‡]** (-1461.5107835)

6	-1.227230	-2.263679	-2.331525
6	-0.821481	-2.913341	-0.989838
6	-2.181014	-3.163228	-0.317953
6	-2.906208	-1.818739	-0.537413
6	-2.542228	-1.487663	-2.021314
6	0.052974	-1.998519	-0.126983
16	-0.628710	-0.294150	0.115911
6	-2.454288	-0.775179	0.519671
6	0.339389	0.309839	1.425723
6	0.472020	-0.464670	2.716982
6	-3.390037	0.464771	0.721095
6	-3.756114	1.183790	-0.591737
6	-4.689589	-0.049536	1.387776
6	-2.764943	1.505126	1.678170
6	2.238064	1.145092	0.439194
7	1.877549	1.817806	-0.642090
6	1.186230	2.976126	-0.422536
8	0.631101	3.357289	0.612313
6	3.093157	-0.054885	0.276978
6	3.363929	-0.574883	-1.000327
6	4.179085	-1.695818	-1.149643
6	4.748173	-2.309476	-0.029408
6	4.504109	-1.785587	1.242357
6	3.686585	-0.665847	1.392526
8	1.131194	3.715200	-1.568017
6	0.415736	4.943280	-1.457558
1	-2.383146	-1.278467	1.491867
1	-3.989031	-1.938906	-0.429896
1	-2.103991	-3.450826	0.737399
1	-2.713657	-3.966695	-0.842239
1	-3.351950	-1.826886	-2.676097

1	-2.425026	-0.417998	-2.196717	6	2.615764	1.442823	-0.523917
1	-0.253137	-3.839415	-1.139955	6	3.563073	2.061062	0.306197
1	-1.406556	-3.043276	-3.079736	6	3.862168	3.413330	0.149852
1	-0.442570	-1.610800	-2.728137	6	3.227274	4.167913	-0.840780
1	0.206217	-2.433013	0.864112	6	2.290994	3.558220	-1.679265
1	1.032387	-1.822170	-0.577994	6	1.988346	2.206514	-1.519948
1	0.092299	1.360890	1.541249	8	3.899695	-2.774612	0.911909
1	2.324390	1.654264	1.403808	6	3.847336	-4.194360	0.801762
1	-2.866836	1.550925	-1.115348	1	-2.619208	-0.702903	1.509783
1	-4.320531	0.541163	-1.275151	1	-4.685718	-0.609801	-0.081015
1	-4.384482	2.053575	-0.367004	1	-3.189935	-2.729681	0.566446
1	-4.481101	-0.520085	2.356267	1	-4.160942	-2.832153	-0.910154
1	-5.369946	0.790707	1.567503	1	-4.428912	-0.414537	-2.398839
1	-5.226731	-0.774531	0.766979	1	-3.082408	0.640752	-2.005840
1	-2.379169	1.040270	2.592576	1	-1.840787	-3.357020	-1.641738
1	-1.953577	2.072834	1.213382	1	-2.988367	-2.023880	-3.267620
1	-3.533643	2.228952	1.973656	1	-1.611639	-0.965769	-2.973982
1	-0.632835	4.769969	-1.192623	1	-0.738785	-2.356226	0.399078
1	0.858447	5.594693	-0.697262	1	0.078149	-1.942495	-1.094038
1	0.482327	5.412673	-2.441467	1	0.542921	1.341161	0.936992
1	3.507324	-0.254328	2.382844	1	1.769778	-0.441195	-1.225651
1	4.957156	-2.245411	2.117112	1	-2.332391	2.577684	-0.438471
1	5.388416	-3.179833	-0.148094	1	-4.038421	2.169587	-0.704449
1	4.383922	-2.085365	-2.144024	1	-3.594486	3.373539	0.507285
1	2.937076	-0.065318	-1.858367	1	-4.617865	0.369405	2.545125
1	1.052629	0.144670	3.420325	1	-4.902807	2.097001	2.290954
1	-0.482341	-0.693017	3.221754	1	-5.386627	0.941719	1.051406
1	1.017917	-1.409238	2.599532	1	-2.161704	1.084953	3.069942
E (CH ₃ CN) = -1461.815227				1	-1.271609	2.077262	1.905569
NImag = 1 (-145.4)				1	-2.682052	2.742188	2.731814
99. 11-re,si-t[‡] (-1461.5143399)				1	2.891519	-4.586797	1.165457
				1	3.979356	-4.518171	-0.235776
				1	4.666314	-4.568432	1.419984
				1	1.261895	1.732075	-2.176934
6	-2.482531	-1.429906	-2.499124	1	1.801539	4.134510	-2.460567
6	-2.083304	-2.339568	-1.313561	1	3.466336	5.221160	-0.963916
6	-3.337391	-2.290898	-0.427303	1	4.599920	3.880392	0.797753
6	-3.651655	-0.781477	-0.392537	1	4.062975	1.453483	1.053238
6	-3.460008	-0.376627	-1.889635	1	1.733532	-0.534690	2.318408
6	-0.859654	-1.823925	-0.548053	1	0.160496	-0.047737	2.993567
16	-0.963316	-0.016829	-0.161603	1	0.322769	-1.545795	2.054320
6	-2.733566	-0.055601	0.631705	E (CH ₃ CN) = -1461.819580			
6	0.444768	0.262006	0.841089	NImag = 1 (-144.9)			
6	0.652428	-0.503786	2.123166	100. 11-re,re-c[‡] (-1461.51503172)			
6	-3.209712	1.338126	1.156090				
6	-3.295118	2.418661	0.059649	6	-3.962768	-0.656242	1.400472
6	-4.611925	1.166077	1.791064	6	-3.420173	-0.127136	0.219588
6	-2.269622	1.834340	2.276840	6	-4.046348	-0.419831	-1.002837
6	2.295089	-0.001079	-0.374273	6	-5.173805	-1.236423	-1.040207
7	3.112057	-0.755387	0.354448	6	-5.702929	-1.765243	0.141506
6	2.955533	-2.103943	0.190559				
8	2.117318	-2.714141	-0.480794				

6	-5.096390	-1.468610	1.363726	1	-0.341527	-3.028171	0.818450
6	-2.239347	0.766563	0.273928	1	-0.689890	-1.919588	2.156141
7	-2.005140	1.560806	-0.763417				
6	-1.110680	2.566908	-0.548599	E (CH ₃ CN) = -1461.818674			
8	-1.070319	3.396505	-1.629285	NImag = 1 (-153.9)			
6	-0.183200	4.505636	-1.514228				
8	-0.395889	2.777436	0.440184	101. 11 - <i>re, re</i> -t [‡] (-1461.51115963)			
6	-0.713954	-0.940216	0.204906				
16	0.860218	-0.160766	0.171786	6	-1.778000	2.436018	-1.281306
6	2.422830	-1.286367	0.080040	6	-2.331843	1.598801	-0.300287
6	3.611200	-0.443046	0.623421	6	-2.877338	2.181172	0.854149
6	3.474978	-0.236462	2.146439	6	-2.832662	3.561977	1.036883
6	2.471617	0.922439	2.229703	6	-2.262023	4.387434	0.062644
6	1.052293	0.444252	1.907934	6	-1.742658	3.820334	-1.103539
6	3.008479	1.917257	1.173130	6	-2.375256	0.130630	-0.517046
6	3.709456	1.025818	0.101003	7	-3.324203	-0.563357	0.107896
6	2.596662	-1.962474	-1.324390	6	-3.458788	-1.858379	-0.319757
6	2.579508	-0.972735	-2.507702	8	-4.576431	-2.418011	0.227362
6	-0.922479	-2.137856	1.106612	6	-4.813600	-3.772956	-0.146861
6	3.942264	-2.727395	-1.345825	8	-2.717458	-2.502770	-1.065453
6	1.482464	-3.011852	-1.535970	6	-0.554364	-0.650917	0.396294
1	2.236597	-2.096146	0.796122	16	0.973250	-0.028994	-0.202305
1	4.526834	-0.994789	0.394560	6	2.633974	-0.771402	0.485295
1	3.153539	-1.138203	2.681966	6	3.740252	0.286205	0.221306
1	4.440460	0.072106	2.567076	6	3.564858	1.498619	1.158488
1	4.765185	1.300950	0.002861	6	2.463990	2.299492	0.447404
1	3.257937	1.153778	-0.884471	6	1.098921	1.623814	0.620851
1	2.431930	1.371791	3.229412	6	2.948449	2.299528	-1.020814
1	3.731570	2.595948	1.638256	6	3.724216	0.957217	-1.189707
1	2.203177	2.527797	0.754461	6	2.910303	-2.228166	-0.011600
1	0.739607	-0.356635	2.583912	6	3.094459	-2.339400	-1.538314
1	0.337623	1.269141	1.937562	6	-0.791726	-0.774234	1.883028
1	-0.994586	-1.104612	-0.834756	6	4.199705	-2.733972	0.682485
1	1.649545	-0.396413	-2.554787	6	1.768575	-3.174684	0.421404
1	3.414826	-0.267189	-2.464995	1	2.466459	-0.831676	1.567586
1	2.670027	-1.527706	-3.448898	1	4.702877	-0.201648	0.398074
1	4.047094	-3.389942	-0.477579	1	3.310928	1.221012	2.188288
1	3.991300	-3.351759	-2.245208	1	4.492323	2.084186	1.191927
1	4.806368	-2.056262	-1.370796	1	4.753991	1.148459	-1.509584
1	1.482811	-3.757500	-0.731775	1	3.271040	0.321838	-1.952089
1	0.488683	-2.560342	-1.579469	1	2.362295	3.316617	0.844504
1	1.646070	-3.543549	-2.480311	1	3.613917	3.152635	-1.190613
1	-1.929603	1.065658	1.278730	1	2.117942	2.394879	-1.728349
1	-0.418904	5.114896	-0.636072	1	0.864867	1.480864	1.678514
1	0.858734	4.175607	-1.436332	1	0.297310	2.206953	0.164941
1	-0.321587	5.089058	-2.427021	1	-0.752380	-1.566648	-0.158954
1	-3.640205	0.024708	-1.905549	1	2.223805	-1.960858	-2.085119
1	-5.650168	-1.455029	-1.992750	1	3.981093	-1.800326	-1.887776
1	-6.586840	-2.397109	0.110091	1	3.222345	-3.391915	-1.816516
1	-5.508730	-1.864916	2.288220	1	4.129442	-2.648350	1.773864
1	-3.494037	-0.420875	2.353728	1	4.351283	-3.792638	0.443140
1	-1.979746	-2.421546	1.071488	1	5.096500	-2.198584	0.355259

1	1.557139	-3.085418	1.493408	1	0.100601	3.830039	0.423329
1	0.839808	-2.991001	-0.123222	1	-0.777010	2.431970	-0.191364
1	2.058251	-4.213467	0.226290	1	0.109870	0.084575	2.580272
1	-2.022615	-0.200568	-1.498289	1	-1.308444	0.630714	1.631718
1	-4.943065	-3.869568	-1.229856	1	-2.760902	-2.235067	0.039762
1	-3.985162	-4.420579	0.159137	1	1.421099	-1.285544	-2.154059
1	-5.730836	-4.065093	0.369238	1	2.253083	0.232965	-2.518197
1	-3.348212	1.531322	1.584305	1	3.049973	-1.311546	-2.834261
1	-3.255031	4.000335	1.937808	1	4.917897	-0.061420	0.145184
1	-2.237010	5.464826	0.204466	1	5.077822	-0.832969	-1.437691
1	-1.319766	4.455544	-1.878099	1	4.437881	0.807872	-1.327629
1	-1.379575	1.994748	-2.193101	1	3.801328	-2.273735	0.678150
1	-1.863711	-0.965778	2.019570	1	2.249033	-2.726075	-0.036199
1	-0.245343	-1.603247	2.356537	1	3.729141	-2.836286	-0.999243
1	-0.559024	0.143993	2.435058	1	-2.747384	1.784890	-2.722243
E (CH ₃ CN) = -1461.819353				1	-4.440557	1.255306	-2.678551
NImag = 1 (-168.0)				1	-4.007433	2.887082	-2.074264
System 12 (R = Me; X = Me; Y = CO₂Me)				1	0.514939	-3.404683	-0.798145
102. 12-<i>si</i>,<i>si</i>-c[‡] (-1269.76939036)				1	-1.111699	-3.742820	-0.225534
6	-2.798719	-2.039795	2.251137	1	-0.870628	-2.473056	-1.420766
6	-2.659896	-1.508985	0.848920	1	-2.428413	-1.321177	2.988153
7	-3.000905	-0.250167	0.628863	1	-2.283855	-2.995770	2.382889
6	-3.093575	0.092254	-0.703737	1	-3.866681	-2.198105	2.460432
8	-3.507159	1.391236	-0.815217	E (CH ₃ CN) = -1270.027556			
6	-3.682394	1.847721	-2.156545	NImag = 1 (-142.4)			
8	-2.841252	-0.585771	-1.695599	103. 12-<i>si</i>,<i>si</i>-t[‡] (-1269.76846665)			
6	-0.379584	-1.923264	0.611379	6	2.760046	-2.680044	0.160650
6	-0.437690	-2.928190	-0.523298	6	1.728300	-2.445302	-0.971112
16	0.284639	-0.361772	0.218170	6	2.491702	-1.515061	-1.923913
6	2.188039	-0.010676	0.344458	6	3.092232	-0.477905	-0.953101
6	2.333547	1.536456	0.422625	6	3.623142	-1.379407	0.203021
6	1.881978	2.045245	1.807333	6	0.442923	-1.777823	-0.467865
6	0.353886	2.058825	1.662523	16	0.738735	-0.308282	0.615799
6	-0.214572	0.635157	1.689693	6	2.018885	0.572778	-0.560369
6	1.425178	2.364659	-0.539848	6	-0.857625	0.348248	0.790305
6	0.156021	2.744573	0.288069	6	-2.636137	-1.127406	0.985177
6	3.027252	-0.784715	-0.727809	7	-3.659771	-0.316248	0.834440
6	4.442821	-0.171178	-0.837382	6	-3.925538	0.028015	-0.476769
6	3.205279	-2.240967	-0.242458	8	-3.224503	-0.153564	-1.471380
6	2.392749	-0.782627	-2.133985	6	2.499405	1.952244	0.006828
1	-0.007241	-2.306603	1.565174	6	2.847372	1.922603	1.510050
1	2.471575	-0.416310	1.323470	6	-2.390788	-1.721114	2.344848
1	3.386895	1.773000	0.253163	8	-5.124287	0.665119	-0.553325
1	2.240689	1.425368	2.637895	6	-5.499945	1.086004	-1.863964
1	2.254648	3.064884	1.969265	6	-1.068874	1.257547	1.982740
1	1.962101	3.267456	-0.850134	6	3.749301	2.432199	-0.767849
1	1.169926	1.820218	-1.451922	6	1.388904	2.998718	-0.237828
1	-0.140778	2.613662	2.468660	1	-1.271172	0.690680	-0.157456
				1	1.428587	0.788893	-1.459260

1	3.916958	0.056842	-1.431087	6	-2.994687	-1.139317	0.738626
1	1.861015	-1.070818	-2.702624	6	-2.435430	-1.027972	2.172103
1	3.296187	-2.069479	-2.423857	6	-4.512899	-0.846458	0.790495
1	4.677023	-1.616791	0.023157	6	-2.838092	-2.592715	0.236061
1	3.571270	-0.888130	1.177263	1	0.093503	-2.116720	-1.463968
1	1.432395	-3.385087	-1.452962	1	-2.501687	-0.590523	-1.285108
1	3.384245	-3.546236	-0.083300	1	-3.829005	1.337099	-0.154127
1	2.278565	-2.892748	1.121226	1	-2.597986	1.322320	-2.520344
1	-0.208767	-1.454143	-1.286462	1	-2.938914	2.897199	-1.785753
1	-0.127217	-2.456077	0.171837	1	-2.734119	3.022695	1.048521
1	-2.257864	-1.682251	0.124330	1	-1.689747	1.725174	1.606574
1	1.980116	1.677939	2.131763	1	-0.496635	2.942165	-2.241431
1	3.640008	1.201430	1.735010	1	-0.986590	3.986583	-0.145438
1	3.205175	2.910490	1.823268	1	0.123558	2.739312	0.424173
1	3.594334	2.397730	-1.853169	1	-0.209430	0.433720	-2.481527
1	3.963484	3.473103	-0.499357	1	1.014230	1.203067	-1.418529
1	4.641799	1.844245	-0.529443	1	-1.374704	-1.292209	2.227730
1	1.211786	3.136276	-1.311542	1	-2.553226	-0.018377	2.578708
1	0.441042	2.711156	0.221060	1	-2.979071	-1.713404	2.833065
1	1.684045	3.969295	0.177766	1	-4.957778	-0.820669	-0.211975
1	-4.773874	1.795852	-2.273398	1	-5.015501	-1.641514	1.353457
1	-5.573359	0.234160	-2.547519	1	-4.740940	0.100049	1.291171
1	-6.474434	1.565338	-1.751196	1	-3.346959	-2.728490	-0.726545
1	-0.710593	2.291348	1.864342	1	-1.792136	-2.874594	0.102681
1	-2.151152	1.317155	2.157035	1	-3.288540	-3.291674	0.950554
1	-0.603908	0.852667	2.890785	1	2.409760	-0.274999	-1.822501
1	-1.396275	-2.170790	2.426020	1	4.569592	2.523206	1.322339
1	-2.512427	-0.967632	3.127693	1	3.361379	1.955299	2.494307
1	-3.137861	-2.506362	2.528753	1	5.103398	1.659061	2.800776
E (CH ₃ CN) = -1270.027528				1	0.007873	-2.953514	1.142943
NImag = 1 (-131.8)				1	1.452437	-3.351046	0.221899
104. 12-si, re-c[‡] (-1269.76996595)				1	1.484001	-1.978595	1.313320
				1	2.154042	-2.611104	-2.698071
				1	3.118405	-3.250430	-1.331062
				1	3.898107	-2.312189	-2.605714
6	2.978376	-2.404944	-2.009874	E (CH ₃ CN) = -1270.026881			
6	2.778556	-1.124687	-1.246356	NImag = 1 (-121.6)			
7	3.478400	-0.939046	-0.151663	105. 12-re, si-c[‡] (-1269.77060855)			
6	3.410963	0.328019	0.382195	6	-0.208037	-2.428912	1.401865
8	4.306659	0.452075	1.395440	6	-0.431185	-1.235874	2.360995
6	4.328660	1.727771	2.034686	6	-1.960895	-1.096614	2.375824
8	2.667926	1.260525	0.066518	6	-2.313959	-1.190770	0.875752
6	0.504157	-1.619225	-0.582427	6	-1.403320	-2.369173	0.400377
6	0.852718	-2.512535	0.592670	6	0.229396	0.048929	1.853731
16	-0.370152	-0.179726	-0.148847	16	-0.184405	0.431273	0.093889
6	-0.046796	0.981436	-1.546125	6	-2.085487	0.178415	0.172161
6	-0.886023	2.262922	-1.473344	6	0.468435	2.039674	-0.100405
6	-2.379525	1.961731	-1.656433	6	-0.111814	3.188991	0.696926
6	-2.746830	1.313118	-0.305740	6	-2.786262	0.400296	-1.211046
6	-2.304219	-0.177419	-0.287834				
6	-2.030252	2.253310	0.713136				
6	-0.842072	2.903841	-0.063941				

6	-2.248779	-0.505072	-2.338392	16	-0.614982	-0.224849	0.439154
6	-4.301812	0.133670	-1.042845	6	-2.252367	0.012537	-0.596052
6	-2.636923	1.876183	-1.643498	6	0.564163	-1.412925	-0.007784
6	2.734141	1.603929	0.122725	6	1.048931	-1.562092	-1.428959
7	2.963275	0.310736	0.302288	6	-3.234617	-1.197136	-0.487351
6	2.938019	-0.438933	-0.851901	6	-3.728365	-1.464617	0.948338
8	2.698348	-0.082813	-2.001888	6	-4.462034	-0.917210	-1.389040
6	3.046213	2.529916	1.266922	6	-2.562925	-2.476581	-1.034744
8	3.210481	-1.748754	-0.553131	6	2.525979	-1.162671	1.295402
6	3.259645	-2.617941	-1.683497	7	3.521927	-1.149123	0.437841
1	-2.452226	0.965678	0.842070	6	3.861424	0.098103	-0.043983
1	-3.369249	-1.446389	0.747250	8	3.305873	1.180160	0.147029
1	-2.314772	-0.173217	2.850271	6	2.309769	-2.412070	2.107247
1	-2.409721	-1.939760	2.916138	8	4.971772	0.001525	-0.823367
1	-1.978602	-3.300724	0.433672	6	5.438179	1.235417	-1.366463
1	-1.059425	-2.248136	-0.627991	1	-1.906220	0.046667	-1.636662
1	-0.018212	-1.431616	3.357966	1	-3.835758	1.472361	-0.594071
1	-0.229005	-3.366708	1.967364	1	-1.653030	2.318510	-1.888138
1	0.763961	-2.373004	0.901018	1	-2.483384	3.477129	-0.837846
1	-0.058849	0.911910	2.461326	1	-3.632375	2.404508	1.539799
1	1.321006	-0.033012	1.815538	1	-2.800898	0.912651	1.944917
1	0.524818	2.220321	-1.173874	1	-0.126476	3.475039	-0.038531
1	2.818368	2.025031	-0.881609	1	-1.672004	3.633693	1.785496
1	-1.170116	-0.386919	-2.487899	1	-0.810818	2.180762	2.285149
1	-2.452826	-1.562897	-2.145952	1	0.466846	1.268255	-1.120001
1	-2.742570	-0.245504	-3.282190	1	1.089919	1.429682	0.512686
1	-4.722121	0.701634	-0.203502	1	0.277434	-2.343904	0.478882
1	-4.829855	0.446412	-1.950880	1	2.167624	-0.229135	1.736709
1	-4.528169	-0.925444	-0.886526	1	-2.898846	-1.650913	1.639382
1	-3.019958	2.557176	-0.873876	1	-4.317461	-0.629574	1.341161
1	-1.598247	2.145941	-1.848739	1	-4.372087	-2.352059	0.958949
1	-3.212472	2.054043	-2.559061	1	-4.159160	-0.667564	-2.413330
1	2.303449	-2.632196	-2.216723	1	-5.092088	-1.812901	-1.439297
1	4.039249	-2.307627	-2.386595	1	-5.088442	-0.103222	-1.011048
1	3.485806	-3.609315	-1.284632	1	-2.185004	-2.323186	-2.052551
1	0.461230	4.097290	0.474293	1	-1.726897	-2.806666	-0.413927
1	-1.164804	3.422005	0.469630	1	-3.293198	-3.293442	-1.070549
1	-0.038148	3.030963	1.779986	1	4.683438	1.692939	-2.014556
1	4.138565	2.636850	1.334299	1	5.689373	1.947031	-0.573462
1	2.620984	3.526507	1.125951	1	6.329429	0.984152	-1.944952
1	2.704574	2.117436	2.221038	1	2.074002	-1.957568	-1.401095
E (CH ₃ CN) = -1270.030227				1	0.437708	-2.242859	-2.039616
NImag = 1 (-149.4)				1	1.104988	-0.603720	-1.957083
106. 12-<i>re</i>,<i>si</i>-t[‡] (-1269.77244160)				1	2.421132	-3.307100	1.488036
				1	3.082487	-2.458132	2.888110
				1	1.333158	-2.420488	2.599955
				E (CH ₃ CN) = -1270.030341			
				NImag = 1 (-106.1)			
6	-1.444906	2.601628	1.497710				
6	-0.747066	2.584776	0.117167				
6	-1.939728	2.523732	-0.850035				
6	-2.808483	1.414716	-0.222298				
6	-2.760940	1.787975	1.294324				
6	0.169933	1.370920	-0.072337				

107. 12-<i>re, re</i>-c[‡] (-1269.77248537)				1	-4.253096	3.056967	-0.863638
				1	-2.652352	3.446649	-1.512869
6	-3.172617	2.965951	-0.681159	E (CH ₃ CN) = -1270.028780 NImag = 1 (-131.3)			
6	-2.838079	1.504164	-0.561686				
7	-3.198031	0.885515	0.542381				
6	-3.137235	-0.485077	0.503111	108. 12-<i>re, re</i>-t[‡] (-1269.76805877)			
8	-3.721235	-1.006192	1.615224				
6	-3.735536	-2.430395	1.686296				
8	-2.641805	-1.216601	-0.359434	6	-3.531639	-0.386370	-1.439994
6	-0.487569	1.884214	-0.485780	6	-3.451179	0.100093	0.042029
16	0.234137	0.318974	-0.222905	6	-3.725157	-1.199759	0.825893
6	2.160226	0.206436	-0.097822	6	-2.871622	-2.224713	0.064101
6	2.550692	-1.259315	-0.439730	6	-3.217414	-1.913489	-1.411055
6	2.330470	-1.540570	-1.940802	6	-1.382302	-2.036469	0.374577
6	0.820625	-1.811069	-2.003056	16	-0.683972	-0.424274	-0.205705
6	0.021607	-0.511808	-1.862765	6	-2.099817	0.723122	0.482790
6	0.595721	-2.768315	-0.809169	6	0.901004	-0.376666	0.528655
6	1.687181	-2.373875	0.233430	6	2.547386	-1.651496	-0.279866
6	2.716173	0.803462	1.240370	7	3.617453	-1.088839	0.255583
6	2.103205	0.178004	2.510359	6	4.026823	0.077347	-0.345702
6	0.126513	2.822442	-1.506309	8	3.404959	0.793437	-1.131492
6	4.249341	0.592546	1.281079	6	-1.857064	2.233902	0.151129
6	2.476420	2.329484	1.272092	6	-0.588019	2.732765	0.877394
1	2.534125	0.847222	-0.905800	6	2.204332	-3.038926	0.197648
1	3.605696	-1.383022	-0.180543	8	5.280068	0.406000	0.077319
1	2.659468	-0.720592	-2.590892	6	5.800736	1.614809	-0.471711
1	2.885050	-2.440416	-2.236124	6	1.044958	-0.386770	2.034369
1	2.326299	-3.233031	0.464587	6	-1.717937	2.529708	-1.356037
1	1.242348	-2.049973	1.175833	6	-3.046103	3.055238	0.707510
1	0.515257	-2.266551	-2.953059	1	-2.020534	0.623897	1.572280
1	0.735181	-3.804818	-1.135301	1	-4.231530	0.839264	0.243689
1	-0.420065	-2.681259	-0.412156	1	-3.478018	-1.127206	1.891560
1	0.291924	0.207352	-2.641373	1	-4.786265	-1.468148	0.748524
1	-1.053451	-0.701799	-1.880122	1	-4.542392	-0.211727	-1.823679
1	-0.642049	2.322828	0.499595	1	-2.847529	0.152714	-2.097187
1	1.013093	0.279069	2.537616	1	-3.122203	-3.258403	0.332287
1	2.349052	-0.884124	2.603740	1	-4.095763	-2.493473	-1.713828
1	2.503000	0.683741	3.397268	1	-2.404011	-2.184549	-2.092731
1	4.731996	0.950425	0.363057	1	-1.187696	-2.118735	1.447782
1	4.673338	1.158056	2.118837	1	-0.772554	-2.781524	-0.140571
1	4.527025	-0.455978	1.426492	1	1.423448	0.437048	0.027220
1	2.922941	2.820059	0.398713	1	-0.901186	1.962234	-1.814688
1	1.414178	2.583459	1.296344	1	-2.639528	2.310496	-1.904514
1	2.941496	2.759990	2.166446	1	-1.498458	3.593782	-1.501571
1	-2.730493	0.950652	-1.498429	1	-3.234940	2.828111	1.764156
1	-4.238315	-2.866232	0.817366	1	-2.815982	4.124323	0.635648
1	-2.718753	-2.834553	1.737033	1	-3.973143	2.886711	0.150369
1	-4.280672	-2.673674	2.600542	1	-0.648382	2.546302	1.956461
1	-0.460971	3.746912	-1.538913	1	0.321581	2.259149	0.502214
1	1.165375	3.123080	-1.291306	1	-0.479941	3.813842	0.733319
1	0.112381	2.406590	-2.521826	1	2.250201	-1.392317	-1.300260
1	-2.957495	3.495449	0.251607	1	5.867342	1.559051	-1.563122

1	5.172368	2.472172	-0.208909
1	6.796694	1.730217	-0.038744
1	2.110932	-0.528695	2.253394
1	0.731064	0.545744	2.527053
1	0.502915	-1.213229	2.512001
1	1.252781	-3.393617	-0.207327
1	2.991649	-3.728756	-0.136063
1	2.178317	-3.083866	1.290436

E (CH₃CN) = -1270.029985
NImag = 1 (-159.8)

Ylide Geometries

109. COMe-In (-1021.30492839)

6	-2.730750	-0.382315	-0.459799
6	-2.578446	-1.920366	-0.654912
6	-1.448993	-2.332401	0.313994
6	-1.633268	-1.346816	1.478361
6	-1.803955	-0.000122	0.741500
6	-0.421232	0.602153	0.372086
16	0.324114	-0.489418	-0.999634
6	-0.052947	-2.178639	-0.290348
6	2.037226	-0.426353	-0.991686
1	2.475073	-0.148221	-1.941163
6	-0.391001	2.132900	0.039786
6	1.037466	2.604406	-0.311649
6	-1.338251	2.545522	-1.103831
6	-0.806435	2.888765	1.326966
1	0.273200	0.430014	1.199094
1	-2.303749	0.727211	1.386756
1	-0.797882	-1.350427	2.185780
1	-2.550173	-1.589100	2.031013
1	-3.768043	-0.124939	-0.220622
1	-2.477736	0.162334	-1.370907
1	-1.544837	-3.378724	0.631239
1	-3.505618	-2.436507	-0.382366
1	-2.355157	-2.190264	-1.693336
1	0.729561	-2.333976	0.454701
1	0.103933	-2.844500	-1.144359
1	-1.106849	2.017798	-2.036260
1	-2.389291	2.363045	-0.857840
1	-1.230579	3.618826	-1.300412
1	-0.164659	2.616071	2.172902
1	-0.704411	3.968254	1.165959
1	-1.846379	2.702153	1.612813
1	1.764317	2.283276	0.441363
1	1.376351	2.223701	-1.278071
1	1.054048	3.700052	-0.359517
6	2.773972	-0.629706	0.198607
8	2.262109	-0.867470	1.317637

6	4.296696	-0.558403	0.089084
1	4.651737	-0.355366	-0.926284
1	4.668595	0.224324	0.760180
1	4.725358	-1.506342	0.433427

E (CH₃CN) = -1021.496505
NImag = 0

110. COMe-Out (-1021.29765356)

6	2.481891	-0.060656	1.206868
6	2.569085	-1.616785	1.112981
6	2.234832	-1.954374	-0.361255
6	2.728788	-0.704287	-1.105308
6	2.167046	0.441011	-0.236342
6	0.666026	0.684965	-0.561274
16	-0.307690	-0.806728	0.130430
6	0.731646	-2.153476	-0.593258
6	-1.830546	-1.066205	-0.591395
1	-1.871536	-1.336235	-1.640932
6	0.018823	2.049735	-0.122213
6	-1.217159	2.320350	-1.011512
6	-0.421145	2.089110	1.357612
6	1.023236	3.198252	-0.371708
1	0.551547	0.613235	-1.650179
1	2.699212	1.371841	-0.444573
1	2.404547	-0.659027	-2.151899
1	3.825736	-0.674399	-1.096931
1	3.441687	0.354096	1.532505
1	1.735374	0.260311	1.935757
1	2.739831	-2.868870	-0.695482
1	3.582077	-1.959848	1.348714
1	1.890837	-2.114355	1.814545
1	0.495120	-2.219144	-1.661027
1	0.355373	-3.057248	-0.104820
1	-1.207394	1.357979	1.578087
1	0.418673	1.920261	2.040485
1	-0.824292	3.083714	1.583667
1	1.425530	3.179417	-1.392719
1	0.510225	4.157501	-0.239080
1	1.863997	3.180202	0.329860
1	-0.936650	2.372049	-2.071691
1	-1.977767	1.545571	-0.897843
1	-1.667508	3.281972	-0.738981
6	-2.975711	-0.808199	0.215653
8	-2.946366	-0.330237	1.363896
6	-4.329239	-1.167154	-0.402241
1	-4.256930	-1.561666	-1.421016
1	-4.819808	-1.913679	0.232458
1	-4.969351	-0.277866	-0.406612

E (CH₃CN) = -1021.494838
NImag = 0

111. Ph-In (-1099.68685684)

6	-3.376058	-0.667865	-0.350853
6	-3.021076	-2.164695	-0.605453
6	-1.840703	-2.467626	0.346856
6	-2.126613	-1.532125	1.531448
6	-2.463876	-0.199568	0.827728
6	-1.166826	0.556563	0.430451
16	-0.363575	-0.429250	-1.035273
6	-0.482256	-2.143260	-0.280485
6	1.245121	-0.136813	-1.407958
1	1.347871	0.206937	-2.430915
6	-1.285124	2.090075	0.128694
6	0.126607	2.714198	0.035412
6	-2.062599	2.417675	-1.162529
6	-2.003658	2.773539	1.317800
1	-0.460436	0.462571	1.261716
1	-3.023951	0.452381	1.503507
1	-1.292669	-1.452535	2.238596
1	-3.000759	-1.891923	2.089226
1	-4.427214	-0.568176	-0.059774
1	-3.239215	-0.064155	-1.249807
1	-1.819951	-3.523907	0.644548
1	-3.871494	-2.808916	-0.356420
1	-2.766717	-2.360576	-1.652940
1	0.334087	-2.245445	0.438499
1	-0.263622	-2.788518	-1.136650
1	-1.612181	1.949740	-2.044268
1	-3.109654	2.102734	-1.104943
1	-2.058027	3.501667	-1.327392
1	-1.533516	2.516884	2.275245
1	-1.942486	3.861823	1.202070
1	-3.065660	2.514163	1.377242
1	0.716484	2.501463	0.934620
1	0.687663	2.336327	-0.821269
1	0.042478	3.803473	-0.060174
6	2.413807	-0.182275	-0.560219
6	3.685642	0.026825	-1.153030
6	4.857405	-0.013673	-0.408072
6	4.824593	-0.264331	0.968315
6	3.585526	-0.465902	1.576782
6	2.405733	-0.422457	0.835302
1	3.737029	0.218586	-2.222787
1	5.809914	0.151406	-0.907236
1	5.741604	-0.296916	1.549681
1	3.530311	-0.654206	2.647073
1	1.463448	-0.566609	1.355778

E (CH₃CN) = -1099.890487
NImag = 0

112. Ph-Out (-1099.68669428)

6	2.977617	-0.333238	1.382298
6	2.969660	-1.884376	1.225581
6	2.739982	-2.131128	-0.283275
6	3.423947	-0.912692	-0.921792
6	2.884922	0.251906	-0.065079
6	1.464200	0.663157	-0.532633
16	0.230998	-0.755147	-0.000050
6	1.251713	-2.171339	-0.646043
6	-1.191437	-0.894089	-0.880848
1	-1.092380	-0.974015	-1.960741
6	0.976558	2.092170	-0.130355
6	-0.439339	2.371620	-0.683191
6	0.963422	2.332285	1.392325
6	1.928779	3.123449	-0.785595
1	1.427921	0.613987	-1.628755
1	3.533457	1.128274	-0.158367
1	3.211929	-0.800293	-1.991569
1	4.512330	-0.993582	-0.805501
1	3.909584	-0.000550	1.851524
1	2.163611	0.009098	2.023136
1	3.180898	-3.079991	-0.614191
1	3.934207	-2.307409	1.526690
1	2.202239	-2.362433	1.844374
1	1.100122	-2.182416	-1.731387
1	0.749350	-3.047779	-0.227043
1	0.315058	1.617442	1.911196
1	1.965372	2.270581	1.830164
1	0.575771	3.336098	1.602417
1	1.980382	2.985818	-1.872606
1	1.556233	4.137286	-0.597795
1	2.947673	3.075394	-0.387593
1	-0.507267	2.146169	-1.753916
1	-1.214864	1.795094	-0.174949
1	-0.675903	3.434250	-0.549485
6	-2.495451	-0.599118	-0.322370
6	-3.613399	-0.567776	-1.191809
6	-4.901094	-0.331467	-0.721177
6	-5.136729	-0.102108	0.636969
6	-4.047414	-0.118552	1.511975
6	-2.756962	-0.359748	1.049191
1	-3.455176	-0.741056	-2.254405
1	-5.729717	-0.321252	-1.426298
1	-6.141595	0.087509	1.003596
1	-4.202608	0.057843	2.574468
1	-1.936426	-0.375442	1.762806

E (CH₃CN) = -1099.892075
NImag = 0

113. Me-In (-907.936562515)

6	1.532004	-1.694490	-0.805471	6	-1.523858	1.630812	-0.587175
6	2.756999	-0.729181	-0.832121	6	1.086374	2.458624	-0.390072
6	2.613662	0.136875	0.441583	1	1.123302	2.562171	-1.474947
6	1.913938	-0.824966	1.413321	6	1.482842	-1.382732	-0.059910
6	0.787063	-1.412476	0.538692	6	2.754593	-0.543171	-0.312912
6	-0.402410	-0.420768	0.455773	6	1.463821	-1.799707	1.424377
16	0.152464	1.093591	-0.682140	6	1.602858	-2.656906	-0.931581
6	1.763017	1.390985	0.204627	1	0.297582	-0.434121	-1.580639
6	-0.644151	2.564887	-0.623825	1	-1.026166	-2.382268	-0.408255
1	-1.274023	2.685294	-1.501825	1	-1.910891	-0.577397	-2.181601
6	-1.792803	-0.998702	0.035724	1	-3.113588	-1.402724	-1.176712
6	-2.883199	0.078051	0.241648	1	-2.278641	-1.979631	1.521338
6	-1.844474	-1.485418	-1.427689	1	-0.998437	-0.854462	1.940486
6	-2.153789	-2.187285	0.958977	1	-3.551831	1.009199	-0.811582
1	-0.537340	0.026269	1.449540	1	-3.795563	-0.239878	1.217597
1	0.419940	-2.349356	0.969787	1	-2.576459	0.915185	1.751642
1	1.547261	-0.337861	2.324700	1	-1.306252	1.825931	-1.643888
1	2.608226	-1.619322	1.717280	1	-1.802151	2.580611	-0.122640
1	1.867338	-2.737369	-0.825006	1	1.358397	-0.932880	2.086349
1	0.889804	-1.552401	-1.676357	1	0.651378	-2.500056	1.645710
1	3.589469	0.470527	0.817503	1	2.405457	-2.299228	1.682900
1	3.694074	-1.295635	-0.791412	1	1.656844	-2.403536	-1.997390
1	2.787796	-0.120609	-1.742436	1	2.518545	-3.203112	-0.673292
1	1.533152	1.894364	1.149371	1	0.763742	-3.346342	-0.790252
1	2.267009	2.109438	-0.448032	1	2.776114	-0.135291	-1.330315
1	-1.581957	-0.690493	-2.133884	1	2.842746	0.295572	0.381051
1	-1.171850	-2.331706	-1.602485	1	3.642949	-1.173843	-0.183634
1	-2.859780	-1.821743	-1.670895	6	2.277995	2.926521	0.404111
1	-2.069294	-1.913120	2.017996	1	2.430806	4.003541	0.244582
1	-3.191364	-2.493426	0.778130	1	3.235295	2.436449	0.150790
1	-1.523009	-3.064933	0.783713	1	2.121332	2.786665	1.481555
1	-2.894701	0.432340	1.279672	E (CH ₃ CN) = -908.091755			
1	-2.731631	0.944352	-0.406493	NImag = 0			
1	-3.871818	-0.343951	0.023365	115. Benzaldehyde (-345.573455825)			
6	-1.054997	3.273447	0.641148	6	-0.306822	2.023578	0.000000
1	-1.986335	2.898263	1.101891	6	0.000000	0.575378	0.000000
1	-1.217338	4.338613	0.429544	8	-1.427733	2.495560	0.000000
1	-0.278217	3.229256	1.416252	1	0.587937	2.686041	0.000000

E (CH₃CN) = -908.093183

NImag = 0

114. Me-Out (-907.935591404)

6	-1.760810	-1.072425	1.190889	6	-0.741411	-1.726952	0.000000
6	-2.770904	0.105262	1.039903	6	-1.038837	-0.368317	0.000000
6	-2.621337	0.572482	-0.426409	1	2.133718	0.883551	0.000000
6	-2.246350	-0.729915	-1.149011	1	2.664879	-1.548878	0.000000
6	-1.151504	-1.308231	-0.230127	1	0.822564	-3.213135	0.000000
6	0.204259	-0.608360	-0.499919	1	-1.543491	-2.459933	0.000000
16	0.109226	1.243495	0.214885	1	-2.064154	-0.010987	0.000000

E (CH₃CN) = -345.669004

NImag = 0

116. (*E*)-*N*-benzylidenemethanesulfonamide
(-913.588698314)

6	-0.036867	0.465760	-0.019101
6	-1.472779	0.184759	-0.008847
7	0.846419	-0.468417	-0.057303
1	0.258631	1.521273	0.017872
6	-2.371328	1.259946	0.079587
6	-3.745551	1.029432	0.098108
6	-4.230172	-0.277801	0.026624
6	-3.340676	-1.355360	-0.064517
6	-1.969641	-1.128834	-0.083051
1	-1.986694	2.275622	0.133521
1	-4.435661	1.865345	0.166671
1	-5.301403	-0.459768	0.039475
1	-3.722563	-2.370646	-0.123364
1	-1.265860	-1.951411	-0.158359
16	2.477817	0.076719	-0.131367
8	3.033133	-0.404940	-1.398656
8	2.584322	1.500749	0.224065
6	3.169171	-0.902213	1.211278
1	2.968702	-1.955834	1.012563
1	4.244245	-0.708598	1.217671
1	2.718018	-0.585176	2.153178

E (CH₃CN) = -913.759467
NImag = 0

117. (*E*)-*N*-ethylidenemethanesulfonamide
(-721.846136370)

6	-1.706801	-0.163346	-0.185482
6	-3.130961	0.201251	0.083776
7	-0.748116	0.431433	0.416554
1	-1.515072	-0.957426	-0.918117
16	0.833089	-0.173487	0.037428
8	1.386565	-0.711758	1.281918
8	0.813261	-0.998719	-1.180410
6	1.650153	1.385811	-0.334668
1	1.539241	2.049306	0.523948
1	2.703083	1.152423	-0.508353
1	1.202614	1.820181	-1.230361
1	-3.626598	0.493162	-0.850822
1	-3.199067	1.014881	0.808817
1	-3.669762	-0.675243	0.466339

E (CH₃CN) = -721.969245
NImag = 0

118. (*E*)-methyl benzylidenecarbamate
(-553.575502212)

6	-0.110272	0.563050	0.003450
6	1.309254	0.216478	0.002951
7	-1.038286	-0.327663	-0.013738
6	-2.356012	0.190998	-0.016739
8	-2.694582	1.359203	-0.055697
8	-3.221222	-0.837203	0.027608
6	-4.605269	-0.462603	0.030156
1	-0.360405	1.631548	0.018494
1	-4.835609	0.157664	0.900947
1	-4.855482	0.095167	-0.876661
1	-5.160717	-1.400210	0.069327
6	2.264767	1.245554	0.022904
6	3.625467	0.944869	0.022480
6	4.040644	-0.388077	0.002192
6	3.094787	-1.420603	-0.017617
6	1.737129	-1.123775	-0.017185
1	1.933199	2.281248	0.038521
1	4.359444	1.745528	0.037863
1	5.101261	-0.625140	0.001916
1	3.423191	-2.456164	-0.033264
1	0.986572	-1.907337	-0.031818

E (CH₃CN) = -553.724738
NImag = 0

119. (*E*)-methyl ethylidenecarbamate
(-361.832041)

6	-1.754536	0.232309	0.137944
6	-3.152453	-0.282044	0.037339
1	-3.165875	-1.299690	-0.358501
1	-3.634805	-0.264254	1.023635
1	-3.747452	0.374197	-0.611769
1	-1.617197	1.256733	0.509849
7	-0.749862	-0.482911	-0.199026
6	0.510649	0.162828	-0.087978
8	1.468408	-0.774434	-0.001183
8	0.724576	1.359294	-0.096627
6	2.805228	-0.264904	0.111668
1	2.908897	0.353279	1.007779
1	3.446768	-1.144184	0.175726
1	3.061502	0.336286	-0.764904

E (CH₃CN) = -361.933507
NImag = 0

Optimized Cartesian coordinates and energies of stationary points from Figure S3. The coordinates and energies of Addition TSs have been given above (p. S16 – S18).

120. 1a-c (-1934.86872214)				1	0.458564	-2.687409	-3.591531
				1	1.235844	-1.070251	-3.515000
6	-0.358819	1.146894	1.411543	1	1.893187	-2.430668	-2.568276
6	-1.397761	1.492321	2.482178	6	1.943656	2.165944	-1.854943
6	-2.643281	2.113594	1.839030	6	2.387604	3.484145	-1.968044
6	-3.294038	0.885438	1.174673	6	3.058903	4.090936	-0.904826
6	-2.590161	0.544889	-0.181743	6	3.288138	3.361989	0.262737
16	0.936549	-0.269114	0.351792	6	2.842462	2.043089	0.371375
6	-3.185646	-0.190074	2.301886	1	1.449720	1.707764	-2.710247
6	-1.968595	0.235667	3.183488	1	2.216129	4.033272	-2.890571
6	-3.482752	-0.207512	-1.231430	1	3.406542	5.117037	-0.990769
6	-4.792643	0.608108	-1.407417	1	3.820101	3.819206	1.093541
6	0.258076	-0.290186	-1.099681	1	3.019915	1.461193	1.269590
6	0.104535	-1.678789	-1.746675				
6	0.973600	-1.969720	-2.948410	E (CH ₃ CN) = -1935.234046			
6	-2.809091	-0.214788	-2.621440	NImag = 0			
6	-3.845916	-1.644935	-0.814019				
8	-0.692847	-2.489985	-1.316603	121. 1a-R[‡] (-1934.87562435)			
6	1.734459	-0.048712	-0.573242	6	0.820642	-0.778076	-1.965924
7	1.866015	-0.590802	0.751325	6	2.185418	-0.826442	-2.663343
16	2.536475	-2.050833	0.885337	6	3.070022	0.314075	-2.135585
6	4.218896	-1.777634	1.512412	6	3.487596	-0.224732	-0.751060
6	2.153770	1.427800	-0.680088	6	2.391633	0.056908	0.317555
8	1.851894	-2.814422	1.944621	6	0.949285	-1.099253	-0.138313
8	2.726654	-2.703793	-0.444543	16	3.802260	-1.728137	-1.050761
1	-0.063132	0.471666	-1.817707	6	3.012886	-2.088399	-2.344037
1	-2.283345	1.488162	-0.649600	6	2.872282	-0.035388	1.810430
1	-4.339393	1.085440	0.941667	6	3.756517	1.218236	2.038057
1	-2.419545	2.926361	1.137964	6	-0.661614	-0.446985	0.615936
1	-3.311303	2.514040	2.611761	6	-1.279878	-1.656265	1.315532
1	-4.108158	-0.175144	2.891512	6	-2.092051	-1.346338	2.554861
1	-3.076714	-1.205471	1.914528	6	1.708168	0.064466	2.816995
1	-0.899060	2.167954	3.187067	6	3.686984	-1.300518	2.140797
1	-2.298744	0.493436	4.194995	8	-1.115909	-2.791292	0.904670
1	-1.221672	-0.558906	3.278797	6	-1.697454	0.386068	-0.366131
1	-0.138382	1.999208	0.764354	7	-1.735169	1.768262	-0.018703
1	0.571412	0.745945	1.816869	16	-0.419372	2.602326	-0.325704
1	2.358685	-0.589727	-1.300951	6	-1.054615	4.283656	-0.405463
1	-2.957989	-2.270099	-0.690589	6	-3.112242	-0.200776	-0.327700
1	-4.420434	-1.659539	0.118143	8	0.585403	2.599909	0.794103
1	-4.471992	-2.103377	-1.588520	8	0.213151	2.289538	-1.653438
1	-4.594353	1.672976	-1.582827	1	-0.343207	0.300325	1.337289
1	-5.332220	0.225873	-2.280187	1	1.977634	1.058178	0.174247
1	-5.469949	0.520206	-0.553532	1	4.384143	0.286641	-0.391634
1	-2.499730	0.794354	-2.922940	1	2.551320	1.276363	-2.094446
1	-1.949234	-0.879529	-2.668041	1	3.956667	0.420668	-2.773005
1	-3.522078	-0.574222	-3.371203	1	4.878877	-1.845228	-1.212698
1	4.691659	-2.752639	1.653365	1	3.538929	-2.390421	-0.225180
1	4.782712	-1.187030	0.786528	1	1.970771	-0.731641	-3.734601
1	4.154063	-1.250497	2.466454	1	3.700367	-2.295990	-3.170795

1	2.386689	-2.978609	-2.217279	6	-1.719035	0.399597	-0.337612
1	0.387921	0.216965	-2.093173	7	-1.906052	1.745743	0.114691
1	0.142302	-1.559056	-2.322326	16	-0.640985	2.682880	-0.140569
1	-1.336530	0.209378	-1.385833	6	-1.345949	4.320700	0.087544
1	3.102566	-2.216820	1.996650	6	-3.045047	-0.363040	-0.374988
1	4.601058	-1.376981	1.544572	8	0.443846	2.546231	0.899151
1	3.987416	-1.269808	3.194508	8	-0.087510	2.608723	-1.534676
1	3.193361	2.133019	1.826670	1	-0.183713	0.460824	1.189557
1	4.078192	1.248059	3.085414	1	2.018708	1.020853	0.311802
1	4.662616	1.216360	1.423101	1	4.416809	0.286939	-0.383283
1	1.106038	0.960459	2.640729	1	2.601822	1.577950	-1.892121
1	1.066656	-0.824513	2.793203	1	3.971073	0.792334	-2.708629
1	2.118032	0.126356	3.831520	1	4.838262	-1.707251	-1.526927
1	-0.198427	4.948964	-0.534865	1	3.495899	-2.358518	-0.609267
1	-1.739708	4.361867	-1.250632	1	1.936056	-0.140608	-3.801283
1	-1.570926	4.503077	0.530243	1	3.620844	-1.824427	-3.509935
1	-1.402519	-1.178551	3.393533	1	2.298082	-2.603246	-2.648081
1	-2.687682	-0.438068	2.432085	1	0.406600	0.603367	-2.011319
1	-2.736972	-2.195368	2.790130	1	0.096889	-1.099600	-2.513094
6	-3.387994	-1.432891	-0.935712	1	-1.340313	0.359127	-1.364684
6	-4.682093	-1.954363	-0.940955	1	2.974532	-2.502427	1.658900
6	-5.724542	-1.245212	-0.341771	1	4.535604	-1.728218	1.309620
6	-5.461452	-0.011034	0.255149	1	3.930242	-1.797403	2.964484
6	-4.166230	0.509442	0.258660	1	3.417457	1.814900	2.038305
1	-2.586100	-1.996889	-1.406511	1	4.216107	0.714792	3.175152
1	-4.874981	-2.911426	-1.418625	1	4.805047	0.833706	1.519680
1	-6.734146	-1.647853	-0.348039	1	1.218956	0.699065	2.732327
1	-6.269121	0.554935	0.712855	1	1.082841	-1.085918	2.701784
1	-3.950286	1.479606	0.692228	1	2.200413	-0.305482	3.808235
E (CH ₃ CN) = -1935.231169				1	-0.528694	5.039289	-0.001379
NImag = 1-(18.8)				1	-2.097969	4.489876	-0.684191
122. 1a - <i>r</i> (-1934.87608815)				1	-1.794087	4.371034	1.080872
				1	-2.819912	-1.662076	2.810075
				1	-1.431617	-0.801829	3.505586
				1	-2.484745	0.046252	2.359510
6	0.807795	-0.414790	-2.041175	6	-4.237688	0.254818	0.014936
6	2.160199	-0.403235	-2.760501	6	-5.452694	-0.427053	-0.077559
6	3.087954	0.615869	-2.082177	6	-5.494561	-1.733590	-0.566176
6	3.501647	-0.138301	-0.801510	6	-4.310099	-2.355135	-0.966566
6	2.422045	0.002635	0.309318	6	-3.097471	-1.672107	-0.873803
16	0.935888	-1.041215	-0.288058	1	-4.190474	1.276212	0.375713
6	3.767954	-1.586406	-1.330141	1	-6.370733	0.068227	0.229142
6	2.951007	-1.723244	-2.649578	1	-6.441243	-2.262628	-0.639030
6	2.914942	-0.306642	1.766887	1	-4.328313	-3.370693	-1.353408
6	3.898848	0.835430	2.133313	1	-2.183832	-2.172839	-1.188226
6	-0.589608	-0.348453	0.584208	E (CH ₃ CN) = -1935.232707			
6	-1.138502	-1.437123	1.497520	NImag = 0			
6	-2.043025	-0.922952	2.601124				
6	1.772811	-0.242325	2.801334				
6	3.629379	-1.662727	1.919168				
8	-0.844846	-2.613702	1.385266				

123. **1a-E[‡]** (-1934.86233549)

6	2.897504	2.276568	0.236294
6	2.061436	1.552156	-0.621188
6	1.470632	2.216240	-1.703355
6	1.683109	3.579674	-1.912252
6	2.505933	4.296089	-1.042471
6	3.115603	3.638143	0.027798
6	1.829956	0.063668	-0.420052
7	2.841991	-0.556450	0.415396
16	3.133061	-2.132047	0.113440
8	2.110693	-2.740376	-0.790363
6	0.664179	-0.354560	0.487355
6	0.695088	0.221382	1.904718
8	0.417215	1.392520	2.093789
6	1.016413	-0.740357	3.025892
6	4.688853	-2.146874	-0.815844
8	3.411832	-2.821280	1.388663
16	-1.187671	0.207635	-0.392655
6	-0.962433	-0.954319	-1.830401
6	-2.269783	-1.452424	-2.445306
6	-3.091309	-2.203635	-1.389056
6	-3.692827	-1.054557	-0.556446
6	-2.695100	-0.521208	0.506137
6	-4.124843	-0.030340	-1.644329
6	-3.218946	-0.310888	-2.881401
6	-3.281419	0.491044	1.586141
6	-2.990858	1.976968	1.279786
6	-4.814455	0.317393	1.712491
6	-2.680628	0.153005	2.968565
1	0.532237	-1.434238	0.447157
1	-2.313098	-1.395869	1.044164
1	-4.556344	-1.416929	0.005373
1	-2.498988	-2.913032	-0.799015
1	-3.899400	-2.768259	-1.869724
1	-5.177869	-0.192076	-1.897701
1	-4.040021	1.003138	-1.301436
1	-1.986914	-2.092934	-3.289122
1	-3.824300	-0.639122	-3.732736
1	-2.669288	0.578930	-3.206755
1	-0.332727	-1.788537	-1.506726
1	-0.391600	-0.361114	-2.550188
1	1.702426	-0.413451	-1.400652
1	-1.920966	2.203877	1.313408
1	-3.379065	2.288518	0.304488
1	-3.477808	2.597877	2.040303
1	-5.096042	-0.706678	1.984180
1	-5.173831	0.973188	2.512699
1	-5.349976	0.593566	0.799183
1	-2.860097	-0.895786	3.236373
1	-1.609061	0.351347	3.012228
1	-3.150588	0.774368	3.739275

1	4.960158	-3.188950	-1.001950
1	4.545764	-1.617048	-1.760097
1	5.452639	-1.654751	-0.211581
1	1.082954	-0.189512	3.967043
1	0.215138	-1.489009	3.104257
1	1.942852	-1.282982	2.817526
1	0.850694	1.661790	-2.405776
1	1.217998	4.076517	-2.759953
1	2.679444	5.356888	-1.204027
1	3.767640	4.187049	0.702441
1	3.383322	1.753052	1.051866

E (CH₃CN) = -1935.223909

NImag = 1 (-203.4)

124. **1a-PC** (-1934.92758093)

6	-4.751512	-0.411786	0.124432
6	-3.556315	-0.822574	-0.477026
6	-3.491676	-2.090021	-1.072862
6	-4.599971	-2.935100	-1.056346
6	-5.789139	-2.521133	-0.451186
6	-5.862264	-1.258002	0.137048
6	-2.350063	0.060382	-0.543655
7	-2.293127	1.249313	0.310880
16	-1.698401	2.728471	-0.354052
8	-1.188437	2.526824	-1.716086
6	-1.284566	0.196671	0.525010
6	-1.275662	-0.550125	1.837985
8	-0.379619	-1.353253	2.034751
6	-2.350757	-0.267703	2.859158
6	-3.241155	3.650371	-0.448270
8	-0.844392	3.321852	0.677878
16	2.237085	0.232726	-1.151223
6	2.504178	1.868175	-0.330759
6	3.845796	1.992032	0.404820
6	3.942542	0.948974	1.532488
6	4.208943	-0.360056	0.755191
6	2.874450	-0.908592	0.182929
6	5.265145	0.096459	-0.295493
6	5.055081	1.628121	-0.487442
6	2.850463	-2.404223	-0.287314
6	3.896923	-2.740361	-1.366759
6	3.098664	-3.302277	0.946490
6	1.446138	-2.752516	-0.831074
1	-0.285697	0.348994	0.112827
1	2.134633	-0.856978	0.990915
1	4.626333	-1.122947	1.421185
1	3.046619	0.903523	2.163621
1	4.795683	1.180354	2.183656
1	6.270754	-0.107955	0.090998
1	5.169092	-0.436511	-1.241319

1	3.915014	3.018619	0.787714	6	2.802090	-0.882786	-0.675769
1	5.940191	2.184992	-0.158226	8	1.579312	3.090228	-0.962632
1	4.878202	1.888544	-1.536238	8	0.207414	2.692066	1.073828
1	1.676239	2.073512	0.356681	1	0.336008	-1.594199	-0.139746
1	2.434329	2.594779	-1.146918	1	-2.063894	-1.518666	-1.246246
1	-1.926521	0.184319	-1.541448	1	-4.540634	-0.676294	-1.071866
1	3.794513	-2.093954	-2.245040	1	-2.789839	-0.250333	-3.038615
1	4.920542	-2.646119	-0.989414	1	-4.150346	0.873951	-2.897565
1	3.765271	-3.777894	-1.698411	1	-5.031097	1.472804	-0.300575
1	2.359979	-3.108039	1.732855	1	-3.745537	1.178722	0.857091
1	3.013995	-4.357805	0.661013	1	-2.101743	2.316695	-2.852847
1	4.098328	-3.162266	1.371717	1	-3.776344	3.138718	-1.337375
1	0.670249	-2.492142	-0.103207	1	-2.452778	2.896840	-0.193913
1	1.229293	-2.229629	-1.768764	1	-0.556094	0.401048	-2.216840
1	1.381698	-3.829471	-1.030267	1	-0.271961	1.931347	-1.336015
1	-2.994542	4.631790	-0.859639	1	-2.689565	-0.811446	2.452807
1	-3.927957	3.122551	-1.112599	1	-4.349496	-0.769277	1.811338
1	-3.654445	3.744492	0.556510	1	-3.762208	-2.201565	2.657133
1	-2.148276	-0.847950	3.761286	1	-3.875782	-3.222007	-0.982673
1	-2.378951	0.802659	3.091248	1	-4.337065	-3.715263	0.650940
1	-3.336525	-0.532550	2.460351	1	-5.066778	-2.282468	-0.059604
1	-2.567826	-2.414085	-1.546013	1	-1.427041	-3.454740	0.018113
1	-4.535464	-3.916825	-1.517386	1	-1.045041	-2.602739	1.535931
1	-6.653545	-3.179294	-0.440801	1	-2.251404	-3.871317	1.522811
1	-6.785633	-0.927078	0.604905	1	1.401076	0.574481	-1.243153
1	-4.804520	0.572365	0.579916	1	2.709627	3.215096	2.438370
E (CH ₃ CN) = -1935.268554				1	3.661861	3.598376	0.964654
NImag = 0				1	2.254968	4.617875	1.417807
125. 1b-c (-1934.86975200)				1	2.196021	-2.331942	1.747565
				1	2.711940	-0.725070	2.272066
				1	1.773112	-1.756956	3.396964
6	-0.982422	1.119033	-1.508924	6	2.506776	-1.965393	-1.517239
6	-2.329025	1.656600	-2.008310	6	3.501522	-2.858191	-1.917476
6	-3.257211	0.495845	-2.384618	6	4.816652	-2.679720	-1.483880
6	-3.648707	-0.053697	-0.999455	6	5.123861	-1.596015	-0.660454
6	-2.515419	-0.962098	-0.415626	6	4.126343	-0.703194	-0.263942
16	-1.173462	0.278511	0.137137	1	1.493731	-2.111024	-1.890128
6	-3.960980	1.258589	-0.210329	1	3.249812	-3.687838	-2.573419
6	-3.119698	2.383614	-0.893562	1	5.593810	-3.373383	-1.793792
6	-2.977086	-2.023824	0.644859	1	6.147017	-1.439070	-0.327948
6	-4.133120	-2.846708	0.015921	1	4.349542	0.156957	0.357276
6	0.475786	-0.620441	0.339352	E (CH ₃ CN) = -1935.232246			
6	0.634022	-0.831122	1.861317	NImag = 0			
6	1.911253	-1.465881	2.353391	126. 1b-R[‡] (-1934.85282253)			
6	-1.847808	-3.035503	0.941134	6	-1.034939	1.353598	-1.356780
6	-3.469869	-1.402502	1.965666	6	-2.390455	1.899446	-1.795245
8	-0.272889	-0.548856	2.622035	6	-3.248126	0.750739	-2.338779
6	1.724251	0.146495	-0.283929	6	-3.703806	0.046388	-1.046542
7	2.242192	1.140897	0.616837	6	-2.641478	-0.934884	-0.473934
16	1.566269	2.578930	0.444109				
6	2.671318	3.608539	1.421508				

16	-1.123908	0.142797	0.050906	1	-0.000629	3.653695	2.966352
6	-4.079962	1.243969	-0.123466	1	0.747111	5.443686	1.406654
6	-3.233179	2.454204	-0.623401	1	2.051134	4.839045	-0.624579
6	-3.151588	-1.902575	0.682976	1	2.576450	2.435540	-1.095775
6	-4.693648	-2.051611	0.626062				
6	0.612964	-0.624698	-0.263092				
6	0.650413	-2.035424	0.342845				
6	1.079235	-3.162829	-0.556509				
6	-2.573089	-3.316825	0.451778				
6	-2.780084	-1.428495	2.104954				
8	0.325587	-2.185907	1.508156	6	1.008776	-1.445657	-1.666980
6	1.868958	0.243752	0.331410	6	2.301977	-1.213401	-2.449738
7	2.894478	0.108274	-0.638840	6	2.859547	0.194010	-2.180257
16	3.949785	-1.092578	-0.415865	6	3.447115	0.045468	-0.760367
6	5.553566	-0.256908	-0.421423	6	2.342729	0.228305	0.321698
6	1.540983	1.705024	0.622872	16	1.201334	-1.268129	0.176195
8	3.802672	-1.752224	0.911276	6	4.133383	-1.359507	-0.820362
8	3.986743	-2.000573	-1.592558	6	3.461999	-2.124012	-1.998086
1	0.717845	-0.620935	-1.348616	6	2.858202	0.491979	1.784205
1	-2.275067	-1.546883	-1.304432	6	3.439920	1.927403	1.790317
1	-4.578699	-0.571370	-1.254962	6	-0.647525	-0.837445	0.722324
1	-2.712898	0.094797	-3.035782	6	-1.249424	-2.262548	0.828509
1	-4.126655	1.144020	-2.864472	6	-2.161995	-2.587680	1.977666
1	-5.148524	1.457309	-0.230330	6	1.709866	0.460573	2.812936
1	-3.908124	1.031650	0.933992	6	3.946826	-0.489112	2.261261
1	-2.180977	2.667082	-2.549543	8	-0.937974	-3.087023	-0.016353
1	-3.885128	3.256951	-0.982128	6	-1.507858	0.118164	-0.158744
1	-2.603961	2.881901	0.164339	7	-2.725609	0.126357	0.610225
1	-0.528328	0.851923	-2.186293	16	-4.070659	-0.311457	-0.180799
1	-0.377032	2.135849	-0.976130	6	-5.090801	1.186594	-0.191586
1	-1.698935	-1.415413	2.264599	6	-0.921443	1.517835	-0.327916
1	-3.182001	-0.434721	2.329656	8	-3.822699	-0.657610	-1.605939
1	-3.207062	-2.126163	2.834013	8	-4.838842	-1.285023	0.633647
1	-5.039775	-2.444157	-0.337176	1	-0.509879	-0.389043	1.704115
1	-4.995523	-2.772617	1.392749	1	1.720851	1.081385	0.039401
1	-5.223301	-1.116980	0.832532	1	4.187284	0.826513	-0.565914
1	-2.817235	-3.684301	-0.552926	1	2.112343	0.990243	-2.258959
1	-1.493649	-3.354471	0.592164	1	3.663349	0.416334	-2.892587
1	-3.012300	-4.016220	1.171819	1	5.205651	-1.232683	-1.001459
1	2.089850	-0.243972	1.291115	1	4.039975	-1.913679	0.113509
1	5.647636	0.308803	-1.350131	1	2.045057	-1.369707	-3.504507
1	5.607714	0.409878	0.441255	1	4.167478	-2.254175	-2.825477
1	6.329966	-1.023430	-0.363859	1	3.119981	-3.123399	-1.708768
1	2.043890	-2.943192	-1.033934	1	0.236946	-0.739796	-1.972076
1	1.148312	-4.085379	0.023109	1	0.612394	-2.456835	-1.768198
1	0.339987	-3.283566	-1.361722	1	3.591983	-1.525681	2.274088
6	0.831577	2.058933	1.779725	1	4.851859	-0.440076	1.649138
6	0.540775	3.396865	2.059225	1	4.234152	-0.232510	3.287240
6	0.965597	4.401613	1.187680	1	2.688489	2.663576	1.483398
6	1.696009	4.059862	0.045675	1	3.767111	2.183905	2.804109
6	1.986831	2.722761	-0.231176	1	4.310486	2.032135	1.134643
1	0.521196	1.282428	2.475560	1	0.896435	1.137904	2.536392

E (CH₃CN) = -1935.224662

NImag = 1 (-25.4)

127. **1b-*r*** (-1934.86589955)

1	1.304419	-0.548970	2.947363	6	-2.397819	-1.868560	2.426368
1	2.088695	0.779272	3.790197	1	0.556186	-0.006385	-1.479193
1	-1.640820	-0.333184	-1.151614	1	-2.124067	-1.823715	-0.134447
1	-5.224952	1.520473	0.838839	1	-4.046090	-1.404520	-1.400732
1	-4.584456	1.954354	-0.780453	1	-1.561250	-0.791479	-2.306685
1	-6.055821	0.935972	-0.638962	1	-2.959332	-0.379864	-3.293664
1	-1.900268	-2.029676	2.881304	1	-5.394615	0.510561	-1.386449
1	-3.182883	-2.288520	1.696484	1	-4.414894	1.157962	-0.088629
1	-2.132809	-3.665647	2.160651	1	-1.739675	1.770521	-3.002058
6	-0.528317	1.993581	-1.585340	1	-4.192947	1.750255	-3.046316
6	-0.029586	3.291729	-1.742838	1	-3.827951	2.819888	-1.691731
6	0.081312	4.135573	-0.638072	1	-0.493173	2.056780	-1.055591
6	-0.338242	3.683488	0.618174	1	-2.016839	2.450271	-0.281530
6	-0.845562	2.393012	0.766948	1	-1.971067	-2.774031	1.986996
1	-0.647112	1.356191	-2.459374	1	-1.561433	-1.221328	2.709909
1	0.255532	3.644952	-2.730708	1	-2.927212	-2.144875	3.345237
1	0.465627	5.145247	-0.755998	1	-4.819022	0.502997	1.693012
1	-0.291338	4.348064	1.477456	1	-4.241974	-0.198115	3.197264
1	-1.236572	2.063086	1.725484	1	-3.183040	0.873128	2.282604
E (CH ₃ CN) = -1935.233623				1	-5.316640	-1.681119	0.541328
NImag = 0				1	-4.186322	-3.046952	0.666595
128. 1b-E[‡] (-1934.85696499)				1	-5.012698	-2.441868	2.106726
6	1.313318	2.210677	1.704297	1	1.846589	-0.360733	1.282687
6	1.766135	1.649002	0.503054	1	5.589494	-0.139474	-1.213372
6	2.198916	2.504464	-0.520396	1	5.416115	0.355632	0.504063
6	2.156626	3.889533	-0.353638	1	6.253217	-1.177110	0.090626
6	1.690580	4.440408	0.843716	1	1.943907	-2.827332	-1.706003
6	1.274518	3.597015	1.874946	1	0.398570	-3.729132	-1.622595
6	1.793919	0.138267	0.305809	1	0.538941	-2.214871	-2.588661
7	2.789370	-0.315968	-0.639056	1	1.006492	1.557118	2.517802
16	3.886155	-1.393462	-0.091449	1	0.932022	4.015925	2.817875
6	5.452318	-0.487793	-0.188368	1	1.666580	5.518938	0.976681
6	0.602589	-0.428025	-0.475779	1	2.501397	4.541016	-1.153023
6	0.491785	-1.956842	-0.434165	1	2.598064	2.060033	-1.427495
8	0.116208	-2.489304	0.596063	E (CH ₃ CN) = -1935.223900			
6	0.847506	-2.733662	-1.674494	NImag = 1 (132.2)			
8	3.690453	-1.753111	1.333912	129. 1b-PC (-1934.92375565)			
8	4.019958	-2.499884	-1.069558	6	4.416405	-2.341367	-1.254798
16	-1.187762	0.300150	0.349245	6	3.046765	-1.978973	-1.873422
6	-2.640582	-0.889276	0.101235	6	3.191071	-0.467928	-2.126464
6	-3.451304	-0.516365	-1.166627	6	3.813741	0.034062	-0.804074
6	-2.477452	-0.194246	-2.327262	6	4.891345	-1.053617	-0.517425
6	-2.267369	1.320873	-2.154546	6	2.702907	0.185699	0.269705
6	-1.497040	1.676095	-0.852781	16	2.047111	-1.496826	0.746057
6	-4.366728	0.751811	-1.098230	6	1.870061	-2.258904	-0.928118
6	-3.728748	1.791077	-2.054122	6	3.030502	1.049771	1.535870
6	-3.378513	-1.163082	1.462616	6	1.780073	1.126745	2.440358
6	-3.936638	0.083362	2.183171	6	4.211688	0.520379	2.373347
6	-4.541045	-2.137225	1.165880	6	3.356087	2.489585	1.075752

8	-1.643448	-2.463722	-0.671105	Optimized Cartesian coordinates and energies of stationary points from Figure S4 (The coordinates and energies of Addition TSs have been given above; p. S46 – S51)			
6	-1.681916	-2.001798	0.452555				
6	-1.557461	-2.839650	1.701104				
6	-1.843351	-0.495805	0.670423				
7	-3.124918	0.202579	0.428177				
16	-4.534616	-0.683735	-0.042944	130. 5a-c (-2013.2820016)			
8	-4.592785	-0.843839	-1.498498	6	3.705533	-1.926180	-0.576813
6	-2.021009	0.385016	-0.528681	6	2.675137	-3.039093	-0.937834
6	-1.416337	1.742450	-0.660719	6	1.820984	-2.434886	-2.079898
6	-1.565464	2.719564	0.332775	6	2.758436	-1.413997	-2.735708
6	-0.961490	3.968379	0.189668	6	3.390293	-0.721801	-1.514794
6	-0.202664	4.258069	-0.947431	6	2.486882	0.388705	-0.900367
6	-0.056959	3.292306	-1.945031	16	0.933600	-0.495569	-0.208351
6	-0.663371	2.043103	-1.803310	6	0.577390	-1.723996	-1.561984
8	-4.639170	-1.840783	0.854288	6	-0.658424	0.568295	-0.427781
6	-5.776793	0.527192	0.439353	1	-0.830976	0.507910	-1.504921
1	-1.334066	-0.105041	1.549728	6	3.208463	1.301806	0.192554
1	1.865821	0.702947	-0.216672	6	2.839564	2.777999	-0.065996
1	4.276878	1.015731	-0.947796	6	2.848917	0.928754	1.647436
1	2.243480	0.025846	-2.375021	6	4.751371	1.218593	0.068521
1	3.884472	-0.292340	-2.959219	6	-1.776399	-0.272213	0.361418
1	5.858528	-0.719154	-0.910654	7	-1.316701	-1.606794	0.653708
1	5.021633	-1.235783	0.549284	1	2.147888	1.030977	-1.720490
1	2.858531	-2.534520	-2.801360	1	4.307762	-0.213168	-1.815240
1	5.120550	-2.614275	-2.049333	1	2.246307	-0.723760	-3.417754
1	4.343211	-3.198972	-0.577829	1	3.543427	-1.923502	-3.308400
1	0.927805	-1.927556	-1.377095	1	4.726257	-2.271324	-0.774173
1	1.776147	-3.331877	-0.729875	1	3.662458	-1.663838	0.482433
1	4.055950	-0.517588	2.685588	1	1.468574	-3.201233	-2.781076
1	5.158731	0.574770	1.826757	1	3.188702	-3.939880	-1.289156
1	4.322718	1.129218	3.278994	1	2.059105	-3.324274	-0.078785
1	2.546152	2.909719	0.467241	1	0.066167	-1.185620	-2.366773
1	3.486442	3.137595	1.950745	1	-0.133464	-2.378371	-1.054812
1	4.282707	2.541937	0.494722	1	-1.977074	0.308750	1.268478
1	0.909080	1.490713	1.882207	1	1.787168	1.049268	1.873822
1	1.526245	0.153352	2.872328	1	3.112177	-0.104572	1.892862
1	1.960056	1.820700	3.270374	1	3.402532	1.583425	2.330254
1	-2.112120	-0.185148	-1.452435	1	5.109511	1.531391	-0.919148
1	-5.689473	0.711464	1.510545	1	5.191332	1.904185	0.800811
1	-5.614985	1.442552	-0.132126	1	5.144012	0.220338	0.280660
1	-6.749188	0.091876	0.197433	1	3.147487	3.087619	-1.073033
1	-0.709370	-2.497185	2.305300	1	1.772061	2.965988	0.034527
1	-2.470227	-2.730632	2.298121	1	3.359569	3.423797	0.650886
1	-1.418685	-3.887529	1.428802	16	-0.794771	-1.882687	2.149776
1	-0.558311	1.296357	-2.586882	8	0.259765	-2.921029	2.095985
1	0.521231	3.512502	-2.838333	8	-0.483623	-0.623391	2.894033
1	0.263586	5.233159	-1.059026	6	-2.168177	-2.644404	3.059473
1	-1.087534	4.719348	0.965087	1	-1.825443	-2.877251	4.070497
1	-2.171233	2.499822	1.207253	1	-3.003158	-1.940681	3.096134
E (CH ₃ CN) = -1935.264976				1	-2.462135	-3.556706	2.537201
NImag = 0				6	-0.574004	2.011866	-0.021542

6	-0.655697	3.009112	-1.005671	6	-3.336964	2.400552	1.632594
6	-0.677467	4.359685	-0.654841	6	-3.313465	-1.823053	-0.067934
6	-0.613036	4.730103	0.689099	6	-4.855283	-1.949115	-0.153689
6	-0.535254	3.744826	1.677537	6	-2.736786	-2.780414	-1.131927
6	-0.523373	2.394270	1.331851	6	-2.888229	-2.311751	1.332806
1	-0.716952	2.724227	-2.053500	8	0.792392	3.732849	-1.582295
1	-0.747641	5.118480	-1.429446	8	1.495315	3.447277	0.817599
1	-0.629743	5.780693	0.966366	1	0.155924	0.214668	-1.464684
1	-0.491343	4.028451	2.725503	1	-2.592597	-0.295990	-1.467054
1	-0.480627	1.630707	2.105119	1	-4.832816	0.397461	-0.626245
6	-3.045794	-0.258292	-0.493885	1	-3.075329	2.057241	-1.749250
6	-3.485153	-1.413547	-1.150553	1	-4.435413	2.748521	-0.852748
6	-4.632279	-1.387175	-1.945873	1	-5.252241	1.337452	1.477304
6	-5.361129	-0.205768	-2.094303	1	-3.945792	0.305635	2.024035
6	-4.937856	0.949236	-1.433827	1	-2.402549	3.771550	0.174344
6	-3.789969	0.921884	-0.640407	1	-3.986731	3.240865	1.897022
1	-2.927276	-2.331818	-1.001045	1	-2.642174	2.262057	2.467696
1	-4.962818	-2.295619	-2.444008	1	-0.803381	2.208632	-0.792860
1	-6.257216	-0.187312	-2.709469	1	-0.519579	2.431910	0.926886
1	-5.506527	1.871198	-1.527885	1	1.208800	1.158964	1.039810
1	-3.477352	1.823873	-0.120214	1	-1.803215	-2.397730	1.427768
E (CH ₃ CN) = -2013.657538				1	-3.251437	-1.661123	2.134350
NImag = 0				1	-3.305952	-3.310041	1.505198
131. 5a-R[‡] (-2013.2645874)				1	-5.244374	-1.647030	-1.132773
6	2.887048	-0.540348	1.952476	1	-5.123197	-3.001763	-0.013000
6	2.733275	-0.228084	0.597609	1	-5.373554	-1.373780	0.619333
6	3.709685	-0.666509	-0.306424	1	-3.090275	-2.509047	-2.134551
6	4.788720	-1.431907	0.130524	1	-1.647349	-2.781586	-1.144901
6	4.923130	-1.756455	1.484261	1	-3.068051	-3.805539	-0.931053
6	3.972342	-1.300928	2.396593	1	3.254469	4.948166	-0.967807
6	1.574323	0.653837	0.132304	1	4.103403	3.497386	-0.330480
7	1.986762	1.563385	-0.889817	1	3.614749	3.568052	-2.054610
16	1.759313	3.124728	-0.622223	1	0.697745	-1.563474	-2.772177
6	3.355017	3.862475	-1.036125	1	1.206078	-3.961373	-3.110958
6	0.340452	-0.230754	-0.486031	1	1.356133	-5.491982	-1.153999
6	0.561733	-1.710745	-0.626226	1	1.025303	-4.590709	1.140905
6	0.760539	-2.228614	-1.914718	1	0.564748	-2.192866	1.479143
6	1.050639	-3.580646	-2.105235	1	3.621403	-0.372904	-1.347441
6	1.135433	-4.438131	-1.008487	1	5.536046	-1.767591	-0.584536
6	0.945622	-3.932561	0.280164	1	5.771057	-2.345410	1.824814
6	0.672144	-2.579726	0.470589	1	4.079561	-1.523455	3.455566
16	-1.249927	0.196134	0.500384	1	2.159044	-0.171711	2.673477
6	-2.857631	-0.337697	-0.404938	E (CH ₃ CN) = -2013.648636			
6	-3.923484	0.767034	-0.149948	NImag = 1 (-34.6)			
6	-3.536009	2.127796	-0.757334	132. 5a-t (-2013.27608473)			
6	-2.597382	2.701899	0.308787	6	-4.293462	0.354735	1.549274
6	-1.231396	2.038568	0.197376	6	-3.571183	1.398514	2.454568
6	-4.186407	1.124948	1.342799	6	-2.718666	2.253705	1.487835

6	-3.487461	2.167426	0.164486	6	2.428978	0.049894	1.387199
6	-3.843994	0.671059	0.093429	6	3.672460	-0.458807	0.997096
6	-2.677364	-0.191827	-0.457496	6	4.422656	-1.245693	1.871454
16	-1.197014	-0.049464	0.752431	6	3.943236	-1.535378	3.150857
6	-1.295705	1.739593	1.289523	6	2.709141	-1.023287	3.554900
6	0.433310	0.072301	-0.298677	6	1.963632	-0.232836	2.677820
1	0.086736	0.696628	-1.123423	1	4.036513	-0.212451	0.005824
6	-3.032601	-1.698002	-0.822244	1	5.387940	-1.632235	1.553637
6	-2.288208	-2.085983	-2.117623	1	4.530835	-2.145831	3.831942
6	-2.680726	-2.715198	0.283958	1	2.333090	-1.226389	4.554690
6	-4.545580	-1.837344	-1.122085	1	1.013196	0.180366	3.013814
6	1.601074	0.905987	0.441415				
7	2.406814	1.462790	-0.606071	E (CH ₃ CN) = -2013.651503			
1	-2.311806	0.299184	-1.366039	NImag = 0			
1	-4.666379	0.520713	-0.608124				
1	-2.912650	2.529774	-0.695026	133. 5a -E [‡] (-2013.27504969)			
1	-4.410417	2.757169	0.221904				
1	-5.379530	0.472500	1.624646	6	-0.947219	2.420063	-0.024536
1	-4.071185	-0.672578	1.846840	6	-0.887022	1.301507	-0.870032
1	-2.608908	3.285475	1.841861	6	-1.206193	1.452897	-2.230266
1	-4.302445	2.032930	2.965735	6	-1.562084	2.704115	-2.733101
1	-2.961809	0.927433	3.233752	6	-1.592167	3.817925	-1.891066
1	-0.758353	2.345663	0.549842	6	-1.284366	3.672989	-0.536809
1	-0.737239	1.752457	2.229131	6	-0.571530	-0.071776	-0.373708
1	1.120572	1.683961	1.045554	16	1.295018	-0.060194	0.711641
1	-1.601759	-2.799657	0.438022	6	2.766475	0.066099	-0.486845
1	-3.146607	-2.472037	1.244385	6	3.891942	-0.883767	0.006925
1	-3.040521	-3.706217	-0.014612	6	3.455373	-2.360939	-0.030333
1	-4.872837	-1.168604	-1.926295	6	2.660540	-2.498694	1.274336
1	-4.737553	-2.861944	-1.458029	6	1.272884	-1.881118	1.102326
1	-5.173255	-1.657814	-0.243642	6	3.546401	-1.760123	2.306410
1	-2.584252	-1.434577	-2.949002	6	4.336066	-0.695946	1.485380
1	-1.204540	-2.026235	-2.010885	6	3.181422	1.572236	-0.768165
1	-2.537607	-3.115771	-2.398041	6	2.905900	2.533374	0.408020
16	1.668261	2.650109	-1.398449	6	-1.670871	-0.818863	0.442743
8	0.951197	2.195689	-2.632919	7	-2.576983	-1.159199	-0.626498
8	0.820094	3.515921	-0.512122	16	-2.084438	-2.429063	-1.509856
6	3.062368	3.638664	-1.966976	8	-1.281036	-3.410197	-0.716367
1	2.665526	4.427966	-2.609010	6	-2.349496	0.012013	1.520599
1	3.573093	4.060774	-1.100412	6	-1.756449	0.157543	2.781791
1	3.734967	2.989759	-2.530175	6	-2.365985	0.920723	3.779169
6	0.881528	-1.262272	-0.828087	6	-3.590199	1.543572	3.528935
6	1.299475	-1.311757	-2.168225	6	-4.195716	1.392280	2.279958
6	1.805460	-2.497316	-2.703289	6	-3.580841	0.632644	1.283640
6	1.892337	-3.645822	-1.914671	6	-3.656863	-3.205751	-1.927936
6	1.489895	-3.599833	-0.578439	8	-1.463320	-2.029350	-2.805283
6	1.000723	-2.412233	-0.034012	6	4.688839	1.660966	-1.107416
1	1.240762	-0.409712	-2.770764	6	2.412893	2.073793	-2.008541
1	2.130348	-2.521276	-3.740040	1	-0.204656	-0.717521	-1.168775
1	2.279200	-4.570175	-2.335645	1	2.391619	-0.351884	-1.427979
1	1.570517	-4.484522	0.047405	1	4.729885	-0.728019	-0.675386
1	0.730439	-2.377196	1.017365	1	2.877536	-2.628763	-0.922324

1	4.343120	-3.004789	-0.004085	6	-3.753461	1.748159	2.155324
1	5.413499	-0.876015	1.564596	6	2.207583	-1.079235	-0.250959
1	4.159861	0.317651	1.851850	7	1.764592	-0.614809	1.079321
1	2.492223	-3.545550	1.553293	1	-2.474641	-0.183030	0.876287
1	4.234995	-2.468602	2.778668	1	-5.001660	-0.381470	1.121540
1	2.952654	-1.310909	3.109886	1	-3.224022	-2.345970	0.738178
1	0.706778	-2.399399	0.321039	1	-4.928442	-2.705460	0.405508
1	0.702701	-1.937673	2.033426	1	-6.446575	-0.558107	-0.720083
1	-1.234136	-1.704446	0.917700	1	-5.334027	0.566299	-1.492566
1	1.835946	2.646405	0.605653	1	-3.759394	-3.322905	-1.682835
1	3.391539	2.214727	1.335635	1	-5.823021	-2.244310	-2.201122
1	3.293417	3.527187	0.156407	1	-4.741390	-1.125301	-3.032386
1	4.961921	1.017597	-1.951753	1	-1.644160	-2.114828	-1.198946
1	4.920746	2.691141	-1.398762	1	-2.236943	-1.765533	-2.837053
1	5.330825	1.408290	-0.257441	1	1.622090	-1.898549	-0.667301
1	2.653451	1.468219	-2.891069	1	-4.068634	2.623168	-1.201916
1	1.331730	2.047465	-1.865883	1	-5.339735	2.245159	-0.023061
1	2.692465	3.110048	-2.230774	1	-4.297481	3.649528	0.222759
1	-3.444556	-4.026207	-2.617027	1	-3.065489	1.151600	2.765697
1	-4.123527	-3.575942	-1.014003	1	-3.757325	2.769248	2.555245
1	-4.290478	-2.458150	-2.407815	1	-4.764293	1.346602	2.284952
1	-1.203652	0.575551	-2.871019	1	-1.178326	1.872411	1.173214
1	-1.817404	2.807238	-3.784281	1	-1.566883	2.582155	-0.404726
1	-1.861226	4.793930	-2.286514	1	-1.983180	3.448380	1.078087
1	-1.318002	4.533415	0.126004	16	0.498016	-1.465978	1.860661
1	-0.731849	2.311655	1.033636	8	-0.310383	-0.470397	2.571913
1	-4.044478	0.497003	0.312957	8	-0.158137	-2.415303	0.944487
1	-5.153473	1.866484	2.080102	6	1.464194	-2.408086	3.051282
1	-4.071740	2.133603	4.304579	1	0.757289	-3.016989	3.619168
1	-1.891618	1.017512	4.752643	1	2.167033	-3.044251	2.510057
1	-0.812072	-0.338946	2.998075	1	1.988007	-1.709469	3.704469
				6	1.948832	1.575608	-0.201123
				6	2.532044	2.231970	0.887488
				6	3.020500	3.532171	0.747323
				6	2.930066	4.188353	-0.480583
134. 5a -PC (-2013.34282620)				6	2.341025	3.540717	-1.569284
				6	1.850198	2.243830	-1.429585
6	-5.406555	-0.423136	-1.040502	1	2.585255	1.723334	1.844701
6	-4.998907	-1.536932	-2.050623	1	3.467034	4.033945	1.601813
6	-3.799498	-2.263050	-1.398305	1	3.310006	5.200753	-0.588590
6	-4.077537	-2.080030	0.104223	1	2.260344	4.047387	-2.527256
6	-4.464701	-0.585794	0.189312	1	1.383973	1.744815	-2.275622
6	-3.180276	0.286883	0.182039	6	3.669711	-1.152033	-0.536678
16	-2.363816	0.189950	-1.496978	6	4.637797	-0.619135	0.323725
6	-2.446986	-1.636642	-1.769256	6	5.991890	-0.705550	0.000161
6	1.396380	0.190920	-0.097789	6	6.396447	-1.323695	-1.184311
1	0.368666	0.086858	-0.454023	6	5.437537	-1.861520	-2.044819
6	-3.309988	1.768722	0.673794	6	4.084256	-1.779361	-1.720037
6	-1.925916	2.452628	0.621320	1	4.323922	-0.145647	1.247226
6	-4.314126	2.612389	-0.134476	1	6.733071	-0.289181	0.677261

E (CH₃CN) = -2013.647108

NImag = 1 (-155.5)

1	7.452080	-1.389700	-1.433475
1	5.742514	-2.350138	-2.966294
1	3.340102	-2.203998	-2.390263

E (CH₃CN) = -2013.695123

NImag = 0

135. **5b-c** (-2013.28158901)

6	1.391233	-1.719219	-1.173895
6	2.744000	-2.427170	-1.051690
6	3.852587	-1.553948	-1.646102
6	3.985595	-0.452014	-0.577265
6	2.862618	0.628507	-0.734726
16	1.292428	-0.240675	-0.051234
6	3.978264	-1.285281	0.743957
6	3.186365	-2.594146	0.422567
6	3.179143	2.049063	-0.138013
6	4.651494	2.421581	-0.448026
6	-0.344027	0.554764	-0.625126
6	-0.718591	1.723197	0.260243
6	2.311104	3.103984	-0.853274
6	2.973724	2.144092	1.386169
6	-1.376076	-0.636333	-0.541827
7	-1.179249	-1.216190	0.765043
16	-1.263745	-2.811309	0.908235
6	-2.948059	-3.252136	1.419963
6	-2.778394	-0.101515	-0.857505
8	-1.067301	-3.514961	-0.399714
8	-0.391908	-3.233008	2.026744
1	-0.196387	0.886018	-1.658227
1	2.681324	0.762560	-1.807685
1	4.933139	0.073561	-0.692286
1	3.625342	-1.169825	-2.648124
1	4.791519	-2.117974	-1.712120
1	5.013316	-1.521967	1.012175
1	3.551150	-0.744902	1.591874
1	2.631053	-3.391310	-1.559958
1	3.839312	-3.467968	0.514329
1	2.333111	-2.756785	1.089406
1	1.213015	-1.361907	-2.194432
1	0.576592	-2.382451	-0.871390
1	1.932106	1.983049	1.677840
1	3.597358	1.425799	1.927826
1	3.254583	3.146578	1.729394
1	4.902660	2.267824	-1.504730
1	4.798289	3.484539	-0.228326
1	5.367867	1.864385	0.163067
1	2.512103	3.110371	-1.932293
1	1.244868	2.941864	-0.700530

1	2.542556	4.103503	-0.468241
1	-1.134469	-1.331834	-1.358030
1	-3.159556	-2.761779	2.372295
1	-3.652667	-2.920934	0.653964
1	-2.993958	-4.337679	1.534850
6	-1.182279	2.902176	-0.341314
6	-1.620229	3.976132	0.433959
6	-1.594940	3.886869	1.825978
6	-1.145438	2.712915	2.434036
6	-0.716709	1.632522	1.661659
1	-1.215403	2.974639	-1.425820
1	-1.980533	4.879084	-0.051288
1	-1.930483	4.723335	2.433222
1	-1.138601	2.629642	3.517546
1	-0.425482	0.698967	2.129887
6	-3.170364	0.093337	-2.188395
6	-4.440040	0.583433	-2.497195
6	-5.339987	0.881232	-1.471978
6	-4.961185	0.681342	-0.142737
6	-3.689168	0.194979	0.162122
1	-2.480805	-0.157421	-2.993474
1	-4.730456	0.720669	-3.535938
1	-6.332339	1.256853	-1.708139
1	-5.659793	0.903242	0.660332
1	-3.384679	0.026917	1.189945

E (CH₃CN) = -2013.661111

NImag = 0

136. **5b-R[‡]** (-2013.25704571)

6	1.395008	2.453498	-0.136800
6	2.686361	2.626306	0.677737
6	2.947724	1.412835	1.594000
6	3.585012	0.399583	0.618293
6	2.503628	-0.344135	-0.221835
16	0.976696	0.704574	-0.622413
6	4.620860	1.300080	-0.095661
6	3.951734	2.691597	-0.222835
6	2.923442	-1.138908	-1.511541
6	3.141842	-0.255343	-2.759046
6	-0.490054	0.276901	0.635666
6	-0.205826	-0.904557	1.507345
6	4.215667	-1.923800	-1.183353
6	1.828188	-2.173723	-1.851319
6	-1.827641	0.296558	-0.284771
7	-2.732162	-0.748365	0.064605
16	-2.833570	-1.948501	-0.990647
6	-4.256390	-1.596742	-2.067440
6	-2.458232	1.677000	-0.093378

8	-1.657929	-1.988182	-1.928653	137. 5b -E [‡] (-2013.26301747)			
8	-3.175603	-3.211115	-0.306184				
1	-0.467866	1.172066	1.260411	6	2.082459	3.066907	0.191551
1	2.059413	-1.075108	0.462745	6	1.643696	1.953066	0.917258
1	4.097349	-0.397333	1.167543	6	1.001198	2.167541	2.145370
1	2.056546	1.035520	2.103374	6	0.770162	3.460160	2.620935
1	3.678625	1.680566	2.365379	6	1.190604	4.563803	1.875968
1	5.494235	1.369194	0.563454	6	1.852804	4.360845	0.662888
1	4.984976	0.913296	-1.046189	6	1.923018	0.534739	0.418944
1	2.561414	3.550550	1.252903	7	2.796630	0.539305	-0.713306
1	4.626616	3.485181	0.113172	16	3.667465	-0.806869	-0.936772
1	3.689455	2.927024	-1.260536	8	3.120779	-1.669708	-2.019968
1	0.512338	2.794608	0.408587	6	0.667235	-0.300285	-0.074718
1	1.432642	3.010188	-1.076985	16	-1.167893	0.630919	0.303501
1	1.716271	-2.908079	-1.046776	6	-0.990873	1.962332	-0.991744
1	0.841636	-1.733281	-2.034756	6	-1.939206	1.836662	-2.184033
1	2.109416	-2.718857	-2.759465	6	-2.025882	0.370684	-2.661484
1	3.871367	0.545041	-2.609968	6	-3.095394	-0.215592	-1.718046
1	3.507131	-0.879441	-3.582201	6	-2.499533	-0.567670	-0.321897
1	2.202859	0.197149	-3.095139	6	-4.181248	0.879738	-1.815580
1	5.083930	-1.277393	-1.026830	6	-3.407323	2.218868	-1.836355
1	4.087248	-2.546200	-0.289718	6	-3.491458	-0.909943	0.852243
1	4.449166	-2.594839	-2.017044	6	-2.737814	-1.702818	1.941178
1	-1.473083	0.227061	-1.323487	6	-4.131763	0.317432	1.536062
1	-5.145815	-1.509205	-1.440430	6	-4.597314	-1.833500	0.289617
1	-4.078748	-0.661761	-2.604819	6	0.584571	-1.718877	0.380292
1	-4.369357	-2.422923	-2.773750	6	0.383444	-2.739473	-0.563663
6	0.052767	-0.672650	2.869996	6	0.313397	-4.074361	-0.164278
6	0.289008	-1.730053	3.748462	6	0.445308	-4.406891	1.183947
6	0.272977	-3.041420	3.272464	6	0.660109	-3.401396	2.131556
6	0.013380	-3.285532	1.921895	6	0.732826	-2.070637	1.732273
6	-0.229638	-2.231074	1.043295	6	5.199412	-0.115135	-1.600909
1	0.035868	0.345592	3.253664	8	4.005571	-1.500838	0.335470
1	0.474252	-1.528590	4.800054	1	0.633829	-0.219621	-1.159587
1	0.449090	-3.870431	3.952836	1	-1.905288	-1.474339	-0.487203
1	-0.030046	-4.304501	1.548902	1	-3.480431	-1.165513	-2.104102
1	-0.453392	-2.438011	0.003973	1	-1.064950	-0.153735	-2.636830
6	-2.143361	2.741279	-0.947739	1	-2.392477	0.328786	-3.693162
6	-2.697017	4.010826	-0.749694	1	-4.697371	0.735534	-2.772632
6	-3.574591	4.230058	0.311609	1	-4.949070	0.836106	-1.044011
6	-3.905857	3.169445	1.161362	1	-1.529369	2.491285	-2.961484
6	-3.357246	1.904207	0.958193	1	-3.824659	2.910145	-2.575139
1	-1.484461	2.570784	-1.798524	1	-3.458859	2.729087	-0.867446
1	-2.454221	4.820369	-1.434159	1	0.050578	1.898303	-1.310790
1	-4.010548	5.213611	0.467129	1	-1.119999	2.903583	-0.452422
1	-4.604380	3.328722	1.979385	1	-2.276613	-2.610830	1.540188
1	-3.637018	1.061784	1.583231	1	-1.949332	-1.106540	2.411954
				1	-3.436482	-1.998140	2.732377

E (CH₃CN) = -2013.645831
NImag = 1 (-26.7)

1	-4.708721	0.946905	0.855127	6	-3.327141	0.774448	-2.226950
1	-4.817189	-0.025581	2.319716	6	-3.939628	-0.506728	-1.633384
1	-3.375962	0.946112	2.017683	6	-4.410775	-0.034521	-0.239148
1	-5.246896	-1.325832	-0.428867	6	-3.198130	0.011787	0.730949
1	-4.170219	-2.716686	-0.200823	6	-5.067976	1.338681	-0.567862
1	-5.228518	-2.188136	1.112042	6	-4.390643	1.841785	-1.878561
1	2.333533	-0.030326	1.269240	6	-3.496656	0.053590	2.268705
1	4.960216	0.489958	-2.477268	6	-4.317477	1.279204	2.715034
1	5.677002	0.494266	-0.831936	6	-4.271306	-1.227294	2.654161
1	5.841419	-0.952799	-1.883144	6	-2.162237	0.040460	3.048091
1	0.349500	-2.487678	-1.618993	1	0.866346	0.338157	0.610865
1	0.180297	-4.853470	-0.909412	1	-2.637095	-0.919073	0.574869
1	0.401454	-5.446963	1.495780	1	-5.147548	-0.732103	0.173226
1	0.784418	-3.658275	3.179763	1	-3.238212	-1.348889	-1.594937
1	0.917788	-1.298998	2.474149	1	-4.803669	-0.820042	-2.234039
1	0.689698	1.315443	2.746706	1	-6.144193	1.196748	-0.722085
1	0.276199	3.603394	3.578815	1	-4.949873	2.060360	0.240696
1	1.018347	5.571317	2.245969	1	-3.171091	0.691473	-3.310576
1	2.203020	5.213920	0.086493	1	-5.123651	1.913380	-2.690453
1	2.620150	2.886571	-0.733539	1	-3.945222	2.834157	-1.753481
E (CH ₃ CN) = -2013.645263				1	-1.273577	0.231226	-1.775119
NImag = 1 (-75.3)				1	-1.515081	1.971261	-2.004513
138. 5b -PC (-2013.33378481)				1	-3.834616	2.218164	2.424851
				1	-5.328049	1.269816	2.293904
				1	-4.418899	1.278882	3.807209
				1	-3.730249	-2.130860	2.346567
6	0.244687	-2.599763	0.063676	1	-4.400776	-1.271459	3.741923
6	0.981948	-2.001461	-0.967334	1	-5.270315	-1.262011	2.207490
6	0.695723	-2.346408	-2.295029	1	-1.527093	-0.797475	2.735425
6	-0.316243	-3.261169	-2.590003	1	-1.591860	0.962907	2.902519
6	-1.049915	-3.849571	-1.558265	1	-2.354594	-0.066067	4.122474
6	-0.763443	-3.517812	-0.231092	1	2.805988	-0.895391	-1.467333
6	2.051479	-0.996998	-0.687845	1	3.983565	-2.742768	2.323761
7	2.578546	-0.909975	0.690746	1	4.214659	-3.222176	0.604399
16	4.284478	-0.848592	0.902077	1	5.617183	-2.673878	1.577329
8	4.541725	0.024484	2.050044	1	2.707186	2.176566	1.806011
6	1.835940	0.247195	0.119244	1	3.604024	4.411165	1.235047
6	2.459168	1.563774	-0.245291	1	3.871803	5.077110	-1.146697
6	2.813215	2.468308	0.765890	1	3.228496	3.489984	-2.950474
6	3.323015	3.724024	0.441702	1	2.326201	1.261315	-2.376154
6	3.474756	4.097158	-0.895545	1	1.271919	-1.898446	-3.101722
6	3.115089	3.206960	-1.907422	1	-0.524697	-3.519494	-3.624765
6	2.609415	1.947486	-1.582917	1	-1.832431	-4.568424	-1.785502
6	4.544188	-2.559519	1.406797	1	-1.321627	-3.981970	0.577899
8	4.988739	-0.637412	-0.370868	1	0.480952	-2.351581	1.094132
16	-2.037047	1.383050	0.231058	E (CH ₃ CN) = -2013.686497			
6	-1.961441	1.063275	-1.584525	NImag = 0			

Full list of citations for *Gaussian03* (Reference 27 in the text)

Gaussian03:

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A., Gaussian, Inc., Wallingford CT, **2004.**