

## SUPPLEMENTARY MATERIAL

### A new insight on the molecular mechanism of the reaction between 2-methoxyfuran and ethyl (Z)-3-phenyl-2-nitroprop-2-enoate: MEDT computational study and considerations

Mikołaj Sadowski<sup>1</sup>, Ewa Dresler<sup>2</sup>, Aneta Wróblewska<sup>3</sup>, Radomir Jasiński<sup>1\*</sup>

<sup>1</sup> Department of Organic Chemistry and Technology, Cracow University of Technology, Warszawska 24, 31-155 Krakow, Poland

<sup>2</sup> Łukasiewicz Research Network—Institute of Heavy Organic Synthesis “Błachownia”, Energetyków 9, 47-225 Kędzierzyn-Koźle, Poland

<sup>3</sup> Department of Organic Chemistry, University of Lodz, Tamka 12, 91-403 Łódź, Poland

\* Correspondence: [radomir.jasinski@pk.edu.pl](mailto:radomir.jasinski@pk.edu.pl)

## CARTESIAN COORDINATES FOR TRANSITION STATES

### **TSA**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.674021	-1.927962	-0.788408
2	6	0	1.460258	-1.917437	-0.371698
3	6	0	-1.036994	0.107123	-0.602044
4	1	0	-0.843366	0.228567	-1.663957
5	6	0	0.033221	0.676221	0.102830
6	8	0	0.588955	-1.815341	-1.360015
7	6	0	1.205483	1.136138	-0.667619
8	8	0	1.173854	1.286688	-1.873284
9	8	0	2.315927	1.297733	0.049793
10	7	0	-0.031211	0.874549	1.507618
11	8	0	-0.765905	0.130968	2.158639
12	8	0	0.604368	1.784992	2.029710
13	6	0	-2.502183	0.214378	-0.327808
14	6	0	-3.234366	0.923795	-1.288510
15	6	0	-3.189673	-0.338147	0.754026
16	6	0	-4.604128	1.107551	-1.155039
17	1	0	-2.721735	1.346027	-2.146605
18	6	0	-4.563100	-0.165667	0.880135
19	1	0	-2.654014	-0.898478	1.504077
20	6	0	-5.274957	0.561017	-0.066973
21	1	0	-5.146040	1.670381	-1.906389
22	1	0	-5.077894	-0.604542	1.727293
23	1	0	-6.345698	0.693945	0.038073
24	6	0	3.489362	1.726205	-0.666150
25	1	0	3.770743	0.941148	-1.372377
26	1	0	3.247426	2.625728	-1.235259
27	6	0	4.573803	1.986606	0.352942
28	1	0	4.806618	1.085072	0.923411
29	1	0	5.481836	2.309972	-0.160949
30	1	0	4.272839	2.771781	1.049213
31	1	0	-1.457448	-2.176336	-1.487018
32	8	0	2.700450	-1.696316	-0.716118
33	6	0	3.664089	-1.736676	0.346987
34	1	0	4.618100	-1.496946	-0.113896
35	1	0	3.409107	-0.989826	1.100920
36	1	0	3.699489	-2.735624	0.785210
37	6	0	0.852527	-2.281236	0.822940
38	6	0	-0.503484	-2.360856	0.527701
39	1	0	1.339286	-2.439766	1.770088
40	1	0	-1.296996	-2.629059	1.205149

**TSB**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.456393	-1.514686	-0.683872
2	6	0	2.622047	-1.702416	-0.466084
3	6	0	-0.244925	0.024887	0.572897
4	1	0	-0.428906	-0.577199	1.455555
5	6	0	-1.500119	0.414489	0.048168
6	8	0	1.688221	-1.113069	-1.191118
7	6	0	-2.684817	-0.165338	0.685665
8	8	0	-2.615411	-0.811173	1.719859
9	8	0	-3.832837	0.010301	0.032740
10	7	0	-1.599015	1.114290	-1.171815
11	8	0	-2.574431	1.819096	-1.414316
12	8	0	-0.666058	0.992750	-1.981074
13	6	0	1.002548	0.802396	0.730030
14	6	0	1.863336	0.391756	1.756951
15	6	0	1.365063	1.921536	-0.032694
16	6	0	3.054047	1.063840	2.011059
17	1	0	1.587609	-0.454300	2.376071
18	6	0	2.541564	2.602682	0.237004
19	1	0	0.734598	2.256580	-0.843049
20	6	0	3.396219	2.172492	1.250815
21	1	0	3.703923	0.723432	2.808634
22	1	0	2.800241	3.472613	-0.355845
23	1	0	4.319882	2.705110	1.446495
24	6	0	-5.007956	-0.572892	0.623077
25	1	0	-4.867411	-1.653618	0.699759
26	1	0	-5.131034	-0.173615	1.632205
27	6	0	-6.179590	-0.222443	-0.264310
28	1	0	-6.041644	-0.624342	-1.270320
29	1	0	-7.092816	-0.650550	0.155554
30	1	0	-6.305955	0.859863	-0.333746
31	1	0	-0.338292	-1.448090	-1.406675
32	8	0	3.871540	-1.400999	-0.660775
33	6	0	4.175211	-0.365887	-1.618569
34	1	0	5.252850	-0.243129	-1.569496
35	1	0	3.869937	-0.680775	-2.616393
36	1	0	3.667738	0.556804	-1.336334
37	6	0	2.082593	-2.599701	0.449096
38	6	0	0.710046	-2.515363	0.262974
39	1	0	-0.056054	-3.062801	0.791387
40	1	0	2.640291	-3.193376	1.153134

## TSC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.456256	-1.515151	-0.683181
2	6	0	2.622021	-1.702412	-0.466128
3	6	0	-0.244895	0.024879	0.573138
4	1	0	-0.428927	-0.576997	1.455928
5	6	0	-1.500040	0.414493	0.048315
6	8	0	1.687832	-1.113474	-1.191013
7	6	0	-2.684809	-0.165235	0.685757
8	8	0	-2.615584	-0.810650	1.720225
9	8	0	-3.832659	0.009960	0.032412
10	7	0	-1.598912	1.114223	-1.171713
11	8	0	-2.574267	1.819147	-1.414146
12	8	0	-0.666044	0.992544	-1.981035
13	6	0	1.002615	0.802375	0.730092
14	6	0	1.863391	0.391972	1.757117
15	6	0	1.365116	1.921382	-0.032837
16	6	0	3.054057	1.064166	2.011145
17	1	0	1.587671	-0.453958	2.376408
18	6	0	2.541573	2.602639	0.236775
19	1	0	0.734661	2.256240	-0.843278
20	6	0	3.396205	2.172691	1.250707
21	1	0	3.703915	0.723944	2.808815
22	1	0	2.800228	3.472469	-0.356231
23	1	0	4.319831	2.705396	1.446327
24	6	0	-5.007922	-0.572974	0.622709
25	1	0	-4.867616	-1.653737	0.699345
26	1	0	-5.130938	-0.173715	1.631847
27	6	0	-6.179456	-0.222245	-0.264703
28	1	0	-6.041483	-0.623995	-1.270768
29	1	0	-7.092762	-0.650315	0.155024
30	1	0	-6.305690	0.860087	-0.333974
31	1	0	-0.338680	-1.449212	-1.405761
32	8	0	3.871388	-1.400837	-0.661358
33	6	0	4.174539	-0.365925	-1.619534
34	1	0	5.252175	-0.242975	-1.570886
35	1	0	3.868949	-0.681121	-2.617164
36	1	0	3.667011	0.556750	-1.337349
37	6	0	2.083064	-2.599511	0.449542
38	6	0	0.710445	-2.515505	0.263877
39	1	0	-0.055376	-3.062923	0.792717
40	1	0	2.641136	-3.192846	1.153571

## TSD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.120695	-0.699751	-0.084880
2	6	0	-1.015157	2.054772	0.250127
3	6	0	0.694311	1.504135	1.469963
4	6	0	0.988089	-0.393528	0.725787
5	1	0	0.883003	-0.891401	1.683172
6	8	0	0.299226	2.136813	0.296069
7	7	0	-0.076025	-0.575995	-1.503554
8	8	0	0.620474	0.307121	-1.995969
9	8	0	-0.699443	-1.379228	-2.192638
10	6	0	2.418271	-0.363562	0.288275
11	6	0	3.219999	-1.415791	0.742132
12	6	0	2.999179	0.632192	-0.498513
13	6	0	4.562098	-1.491127	0.391152
14	1	0	2.785723	-2.187826	1.368898
15	6	0	4.345639	0.564575	-0.834672
16	1	0	2.397051	1.458960	-0.846826
17	6	0	5.129791	-0.498145	-0.399037
18	1	0	5.163774	-2.321358	0.743042
19	1	0	4.782579	1.347723	-1.443876
20	1	0	6.178701	-0.548420	-0.668502
21	6	0	-1.293765	-1.294764	0.571237
22	8	0	-1.259385	-1.685633	1.723848
23	8	0	-2.413435	-1.287360	-0.152890
24	6	0	-3.595238	-1.804714	0.482957
25	1	0	-3.398704	-2.824541	0.819866
26	1	0	-3.817764	-1.193548	1.361616
27	6	0	-4.712989	-1.756953	-0.532357
28	1	0	-4.471020	-2.365155	-1.406017
29	1	0	-5.628307	-2.147470	-0.081960
30	1	0	-4.903856	-0.733015	-0.861291
31	1	0	1.692128	1.756234	1.792642
32	8	0	-1.553993	2.459247	-0.865858
33	6	0	-2.970133	2.251864	-0.993048
34	1	0	-3.225557	2.587794	-1.993444
35	1	0	-3.193756	1.189331	-0.881275
36	1	0	-3.505607	2.844234	-0.249173
37	6	0	-1.548614	1.598848	1.456562
38	6	0	-0.451085	1.323108	2.255438
39	1	0	-2.592828	1.466303	1.685023
40	1	0	-0.459139	0.919502	3.255754

## TSE

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.225170	-1.013727	0.056124
2	6	0	-0.845074	2.900414	-0.212189
3	6	0	0.567864	1.470285	-1.077906
4	6	0	0.773548	-0.072274	0.314321
5	1	0	0.465210	0.560316	1.142947
6	8	0	-0.781832	1.792792	-0.932747
7	7	0	-0.026781	-2.043678	-0.906663
8	8	0	-0.490518	-3.159666	-0.714629
9	8	0	0.632674	-1.765623	-1.911058
10	6	0	2.245818	-0.318689	0.314848
11	6	0	2.869207	-0.250859	1.565841
12	6	0	3.029577	-0.568793	-0.812344
13	6	0	4.235879	-0.460037	1.692395
14	1	0	2.275561	-0.038807	2.448897
15	6	0	4.400140	-0.764796	-0.684845
16	1	0	2.573483	-0.608487	-1.790906
17	6	0	5.007358	-0.717285	0.564352
18	1	0	4.697628	-0.413441	2.671999
19	1	0	4.994876	-0.954455	-1.571128
20	1	0	6.076135	-0.872484	0.657890
21	6	0	-1.533997	-0.838976	0.691044
22	8	0	-1.740811	0.000799	1.550189
23	8	0	-2.491570	-1.630711	0.212757
24	6	0	-3.795039	-1.510813	0.810448
25	1	0	-3.705774	-1.682893	1.885106
26	1	0	-4.163691	-0.493482	0.658844
27	6	0	-4.690918	-2.531739	0.149743
28	1	0	-4.310666	-3.542783	0.307522
29	1	0	-5.692240	-2.467863	0.581622
30	1	0	-4.766235	-2.348587	-0.924141
31	1	0	0.782618	0.860348	-1.941631
32	8	0	-2.006491	3.360050	0.158876
33	6	0	-3.185158	2.625923	-0.227685
34	1	0	-4.017172	3.196059	0.174746
35	1	0	-3.251648	2.569241	-1.314366
36	1	0	-3.153662	1.629696	0.211537
37	6	0	0.412804	3.408716	0.071262
38	6	0	1.301526	2.520818	-0.530664
39	1	0	2.379722	2.574956	-0.523893
40	1	0	0.621492	4.288277	0.656024

**TSF**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.504207	0.442095	-0.120591
2	6	0	2.569245	-1.503632	0.856851
3	6	0	0.417421	-1.630625	0.498621
4	6	0	-0.195007	0.103717	-0.517483
5	1	0	-0.278257	-0.499915	-1.415665
6	8	0	1.677154	-1.895554	-0.039135
7	7	0	-1.775612	1.326903	0.946577
8	8	0	-2.793915	2.010852	0.938792
9	8	0	-0.955783	1.391326	1.871310
10	6	0	1.053176	0.899760	-0.552587
11	6	0	1.793669	0.799893	-1.742097
12	6	0	1.568039	1.695214	0.478172
13	6	0	2.980083	1.496065	-1.913977
14	1	0	1.424870	0.172052	-2.546499
15	6	0	2.761615	2.386720	0.306538
16	1	0	1.039221	1.762146	1.415384
17	6	0	3.470107	2.293397	-0.884470
18	1	0	3.524464	1.410476	-2.847371
19	1	0	3.142570	2.995834	1.118214
20	1	0	4.402024	2.833100	-1.009069
21	6	0	-2.589595	-0.315104	-0.752983
22	8	0	-2.379890	-1.119896	-1.647157
23	8	0	-3.802102	-0.121846	-0.238523
24	6	0	-4.874939	-0.896363	-0.804540
25	1	0	-4.937039	-0.682750	-1.873749
26	1	0	-4.648381	-1.957965	-0.681817
27	6	0	-6.142722	-0.506817	-0.081126
28	1	0	-6.354110	0.556525	-0.209943
29	1	0	-6.981162	-1.077095	-0.487676
30	1	0	-6.065429	-0.722159	0.986685
31	1	0	-0.367597	-2.246339	0.087950
32	8	0	3.836534	-1.519980	0.553037
33	6	0	4.212947	-1.937958	-0.771881
34	1	0	5.295572	-1.857909	-0.797511
35	1	0	3.901938	-2.968677	-0.943436
36	1	0	3.762345	-1.273847	-1.510176
37	6	0	1.974068	-1.098142	2.041701
38	6	0	0.607668	-1.224358	1.820340
39	1	0	-0.187605	-0.982452	2.506758
40	1	0	2.490479	-0.731729	2.912361

**TSG**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.294162	-0.338091	-0.036289
2	6	0	3.041375	-1.238766	-0.571292
3	6	0	0.884022	-1.046916	-1.083585
4	6	0	-0.079089	0.133108	-0.791389
5	1	0	-0.463905	0.437964	-1.763052
6	8	0	2.224847	-0.564820	-1.341239
7	7	0	-1.115544	-0.902858	1.172426
8	8	0	-2.017195	-1.254896	1.945953
9	8	0	0.114188	-1.112348	1.531976
10	6	0	0.554755	1.386704	-0.193644
11	6	0	0.154238	2.610303	-0.735013
12	6	0	1.476085	1.396286	0.856086
13	6	0	0.648268	3.811948	-0.241004
14	1	0	-0.559021	2.621807	-1.553069
15	6	0	1.978222	2.597252	1.344904
16	1	0	1.790403	0.468248	1.311793
17	6	0	1.566401	3.809338	0.802422
18	1	0	0.318649	4.748504	-0.676860
19	1	0	2.693944	2.582655	2.159569
20	1	0	1.959084	4.743205	1.188726
21	6	0	-2.599214	-0.105681	-0.654905
22	8	0	-2.697757	0.399175	-1.763019
23	8	0	-3.662284	-0.477352	0.053284
24	6	0	-4.947278	-0.250248	-0.553770
25	1	0	-5.051398	0.814793	-0.772439
26	1	0	-4.993982	-0.796845	-1.498426
27	6	0	-5.996721	-0.727102	0.423161
28	1	0	-5.934819	-0.173633	1.362360
29	1	0	-6.989245	-0.569723	-0.005455
30	1	0	-5.877580	-1.791578	0.635658
31	1	0	0.561363	-1.542510	-2.002435
32	8	0	4.282508	-0.917105	-0.703588
33	6	0	5.242431	-1.578572	0.147936
34	1	0	6.198499	-1.127188	-0.096657
35	1	0	4.992349	-1.398279	1.193457
36	1	0	5.258093	-2.645387	-0.074989
37	6	0	2.419731	-2.199286	0.229851
38	6	0	1.069550	-2.076593	-0.019263
39	1	0	2.910510	-2.895540	0.887683
40	1	0	0.329736	-2.839818	0.164983



**TSI**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.483807	-1.691113	-0.730914
2	6	0	1.630062	-2.312634	-0.423417
3	6	0	-0.877608	-0.201311	-0.758109
4	1	0	-0.722502	0.120829	-1.790170
5	6	0	0.085065	0.603042	0.068529
6	8	0	0.829864	-1.801841	-1.328732
7	6	0	0.937742	1.572929	-0.613160
8	8	0	0.811430	1.799613	-1.806323
9	8	0	1.861962	2.173092	0.133508
10	7	0	0.119349	0.347615	1.388983
11	8	0	-0.623968	-0.633890	1.792716
12	8	0	0.793858	0.957001	2.229922
13	6	0	-2.344039	0.050038	-0.424009
14	6	0	-2.764065	1.376440	-0.301869
15	6	0	-3.293285	-0.959970	-0.285805
16	6	0	-4.091972	1.684762	-0.042005
17	1	0	-2.039528	2.176708	-0.409460
18	6	0	-4.626188	-0.653906	-0.023137
19	1	0	-3.019354	-2.005032	-0.370124
20	6	0	-5.031497	0.667883	0.100372
21	1	0	-4.393805	2.722141	0.049280
22	1	0	-5.345837	-1.457222	0.088089
23	1	0	-6.068737	0.905414	0.307137
24	6	0	2.714488	3.116364	-0.540990
25	1	0	3.236030	2.604661	-1.353033
26	1	0	2.094969	3.902735	-0.977870
27	6	0	3.677634	3.666989	0.484613
28	1	0	4.286487	2.869667	0.916061
29	1	0	4.343579	4.388553	0.005629
30	1	0	3.142429	4.173630	1.290259
31	1	0	-1.150517	-2.289851	-1.353077
32	8	0	2.854492	-2.438417	-0.810440
33	6	0	3.807231	-2.957992	0.140691
34	1	0	4.764095	-2.931854	-0.370726
35	1	0	3.830266	-2.320238	1.024399
36	1	0	3.544738	-3.983269	0.402144
37	6	0	1.000664	-2.670373	0.767298
38	6	0	-0.318684	-2.278735	0.636192
39	1	0	1.461157	-3.156783	1.609860
40	1	0	-1.150464	-2.672334	1.197818

**TSJ**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.820658	-1.822668	-1.069169
2	6	0	1.183518	-1.764867	-0.306720
3	6	0	-0.957608	-0.264253	-0.825546
4	1	0	-0.758448	0.156178	-1.812783
5	6	0	0.254685	0.114444	-0.003173
6	8	0	0.553259	-1.888144	-1.482432
7	6	0	1.238571	1.004377	-0.691420
8	8	0	1.075783	1.372493	-1.836831
9	8	0	2.339012	1.263731	-0.001962
10	7	0	0.039440	0.281110	1.413283
11	8	0	-0.959199	-0.250583	1.889010
12	8	0	0.847292	0.887876	2.108512
13	6	0	-2.319744	0.248454	-0.416431
14	6	0	-2.482890	1.621451	-0.219399
15	6	0	-3.435638	-0.576290	-0.308151
16	6	0	-3.724011	2.152347	0.102572
17	1	0	-1.626190	2.281307	-0.315883
18	6	0	-4.683343	-0.046155	0.008447
19	1	0	-3.352838	-1.645708	-0.465045
20	6	0	-4.832305	1.318265	0.219626
21	1	0	-3.827068	3.220216	0.259630
22	1	0	-5.539268	-0.706572	0.091818
23	1	0	-5.802940	1.730321	0.470942
24	6	0	3.361789	2.022437	-0.676581
25	1	0	3.654513	1.484544	-1.580952
26	1	0	2.945794	2.987937	-0.971540
27	6	0	4.514360	2.176839	0.287153
28	1	0	4.917047	1.203275	0.574114
29	1	0	5.311426	2.750440	-0.191064
30	1	0	4.200824	2.706382	1.188916
31	1	0	-1.461735	-2.185840	-1.866539
32	8	0	2.481975	-1.629084	-0.415298
33	6	0	3.241191	-1.641281	0.805730
34	1	0	4.262137	-1.413941	0.512767
35	1	0	2.868642	-0.870921	1.481518
36	1	0	3.198299	-2.629882	1.265104
37	6	0	0.429649	-2.512308	0.704905
38	6	0	-0.814061	-2.579470	0.220395
39	1	0	0.794887	-2.811212	1.674454
40	1	0	-1.687166	-2.982537	0.710143

**TSK**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.208444	-0.288998	0.012217
2	6	0	-0.953061	1.824974	0.008783
3	6	0	0.693503	1.572346	1.368287
4	6	0	0.940854	0.062921	0.925326
5	1	0	0.807747	-0.544599	1.820496
6	8	0	0.303721	2.217013	0.150578
7	7	0	0.030991	-0.425797	-1.380633
8	8	0	0.876010	0.298855	-1.899621
9	8	0	-0.623421	-1.239325	-2.037582
10	6	0	2.346692	-0.213997	0.429725
11	6	0	2.798933	-1.533271	0.475903
12	6	0	3.207507	0.772880	-0.043349
13	6	0	4.081924	-1.861795	0.055452
14	1	0	2.136598	-2.310693	0.844649
15	6	0	4.495521	0.449155	-0.454802
16	1	0	2.872695	1.800534	-0.119766
17	6	0	4.937373	-0.868327	-0.408687
18	1	0	4.414374	-2.893021	0.096427
19	1	0	5.151828	1.229920	-0.822743
20	1	0	5.940714	-1.119396	-0.733780
21	6	0	-1.251828	-1.162479	0.612791
22	8	0	-1.092835	-1.763056	1.655440
23	8	0	-2.421435	-1.124306	-0.021845
24	6	0	-3.483379	-1.938463	0.511574
25	1	0	-3.163810	-2.982571	0.494259
26	1	0	-3.659194	-1.650938	1.550363
27	6	0	-4.702978	-1.710192	-0.350083
28	1	0	-4.502506	-1.979725	-1.388841
29	1	0	-5.525058	-2.329756	0.014768
30	1	0	-5.021304	-0.665782	-0.311930
31	1	0	1.576033	2.052517	1.778024
32	8	0	-1.486707	2.122601	-1.137525
33	6	0	-2.898852	1.885942	-1.305029
34	1	0	-3.107448	2.131724	-2.341722
35	1	0	-3.116052	0.836684	-1.110003
36	1	0	-3.466439	2.541115	-0.643010
37	6	0	-1.577954	1.694776	1.327944
38	6	0	-0.553944	1.605036	2.183959
39	1	0	-2.636503	1.607437	1.514551
40	1	0	-0.592490	1.419839	3.247052

## TSL

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.070797	-0.034420	0.300605
2	6	0	2.779046	-2.210663	0.314338
3	6	0	1.155722	-0.726878	0.416662
4	6	0	0.296815	0.285159	-0.328778
5	1	0	0.209319	-0.118369	-1.341447
6	8	0	1.809168	-1.677920	-0.399186
7	7	0	-1.364374	0.612825	1.529653
8	8	0	-2.511690	0.683786	1.959413
9	8	0	-0.399614	1.060223	2.163611
10	6	0	0.748263	1.722678	-0.433239
11	6	0	2.085730	2.079556	-0.285434
12	6	0	-0.183071	2.710956	-0.750692
13	6	0	2.486386	3.402311	-0.444470
14	1	0	2.826695	1.325891	-0.040438
15	6	0	0.214386	4.032910	-0.906505
16	1	0	-1.228477	2.447471	-0.875352
17	6	0	1.551951	4.383845	-0.752857
18	1	0	3.531422	3.664478	-0.322856
19	1	0	-0.523061	4.790331	-1.147219
20	1	0	1.862632	5.415648	-0.871111
21	6	0	-2.153837	-0.429717	-0.627778
22	8	0	-2.008288	-0.386504	-1.835065
23	8	0	-3.239013	-0.924288	-0.046196
24	6	0	-4.299716	-1.359200	-0.919467
25	1	0	-4.607450	-0.517460	-1.543510
26	1	0	-3.916531	-2.146358	-1.572678
27	6	0	-5.429022	-1.852929	-0.046372
28	1	0	-5.796566	-1.055911	0.602903
29	1	0	-6.253272	-2.191311	-0.678371
30	1	0	-5.105168	-2.690673	0.574756
31	1	0	-0.129357	-1.093822	0.745243
32	8	0	3.466696	-3.200481	-0.171532
33	6	0	3.182122	-3.638080	-1.516443
34	1	0	3.883928	-4.444672	-1.704502
35	1	0	2.156217	-3.999653	-1.580517
36	1	0	3.342693	-2.818812	-2.217098
37	6	0	2.899842	-1.619863	1.567190
38	6	0	1.911794	-0.651915	1.607011
39	1	0	1.692962	0.035786	2.407415
40	1	0	3.612879	-1.893366	2.326228

## TSM

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.070773	-0.034621	0.300667
2	6	0	2.779389	-2.210340	0.314212
3	6	0	1.155821	-0.726816	0.416695
4	6	0	0.296797	0.285136	-0.328730
5	1	0	0.209316	-0.118394	-1.341400
6	8	0	1.809349	-1.677769	-0.399209
7	7	0	-1.364379	0.612496	1.529778
8	8	0	-2.511673	0.683223	1.959628
9	8	0	-0.399646	1.060009	2.163694
10	6	0	0.748052	1.722715	-0.433202
11	6	0	2.085428	2.079845	-0.285185
12	6	0	-0.183400	2.710806	-0.750896
13	6	0	2.485873	3.402660	-0.444253
14	1	0	2.826491	1.326332	-0.040024
15	6	0	0.213846	4.032819	-0.906738
16	1	0	-1.228736	2.447125	-0.875723
17	6	0	1.551321	4.384005	-0.752882
18	1	0	3.530843	3.665022	-0.322478
19	1	0	-0.523694	4.790087	-1.147648
20	1	0	1.861840	5.415854	-0.871164
21	6	0	-2.153800	-0.429903	-0.627738
22	8	0	-2.008263	-0.386587	-1.835023
23	8	0	-3.238953	-0.924551	-0.046187
24	6	0	-4.299672	-1.359401	-0.919468
25	1	0	-4.607432	-0.517612	-1.543435
26	1	0	-3.916499	-2.146501	-1.572756
27	6	0	-5.428950	-1.853214	-0.046382
28	1	0	-5.796445	-1.056267	0.603006
29	1	0	-6.253236	-2.191501	-0.678384
30	1	0	-5.105084	-2.691040	0.574629
31	1	0	-0.129218	-1.093913	0.745265
32	8	0	3.467165	-3.200041	-0.171712
33	6	0	3.182507	-3.637759	-1.516566
34	1	0	3.884368	-4.444301	-1.704632
35	1	0	2.156629	-3.999429	-1.580526
36	1	0	3.342940	-2.818525	-2.217291
37	6	0	2.900226	-1.619504	1.567045
38	6	0	1.912030	-0.651720	1.606957
39	1	0	1.693173	0.035944	2.407384
40	1	0	3.613395	-1.892878	2.326006

# TSN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.887896	-0.978210	-0.836802
2	6	0	-2.690515	-2.134783	-0.346284
3	6	0	-0.074839	0.307651	-0.747771
4	1	0	0.341857	0.414556	-1.753876
5	6	0	1.130843	-0.193110	0.067935
6	8	0	-1.867163	-1.237732	0.145114
7	6	0	2.450175	-0.076746	-0.590104
8	8	0	2.552709	0.371076	-1.719103
9	8	0	3.484777	-0.559312	0.085634
10	7	0	0.997517	-0.191371	1.486761
11	8	0	1.947818	-0.470411	2.212941
12	8	0	-0.125196	0.043292	1.940935
13	6	0	-0.763335	1.604486	-0.405165
14	6	0	-2.109830	1.798120	-0.704646
15	6	0	-0.033492	2.659986	0.138521
16	6	0	-2.718773	3.024540	-0.459658
17	1	0	-2.693860	0.991092	-1.134489
18	6	0	-0.639647	3.885587	0.383285
19	1	0	1.016800	2.524560	0.376252
20	6	0	-1.986277	4.071959	0.086567
21	1	0	-3.768479	3.159179	-0.695684
22	1	0	-0.059176	4.695913	0.809787
23	1	0	-2.460939	5.026912	0.281293
24	6	0	4.766675	-0.496450	-0.569588
25	1	0	4.711612	-1.057737	-1.505011
26	1	0	4.988391	0.545506	-0.809911
27	6	0	5.785523	-1.082689	0.379142
28	1	0	5.549852	-2.123318	0.611365
29	1	0	6.773868	-1.048430	-0.084957
30	1	0	5.821931	-0.515123	1.311149
31	1	0	0.327753	-1.384427	-0.341013
32	8	0	-3.634020	-2.618124	0.404236
33	6	0	-3.771901	-2.096422	1.743730
34	1	0	-4.624095	-2.621742	2.163551
35	1	0	-2.869468	-2.304565	2.317246
36	1	0	-3.959485	-1.023461	1.707539
37	6	0	-2.385811	-2.474199	-1.663066
38	6	0	-1.284829	-1.702485	-1.981048
39	1	0	-0.758412	-1.675032	-2.924067
40	1	0	-2.908608	-3.198010	-2.264832

## TSO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.888036	-0.978114	-0.836753
2	6	0	-2.690759	-2.134594	-0.346381
3	6	0	-0.074872	0.307646	-0.747606
4	1	0	0.341831	0.414554	-1.753712
5	6	0	1.130809	-0.193306	0.067962
6	8	0	-1.867328	-1.237672	0.145130
7	6	0	2.450091	-0.076919	-0.590159
8	8	0	2.552550	0.370856	-1.719185
9	8	0	3.484741	-0.559384	0.085562
10	7	0	0.997603	-0.191750	1.486802
11	8	0	1.947852	-0.471320	2.212848
12	8	0	-0.124993	0.043232	1.941102
13	6	0	-0.763205	1.604566	-0.404998
14	6	0	-2.109664	1.798381	-0.704524
15	6	0	-0.033235	2.659972	0.138699
16	6	0	-2.718441	3.024893	-0.459584
17	1	0	-2.693795	0.991430	-1.134373
18	6	0	-0.639223	3.885665	0.383412
19	1	0	1.017026	2.524400	0.376482
20	6	0	-1.985816	4.072222	0.086640
21	1	0	-3.768121	3.159675	-0.695649
22	1	0	-0.058654	4.695918	0.809921
23	1	0	-2.460349	5.027247	0.281323
24	6	0	4.766620	-0.496500	-0.569696
25	1	0	4.711550	-1.057817	-1.505099
26	1	0	4.988294	0.545457	-0.810050
27	6	0	5.785507	-1.082676	0.379034
28	1	0	5.549908	-2.123323	0.611250
29	1	0	6.773852	-1.048344	-0.085058
30	1	0	5.821868	-0.515114	1.311046
31	1	0	0.327628	-1.384574	-0.341105
32	8	0	-3.634355	-2.617890	0.404054
33	6	0	-3.772187	-2.096336	1.743608
34	1	0	-4.624510	-2.621535	2.163320
35	1	0	-2.869823	-2.304748	2.317135
36	1	0	-3.959547	-1.023331	1.707553
37	6	0	-2.386047	-2.473923	-1.663180
38	6	0	-1.284992	-1.702274	-1.981072
39	1	0	-0.758533	-1.674811	-2.924067
40	1	0	-2.908891	-3.197636	-2.265024

## TSP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.395070	-0.566276	0.165941
2	6	0	3.320220	-1.151926	-0.145953
3	6	0	0.937310	-1.296090	0.582864
4	6	0	0.046112	-0.317279	-0.183346
5	1	0	0.163876	-0.560687	-1.239539
6	8	0	2.266083	-1.449976	-0.734006
7	7	0	-1.619377	-1.109439	1.370655
8	8	0	-2.725704	-1.344344	1.873024
9	8	0	-0.553551	-1.406451	2.047915
10	6	0	0.504620	1.119398	0.018330
11	6	0	1.355041	1.711339	-0.911986
12	6	0	0.125605	1.843000	1.148042
13	6	0	1.830258	3.003678	-0.714091
14	1	0	1.642942	1.159778	-1.801203
15	6	0	0.599054	3.134057	1.348220
16	1	0	-0.543551	1.396380	1.875988
17	6	0	1.455403	3.716819	0.418921
18	1	0	2.487615	3.454937	-1.448837
19	1	0	0.296779	3.687140	2.230385
20	1	0	1.822415	4.725050	0.574255
21	6	0	-2.405547	-0.160496	-0.793427
22	8	0	-2.091159	0.341755	-1.861734
23	8	0	-3.673021	-0.373405	-0.441542
24	6	0	-4.676157	0.024289	-1.392960
25	1	0	-4.568208	1.092205	-1.595572
26	1	0	-4.512371	-0.516721	-2.327836
27	6	0	-6.023324	-0.297425	-0.788813
28	1	0	-6.171101	0.246623	0.146370
29	1	0	-6.812407	-0.005942	-1.485978
30	1	0	-6.116709	-1.367120	-0.589971
31	1	0	0.720964	-2.352165	0.484159
32	8	0	4.483029	-1.142388	-0.714570
33	6	0	4.543209	-1.481771	-2.119554
34	1	0	5.593348	-1.406589	-2.383066
35	1	0	4.176250	-2.496318	-2.267012
36	1	0	3.946297	-0.772569	-2.691665
37	6	0	3.195386	-0.798318	1.257823
38	6	0	1.918107	-0.875698	1.623342
39	1	0	1.551884	-0.649551	2.613498
40	1	0	4.030828	-0.513711	1.878625