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ELECTRONIC SUPPORTING INFORMATION

In the searching for zwitterionic intermediates on reaction paths of [3+2] cycloaddition reactions between 2,2,4,4-tetramethyl-3-thiocyclobutanone S-methylide and polymerizable olefins

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[1] Computational details

All calculations reported in this thesis were performed on an SGI-Altix 3700 computer in the CYFRONET regional computational centre in Cracow. Hybrid functional B3LYP [S1] with the 6-31G(d) basis set included in the GAUSSIAN 09 [S2] package was used. Subsequently, similar simulations using more advanced B3LYP/6-31G(d,p) and B3LYP/6-31+G(d) theoretical levels were performed. For the calculations of solvent effect on the reaction paths, the polarizable continuum model (PCM), in which the cavity is created via a series of overlapping spheres, was used.

Transition states were calculated using the QST2 (or QST3) and TS procedures. Subsequently, transition states were localized out by changing gradually the distance between the centers (with optimization after each step). In this way transition states identical as previously have been obtained. Stationary points were characterized by frequency calculations. All reactants, and products, had positive Hessian matrices. All transition states showed only one negative eigenvalue in their diagonalized Hessian matrices, and their

associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration. For all reactions, intrinsic reaction coordinate (IRC) calculations were performed to connect previously computed transition structures (**TS**) with suitable minima.

Values of the global electron density transfer (GEDT) [S3] were calculated according to the formula:

$$GEDT=-\Sigma q_A$$

where q_A is the net charge and the sum is taken over all the atoms of dipolarophile.

Global electronic properties of reactants were estimated according to the equations recommended earlier by *Parr* and *Domingo* [S4-S6]. In particular, the electronic chemical potentials (μ) and chemical hardness (η) were evaluated in terms of one-electron energies of FMO (E_{HOMO} and E_{LUMO}) using the following equations:

$$\mu\approx(E_{HOMO}+E_{LUMO})/2 \qquad \eta\approx E_{LUMO}-E_{HOMO}$$

Next, the values of μ and η were then used for the calculation of global electrophilicity (ω) according to the formula:

$$\omega=\mu^2/2\,\eta$$

Subsequently, global nucleophilicity (N) [S7] can be expressed in terms of equation:

$$N=E_{HOMO\ (addent)}-E_{HOMO\ (tetracyanoethene)}$$

The local electrophilicity (ω_k) condensed to atom k was calculated by projecting the index ω onto any reaction centre k in the molecule by using *Parr* functions P^+_k [S8]:

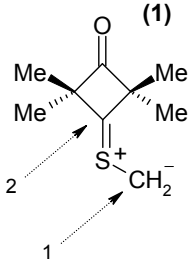
$$\omega_k = P^+_k\cdot\omega$$

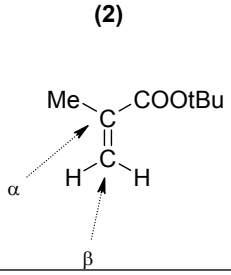
The local nucleophilicity (N_k) condensed to atom *k* was calculated using global nucleophilicity N and *Parr* functions P^-_k [S8] according to the formula:

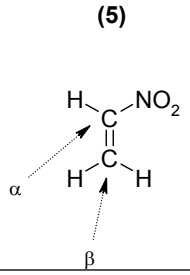
$$N_k = P^-_k\cdot N$$

[2] Selected results of quantumchemical calculations

2.1. Electronic properties of addents







	Global properties					Local properties							
						P^-_k		N_k		P^+_k		ω_k	
	μ [a.u.]	η [a.u.]	ω [eV]	N [eV]	Δω [eV]	C_1/C_α	C_2/C_β	C_1/C_α [eV]	C_2/C_β [eV]	C_1/C_α	C_2/C_β	C_1/C_α [eV]	C_2/C_β [eV]
1	-0.1168	0.1284	1.44	4.19		0.75	0.48	3.14	2.00	0.39	0.09	0.56	0.12
2	-0.1477	0.2258	1.31	2.03	0.13	0.25	0.43	0.51	0.87	0.06	0.54	0.08	0.71
5	-0.1958	0.2001	2.61	1.07	1.16	0.01	0.01	0.01	0.01	0.01	0.44	0.02	1.15

2.2. Key parameters of critical structures according to B3LYP/6-31G(d) calculations

Reaction	Structure	Interatomic distances [Å]		GEDT
		r_{C1-C5}	r_{C3-C4}	[e]
1+**2**	$\mathbf{TS_A}$	2.548	2.547	0.09
	4	1.546	1.547	0.05
	$\mathbf{TS_B}$	2.124		0.12
	8	1.572		0.17
1+**5**	$\mathbf{LM_A}$	3.500	4.519	0.00
	$\mathbf{TS1_A}$	2.449	3.820	0.16
	6	1.571	4.754	0.50
	$\mathbf{TS2_A}$	1.575	3.231	0.47
	7	1.529	1.539	0.07
	$\mathbf{LM_B}$	3.828		0.00
	$\mathbf{TS_B}$	2.349		0.18
	9	1.571		0.49

2.3. Energetic aspects according to DFT calculations

Solvent	Transition	Theory level					
		B3LYP/6-31G(d)			B3LYP/6-31+G(d)		
		ΔH	ΔG	ΔS	ΔH	ΔG	ΔS
Toluene	**1+2→TS$_A$**	10.83	25.86	-50.5	13.48	28.52	-50.5
	1+2→4	-63.11	-46.06	-57.2	-58.04	-41.56	-55.3
	1+2→TS$_B$	9.16	21.17	-40.3	10.99	23.43	-41.7
	1+2→8	0.22	12.89	-42.5	2.73	16.00	-44.5
	1+5→LM$_A$	-0.99	8.71	-32.6			
	1+5→TS1$_A$	-0.45	13.20	-45.8	1.90	14.83	-43.4
	1+5→6	-18.06	-2.51	-52.2	-17.32	-3.09	-47.8
	1+5→TS2$_A$	-17.45	-1.32	-54.1	-15.78	0.46	-54.5
	1+5→7	-67.81	-50.95	-56.6	-62.07	-45.11	-56.9
	1+5→LM$_B$	-0.98	7.27	-27.7			
	1+5→TS$_B$	1.22	13.15	-40.0	2.27	14.55	-41.2
	1+5→9	-13.23	1.36	-49.0	-13.24	0.77	-47.0
Nitromethane	**1+2→TS$_A$**	10.68	25.74	-50.5	13.40	29.08	-52.6
	1+2→4	-63.19	-45.68	-58.8	-57.99	-40.55	-58.5
	1+2→TS$_B$	8.53	20.80	-41.2	10.09	22.38	-41.2
	1+2→8	-0.90	11.83	-42.7	0.99	13.36	-41.5
	1+5→LM$_A$	-0.69	8.48	-30.8			
	1+5→TS1$_A$	-0.98	12.14	-44.1	0.69	12.21	-38.6
	1+5→6	-21.75	-6.67	-50.6	-23.64	-9.58	-47.2
	1+5→TS2$_A$	-21.16	-4.84	-54.8	-20.41	-4.11	-54.7
	1+5→7	-67.24	-49.91	-58.2	-61.16	-43.73	-58.5
	1+5→LM$_B$	-0.33	7.63	-26.7			
	1+5→TS$_B$	0.43	12.18	-39.4	1.06	12.54	-38.5
	1+5→9	-18.73	-4.20	-48.8	-21.99	-8.23	-46.2

2.4. Cartesian coordinates of key structures of reaction **1**+**2** according to B3LYP/6-31G(d) calculations

(1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.392912	-0.279163	-0.000217
2	6	0	-3.174854	-0.068672	0.000074
3	1	0	-3.131115	1.011823	-0.000234
4	1	0	-4.122301	-0.589692	0.000338
5	16	0	-1.842779	-1.045666	0.000187
6	6	0	1.001950	-0.918353	-0.000093
7	6	0	0.089481	1.170065	-0.000040
8	6	0	1.508669	0.546700	0.000341
9	8	0	2.614253	1.030083	0.001049
10	6	0	-0.207305	1.993347	-1.269022
11	1	0	-1.262386	2.287007	-1.302127
12	1	0	0.400565	2.905137	-1.273876
13	1	0	0.014778	1.426764	-2.178874
14	6	0	-0.208395	1.994043	1.268097
15	1	0	0.012172	1.427676	2.178466
16	1	0	0.400115	2.905405	1.273333
17	1	0	-1.263288	2.288486	1.299795
18	6	0	1.401034	-1.699057	-1.266552
19	1	0	2.480873	-1.886224	-1.274568
20	1	0	0.885729	-2.666504	-1.291809
21	1	0	1.138678	-1.151970	-2.177693
22	6	0	1.400933	-1.699312	1.266224
23	1	0	0.885699	-2.666795	1.291334
24	1	0	2.480779	-1.886395	1.274232
25	1	0	1.138540	-1.152324	2.177423

(2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.098414	0.345365	0.000007
2	6	0	2.201314	1.680594	0.000038
3	1	0	1.325826	2.319723	0.000080
4	1	0	3.173223	2.167312	0.000018
5	6	0	3.284498	-0.583500	-0.000067
6	1	0	3.268667	-1.239957	0.877319
7	1	0	3.268617	-1.239867	-0.877518
8	1	0	4.220999	-0.018898	-0.000049
9	6	0	0.763875	-0.339329	0.000062
10	8	0	0.661038	-1.555188	0.000058

11	8	0	-0.267406	0.524910	0.000137
12	6	0	-1.672718	0.070705	-0.000014
13	6	0	-1.963319	-0.729669	-1.273754
14	1	0	-1.692284	-0.145868	-2.160245
15	1	0	-1.409862	-1.669744	-1.286122
16	1	0	-3.034963	-0.951680	-1.327888
17	6	0	-2.447995	1.390531	-0.000091
18	1	0	-3.525049	1.193238	-0.000152
19	1	0	-2.204899	1.982570	0.888290
20	1	0	-2.204790	1.982532	-0.888468
21	6	0	-1.963522	-0.729670	1.273685
22	1	0	-1.692709	-0.145826	2.160214
23	1	0	-3.035153	-0.951792	1.327618
24	1	0	-1.409965	-1.669686	1.286161

(TS_A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.609587	-0.164205	0.160605
2	6	0	-0.200630	1.218936	1.656561
3	6	0	-1.006735	1.584061	-0.732537
4	6	0	-0.136880	0.782471	-1.433929
5	1	0	-0.971269	1.257561	2.419748
6	1	0	0.362936	2.121737	1.458890
7	1	0	-0.393083	-0.242836	-1.659472
8	1	0	0.649160	1.230461	-2.028536
9	16	0	0.465261	-0.294882	1.401464
10	6	0	2.893526	0.731725	0.131621
11	6	0	2.372700	-1.432437	-0.319069
12	6	0	3.630100	-0.545252	-0.327104
13	8	0	4.790299	-0.767290	-0.579042
14	6	0	2.477594	-2.621748	0.651746
15	1	0	1.513372	-3.135964	0.738240
16	1	0	3.213708	-3.341665	0.278246
17	1	0	2.787046	-2.305799	1.653368
18	6	0	1.991194	-1.932311	-1.725576
19	1	0	1.942378	-1.115972	-2.452062
20	1	0	2.734337	-2.657478	-2.075549
21	1	0	1.012738	-2.424808	-1.699030
22	6	0	3.390134	1.220428	1.505882
23	1	0	4.411402	1.604001	1.410973
24	1	0	2.757808	2.029789	1.887039
25	1	0	3.393893	0.416711	2.248723
26	6	0	3.004521	1.868522	-0.896261
27	1	0	2.355066	2.707294	-0.624659
28	1	0	4.038541	2.229712	-0.921998
29	1	0	2.742468	1.541815	-1.906166

30	6	0	-0.882794	3.092755	-0.739903
31	1	0	-1.494848	3.525345	-1.542157
32	1	0	-1.233463	3.536909	0.195055
33	1	0	0.153618	3.399821	-0.911727
34	6	0	-2.325902	1.071543	-0.275894
35	8	0	-3.232771	1.802051	0.098910
36	8	0	-2.417104	-0.278042	-0.362245
37	6	0	-3.655219	-0.998375	-0.024932
38	6	0	-4.013059	-0.784663	1.450227
39	1	0	-3.172103	-1.070715	2.091875
40	1	0	-4.270331	0.257258	1.645602
41	1	0	-4.869504	-1.415367	1.714475
42	6	0	-3.274720	-2.459664	-0.279700
43	1	0	-4.127230	-3.113549	-0.067580
44	1	0	-2.978518	-2.605884	-1.323781
45	1	0	-2.439897	-2.759595	0.362161
46	6	0	-4.786435	-0.565169	-0.964591
47	1	0	-4.481777	-0.692231	-2.009314
48	1	0	-5.669151	-1.190638	-0.789587
49	1	0	-5.056772	0.478728	-0.800079

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(4)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.555959	-0.035705	0.171880
2	6	0	-0.534300	0.915422	1.674425
3	6	0	-0.717887	1.146322	0.157160
4	6	0	0.164630	0.051940	-0.498798
5	1	0	-1.147414	0.081612	2.020520
6	1	0	-0.781965	1.805702	2.259721
7	1	0	-0.342109	-0.906222	-0.359615
8	1	0	0.243648	0.218914	-1.576700
9	16	0	1.245460	0.525107	1.928287
10	6	0	2.816198	0.664435	-0.543574
11	6	0	2.293874	-1.456909	0.043493
12	6	0	3.483192	-0.714318	-0.568349
13	8	0	4.575224	-1.084750	-0.935338
14	6	0	2.656764	-2.196346	1.338043
15	1	0	1.757314	-2.586684	1.825651
16	1	0	3.318185	-3.036711	1.099835
17	1	0	3.173439	-1.554416	2.057267
18	6	0	1.673173	-2.450198	-0.956010
19	1	0	1.391359	-1.980634	-1.903630
20	1	0	2.403669	-3.235325	-1.178180
21	1	0	0.781943	-2.927619	-0.532918
22	6	0	3.626197	1.691101	0.260129
23	1	0	4.576114	1.875651	-0.253301

24	1	0	3.087363	2.640724	0.343853
25	1	0	3.852588	1.347254	1.273229
26	6	0	2.597780	1.187378	-1.975442
27	1	0	2.003291	2.106565	-1.976133
28	1	0	3.572199	1.410424	-2.423117
29	1	0	2.103023	0.458309	-2.625004
30	6	0	-0.302806	2.569140	-0.241787
31	1	0	-0.363218	2.706505	-1.325084
32	1	0	-0.966200	3.305905	0.220186
33	1	0	0.719321	2.773972	0.085572
34	6	0	-2.194354	0.936411	-0.240929
35	8	0	-2.864783	1.778455	-0.805083
36	8	0	-2.628956	-0.286329	0.113971
37	6	0	-4.013720	-0.744308	-0.147606
38	6	0	-5.004510	0.144032	0.610246
39	1	0	-4.750486	0.176339	1.675376
40	1	0	-5.009136	1.161104	0.215328
41	1	0	-6.012968	-0.273367	0.515108
42	6	0	-4.006516	-2.163396	0.424435
43	1	0	-4.991800	-2.623401	0.296554
44	1	0	-3.265829	-2.785307	-0.088809
45	1	0	-3.767397	-2.149954	1.492752
46	6	0	-4.278900	-0.765642	-1.655731
47	1	0	-3.517503	-1.363213	-2.168891
48	1	0	-5.255099	-1.225092	-1.846479
49	1	0	-4.280208	0.242094	-2.073587

(TS_B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.721098	-0.456462	0.210983
2	6	0	0.009251	-0.042570	0.817955
3	6	0	-2.007216	1.430785	-0.605239
4	6	0	-1.034402	0.511266	-0.946782
5	1	0	-0.802820	-0.506234	1.371226
6	1	0	0.295781	0.945697	1.164094
7	1	0	-1.331139	-0.502038	-1.188060
8	1	0	-0.127767	0.862531	-1.435480
9	16	0	1.271746	-1.174379	0.550794
10	6	0	3.349820	0.919068	0.430949
11	6	0	3.964283	-1.106212	-0.405160
12	6	0	4.629771	0.270385	-0.157764
13	8	0	5.744240	0.689434	-0.347773
14	6	0	4.611697	-2.251333	0.396446
15	1	0	4.009017	-3.162821	0.309786
16	1	0	5.613092	-2.463602	0.006105
17	1	0	4.701225	-2.000993	1.458249

18	6	0	3.861320	-1.479009	-1.897787
19	1	0	3.422835	-0.669354	-2.489642
20	1	0	4.855996	-1.700888	-2.300161
21	1	0	3.233286	-2.368785	-2.020194
22	6	0	3.502938	1.368977	1.897146
23	1	0	4.178981	2.229224	1.952966
24	1	0	2.534677	1.669267	2.312858
25	1	0	3.909821	0.569620	2.524294
26	6	0	2.823690	2.077321	-0.442877
27	1	0	1.863815	2.445857	-0.065054
28	1	0	3.539608	2.906494	-0.421535
29	1	0	2.686099	1.770199	-1.484391
30	6	0	-1.721172	2.905309	-0.500591
31	1	0	-2.459864	3.492003	-1.059300
32	1	0	-1.773379	3.264128	0.537415
33	1	0	-0.725420	3.140351	-0.891604
34	6	0	-3.359332	1.015918	-0.222992
35	8	0	-4.255127	1.808824	0.053709
36	8	0	-3.511468	-0.339977	-0.205609
37	6	0	-4.802992	-0.971792	0.088397
38	6	0	-5.242825	-0.639624	1.519309
39	1	0	-4.455604	-0.912950	2.231130
40	1	0	-5.460021	0.423934	1.625195
41	1	0	-6.142515	-1.212490	1.771767
42	6	0	-4.485686	-2.464852	-0.042285
43	1	0	-5.381973	-3.061556	0.157769
44	1	0	-4.133176	-2.698101	-1.052531
45	1	0	-3.708449	-2.758975	0.671124
46	6	0	-5.849731	-0.553450	-0.951210
47	1	0	-5.483803	-0.761650	-1.962837
48	1	0	-6.770956	-1.127255	-0.798147
49	1	0	-6.079528	0.509869	-0.871366

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(8)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.557982	-0.395489	-0.318567
2	6	0	0.081658	0.324486	-1.102029
3	6	0	1.748849	1.368130	0.353423
4	6	0	0.689809	0.355826	0.346880
5	1	0	0.823253	0.009298	-1.840371
6	1	0	-0.314428	1.301898	-1.382484
7	1	0	1.067009	-0.638147	0.587827
8	1	0	-0.149037	0.593071	1.023213
9	16	0	-1.271702	-0.948000	-1.233661
10	6	0	-3.320928	0.930209	-0.211193
11	6	0	-3.599544	-1.228973	0.429594

12	6	0	-4.404670	0.089467	0.512823
13	8	0	-5.488463	0.366994	0.961913
14	6	0	-4.304321	-2.337446	-0.375578
15	1	0	-3.619274	-3.176386	-0.541998
16	1	0	-5.172741	-2.705913	0.180818
17	1	0	-4.647667	-1.976043	-1.350071
18	6	0	-3.140691	-1.766935	1.802121
19	1	0	-2.660769	-0.989962	2.404811
20	1	0	-4.002408	-2.153185	2.357612
21	1	0	-2.422889	-2.582271	1.660792
22	6	0	-3.788222	1.527996	-1.553811
23	1	0	-4.527297	2.315264	-1.370363
24	1	0	-2.941031	1.969483	-2.090291
25	1	0	-4.243321	0.770999	-2.199801
26	6	0	-2.732179	2.032677	0.693448
27	1	0	-1.897321	2.538526	0.196800
28	1	0	-3.506828	2.777559	0.906377
29	1	0	-2.373747	1.629533	1.645071
30	6	0	1.403350	2.826196	0.367087
31	1	0	2.265357	3.412589	0.695093
32	1	0	1.121911	3.216086	-0.626206
33	1	0	0.553873	3.029414	1.034576
34	6	0	3.145598	1.014774	0.239253
35	8	0	4.072380	1.830716	0.243188
36	8	0	3.337356	-0.340775	0.131348
37	6	0	4.676721	-0.925057	0.046411
38	6	0	5.384107	-0.451312	-1.229808
39	1	0	4.767917	-0.672434	-2.108820
40	1	0	5.575339	0.621930	-1.193980
41	1	0	6.338344	-0.978873	-1.342727
42	6	0	4.387347	-2.428056	-0.029404
43	1	0	5.323802	-2.991288	-0.102765
44	1	0	3.850991	-2.763778	0.864550
45	1	0	3.774391	-2.660239	-0.906876
46	6	0	5.486078	-0.601501	1.308878
47	1	0	4.931824	-0.909070	2.202803
48	1	0	6.434014	-1.151696	1.290588
49	1	0	5.697900	0.466221	1.375630

2.5. Cartesian coordinates of key structures of reaction **1**+**5** according to B3LYP/6-31G(d) calculations

(5)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.147838	-1.867126	0.000000
2	1	0	1.230044	-1.801964	0.000000
3	1	0	-0.316357	-2.847236	0.000000
4	6	0	-0.605566	-0.773886	0.000000
5	1	0	-1.685927	-0.727317	0.000000
6	7	0	0.000000	0.557105	0.000000
7	8	0	-0.786767	1.506274	0.000000
8	8	0	1.226593	0.659083	0.000000

(LM_A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.938657	0.514303	-0.400675
2	6	0	-0.811621	2.675907	-0.648267
3	6	0	-3.752998	0.980270	0.203489
4	6	0	-3.359358	-0.116503	0.844037
5	1	0	-0.659099	2.963999	0.382957
6	1	0	-1.378508	3.302850	-1.323036
7	1	0	-4.224041	1.789294	0.750724
8	1	0	-3.615714	1.086325	-0.865447
9	1	0	-3.436017	-0.315309	1.903958
10	16	0	-0.036837	1.403055	-1.372086
11	6	0	1.735787	-0.741543	-0.783201
12	6	0	1.397984	0.560566	1.056023
13	6	0	2.209679	-0.709363	0.691364
14	8	0	2.950938	-1.415269	1.329827
15	6	0	2.288745	1.755459	1.449292
16	1	0	1.689912	2.667340	1.551543
17	1	0	2.775224	1.557647	2.411072
18	1	0	3.066467	1.942683	0.702153
19	6	0	0.327024	0.300261	2.133590
20	1	0	-0.300159	-0.560880	1.884480
21	1	0	0.811444	0.104471	3.096904
22	1	0	-0.321991	1.175518	2.251004
23	6	0	2.887006	-0.535045	-1.786359
24	1	0	3.542310	-1.413336	-1.797592
25	1	0	2.485254	-0.394340	-2.796650
26	1	0	3.491440	0.342964	-1.536069

27	6	0	0.920574	-1.997342	-1.144650
28	1	0	0.512602	-1.900505	-2.157418
29	1	0	1.566075	-2.882745	-1.118364
30	1	0	0.080911	-2.158046	-0.462271
31	7	0	-2.698884	-1.200675	0.128981
32	8	0	-2.619430	-1.156397	-1.098440
33	8	0	-2.243183	-2.112570	0.829202

($TS1_A$)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.742912	-0.414782	0.443579
2	6	0	-1.272896	-2.308726	0.776063
3	6	0	-3.216109	-1.084777	-0.075261
4	6	0	-2.819284	-0.081957	-0.894985
5	1	0	-0.993739	-2.738469	-0.178735
6	1	0	-1.747148	-2.955542	1.506906
7	1	0	-3.545175	-2.024052	-0.503353
8	1	0	-3.476049	-0.878731	0.953838
9	1	0	-2.654900	-0.161824	-1.959411
10	16	0	-0.310041	-1.120533	1.486065
11	6	0	1.629773	0.805825	0.733518
12	6	0	1.354229	-0.727724	-0.925409
13	6	0	2.283246	0.479461	-0.630898
14	8	0	3.198533	0.969646	-1.242643
15	6	0	2.109661	-2.067674	-1.020215
16	1	0	1.406440	-2.906551	-1.065972
17	1	0	2.717513	-2.081478	-1.931156
18	1	0	2.771755	-2.223677	-0.162863
19	6	0	0.474332	-0.505436	-2.170812
20	1	0	-0.097207	0.424536	-2.106863
21	1	0	1.113306	-0.460206	-3.059794
22	1	0	-0.228839	-1.336081	-2.296728
23	6	0	2.602951	0.681227	1.919777
24	1	0	3.344072	1.486573	1.877008
25	1	0	2.059074	0.766951	2.867398
26	1	0	3.133939	-0.276287	1.914185
27	6	0	0.901239	2.163880	0.760876
28	1	0	0.349722	2.273228	1.700803
29	1	0	1.634556	2.974906	0.691172
30	1	0	0.183656	2.271277	-0.057539
31	7	0	-2.500119	1.206288	-0.379062
32	8	0	-2.619285	1.428491	0.838145
33	8	0	-2.110475	2.063615	-1.196740

(6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.680859	-0.111211	0.594153
2	6	0	-1.752586	-1.250358	1.366960
3	6	0	-3.069933	-0.938741	0.605711
4	6	0	-2.838724	-0.403529	-0.763505
5	1	0	-1.190676	-2.050325	0.884440
6	1	0	-1.955367	-1.532527	2.405121
7	1	0	-3.620869	-1.884904	0.550308
8	1	0	-3.662064	-0.241873	1.209561
9	1	0	-2.965836	-0.970135	-1.674535
10	16	0	-0.637375	0.214420	1.491704
11	6	0	1.835710	0.878342	0.363351
12	6	0	1.178504	-1.142975	-0.434390
13	6	0	2.358616	-0.160995	-0.650386
14	8	0	3.335586	-0.209426	-1.352285
15	6	0	1.647466	-2.485682	0.162501
16	1	0	0.794285	-3.127612	0.405706
17	1	0	2.265613	-3.005345	-0.576890
18	1	0	2.243508	-2.346672	1.069960
19	6	0	0.342273	-1.355139	-1.711617
20	1	0	-0.094038	-0.422090	-2.079882
21	1	0	0.992815	-1.775023	-2.487111
22	1	0	-0.471504	-2.062916	-1.526417
23	6	0	2.780963	1.123065	1.550937
24	1	0	3.671836	1.656348	1.203405
25	1	0	2.285122	1.737726	2.310001
26	1	0	3.101994	0.187032	2.019467
27	6	0	1.397507	2.203833	-0.299082
28	1	0	1.019302	2.892598	0.463811
29	1	0	2.261467	2.665300	-0.788827
30	1	0	0.600235	2.056552	-1.034191
31	7	0	-2.322142	0.812871	-0.883465
32	8	0	-2.135590	1.491582	0.241342
33	8	0	-1.973340	1.338268	-1.982150

($TS2_A$)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.525403	0.232457	-0.461269
2	6	0	-1.709710	1.787153	-0.949484
3	6	0	-2.841379	1.165728	-0.048179
4	6	0	-2.363024	0.230439	0.986591
5	1	0	-1.103852	2.494607	-0.380941

6	1	0	-2.138509	2.302449	-1.814429
7	1	0	-3.338028	2.023853	0.420305
8	1	0	-3.553234	0.667825	-0.712620
9	1	0	-2.247259	0.480622	2.029633
10	16	0	-0.616716	0.500759	-1.624236
11	6	0	1.548579	-0.908565	-0.540128
12	6	0	1.256558	0.988512	0.667997
13	6	0	2.315190	-0.140543	0.553663
14	8	0	3.367341	-0.319943	1.110234
15	6	0	1.808426	2.368244	0.256158
16	1	0	1.018693	3.126689	0.264672
17	1	0	2.575894	2.669053	0.976679
18	1	0	2.260947	2.350307	-0.740046
19	6	0	0.626872	1.034916	2.070591
20	1	0	0.175755	0.077937	2.342713
21	1	0	1.414157	1.276104	2.793540
22	1	0	-0.143953	1.809231	2.122776
23	6	0	2.328641	-1.034955	-1.861856
24	1	0	3.162692	-1.729498	-1.719785
25	1	0	1.680621	-1.432285	-2.650281
26	1	0	2.734385	-0.073889	-2.194546
27	6	0	0.996491	-2.277407	-0.085012
28	1	0	0.419392	-2.729229	-0.897131
29	1	0	1.840306	-2.930079	0.162193
30	1	0	0.329148	-2.202493	0.778541
31	7	0	-2.195850	-1.076444	0.672874
32	8	0	-2.360537	-1.429808	-0.550003
33	8	0	-1.856933	-1.917013	1.560012

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(7)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.126811	-0.229010	0.069130
2	6	0	-1.975816	-1.881071	0.681328
3	6	0	-1.856670	-1.483074	-0.790232
4	6	0	-1.102896	-0.145767	-0.852613
5	1	0	-2.092220	-2.960438	0.803276
6	1	0	-2.813121	-1.375795	1.168036
7	1	0	-1.256337	-2.218553	-1.336284
8	1	0	-2.831311	-1.414989	-1.285644
9	1	0	-0.846317	0.110208	-1.877031
10	16	0	-0.403363	-1.345933	1.473091
11	6	0	0.868293	1.115050	0.535324
12	6	0	1.487214	-0.702644	-0.667906
13	6	0	2.161035	0.514466	-0.025800
14	8	0	3.316219	0.863465	0.039475
15	6	0	2.108430	-2.041502	-0.257500

16	1	0	1.517364	-2.881829	-0.638339
17	1	0	3.116992	-2.108106	-0.679366
18	1	0	2.184366	-2.152171	0.826091
19	6	0	1.504964	-0.582765	-2.205865
20	1	0	1.161010	0.390408	-2.569991
21	1	0	2.533873	-0.712023	-2.556475
22	1	0	0.892388	-1.363827	-2.671676
23	6	0	0.926128	1.408838	2.038823
24	1	0	1.594787	2.258745	2.212302
25	1	0	-0.070404	1.657375	2.414553
26	1	0	1.305823	0.560944	2.616438
27	6	0	0.504067	2.407975	-0.226276
28	1	0	-0.397255	2.868379	0.188193
29	1	0	1.328442	3.119739	-0.112331
30	1	0	0.352339	2.251287	-1.298802
31	7	0	-2.089012	0.954382	-0.473000
32	8	0	-2.332915	1.158784	0.713031
33	8	0	-2.622415	1.545492	-1.408993

(LM_B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.564880	-0.484347	-0.191470
2	6	0	-0.605989	-1.975442	-1.128989
3	6	0	-3.526929	-1.389553	1.274479
4	6	0	-4.409041	-0.424349	1.039900
5	1	0	-1.196563	-1.086796	-1.306215
6	1	0	-0.958177	-2.950763	-1.437535
7	1	0	-3.681963	-2.061604	2.111984
8	1	0	-2.649606	-1.534706	0.650195
9	1	0	-5.308139	-0.216069	1.603617
10	16	0	0.949814	-1.957726	-0.564278
11	6	0	2.959044	-0.177627	0.372486
12	6	0	1.089492	0.966922	-0.250151
13	6	0	2.499225	1.300759	0.299765
14	8	0	3.047028	2.340762	0.572163
15	6	0	0.826448	1.551363	-1.651516
16	1	0	-0.120554	1.177162	-2.055296
17	1	0	0.761655	2.643556	-1.591995
18	1	0	1.624879	1.291510	-2.353959
19	6	0	-0.038743	1.362032	0.724398
20	1	0	0.130200	0.951420	1.725392
21	1	0	-0.089455	2.453831	0.805588
22	1	0	-1.007312	1.002869	0.361172
23	6	0	4.155566	-0.488450	-0.545672
24	1	0	5.061851	-0.002779	-0.166502
25	1	0	4.335454	-1.569522	-0.580218

26	1	0	3.980040	-0.140903	-1.568764
27	6	0	3.238957	-0.656090	1.809736
28	1	0	3.405097	-1.739778	1.821721
29	1	0	4.136867	-0.167619	2.205039
30	1	0	2.402405	-0.433803	2.480029
31	7	0	-4.247154	0.501725	-0.078163
32	8	0	-3.250495	0.416483	-0.800256
33	8	0	-5.147918	1.328283	-0.227714

(TS_B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.344470	-0.433020	-0.230634
2	6	0	-1.195883	-1.306433	-1.009074
3	6	0	-2.579520	-1.239076	0.887544
4	6	0	-3.828548	-0.903745	0.472027
5	1	0	-1.450969	-0.282619	-1.254990
6	1	0	-1.699991	-2.096295	-1.554844
7	1	0	-2.382842	-2.264570	1.176354
8	1	0	-1.901923	-0.477347	1.250033
9	1	0	-4.632705	-1.594958	0.263448
10	16	0	0.404982	-1.715281	-0.648393
11	6	0	2.777097	-0.472764	0.315461
12	6	0	1.230162	1.091144	-0.265843
13	6	0	2.698410	1.073410	0.231271
14	8	0	3.497246	1.946332	0.458148
15	6	0	1.051539	1.733105	-1.654527
16	1	0	0.023783	1.608380	-2.010831
17	1	0	1.259969	2.806174	-1.588124
18	1	0	1.728830	1.295923	-2.394838
19	6	0	0.270322	1.727928	0.763033
20	1	0	0.396458	1.290238	1.758734
21	1	0	0.480527	2.800650	0.835183
22	1	0	-0.773672	1.601902	0.459580
23	6	0	3.844371	-1.083709	-0.610785
24	1	0	4.844479	-0.828367	-0.244437
25	1	0	3.753300	-2.175823	-0.628430
26	1	0	3.749312	-0.715930	-1.637331
27	6	0	2.934104	-0.999583	1.755383
28	1	0	2.820753	-2.089446	1.773223
29	1	0	3.930432	-0.750076	2.136040
30	1	0	2.189503	-0.567415	2.431074
31	7	0	-4.162283	0.444507	0.176857
32	8	0	-3.272959	1.319783	0.216490
33	8	0	-5.344053	0.690007	-0.119225

(9)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.183129	-0.444622	-0.148297
2	6	0	-1.439279	-1.368906	-0.679262
3	6	0	-2.102565	-1.271393	0.741702
4	6	0	-3.496867	-0.831128	0.589347
5	1	0	-1.569206	-0.409734	-1.180946
6	1	0	-1.881180	-2.173002	-1.272126
7	1	0	-2.068982	-2.248150	1.233339
8	1	0	-1.498508	-0.568948	1.330456
9	1	0	-4.352401	-1.475479	0.730687
10	16	0	0.340910	-1.792455	-0.614553
11	6	0	2.664829	-0.407707	0.232161
12	6	0	0.992417	1.073553	-0.152672
13	6	0	2.519016	1.129250	0.110192
14	8	0	3.308061	2.035297	0.166892
15	6	0	0.526040	1.712785	-1.474689
16	1	0	-0.561417	1.644630	-1.569605
17	1	0	0.803021	2.772179	-1.460053
18	1	0	0.998844	1.247741	-2.345359
19	6	0	0.200780	1.663535	1.043496
20	1	0	0.469552	1.185754	1.990840
21	1	0	0.445107	2.728654	1.116430
22	1	0	-0.873526	1.551241	0.866902
23	6	0	3.636451	-1.022335	-0.792636
24	1	0	4.658257	-0.718661	-0.544304
25	1	0	3.582319	-2.115983	-0.763729
26	1	0	3.417849	-0.690255	-1.812184
27	6	0	2.977994	-0.903996	1.660253
28	1	0	2.894883	-1.994775	1.706841
29	1	0	4.002483	-0.619637	1.920871
30	1	0	2.302426	-0.473075	2.404533
31	7	0	-3.776565	0.413238	0.122330
32	8	0	-2.804393	1.200369	-0.174595
33	8	0	-4.973642	0.785572	-0.011501

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