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Waste Management in Zinc Promoted Allylation of aldehyde

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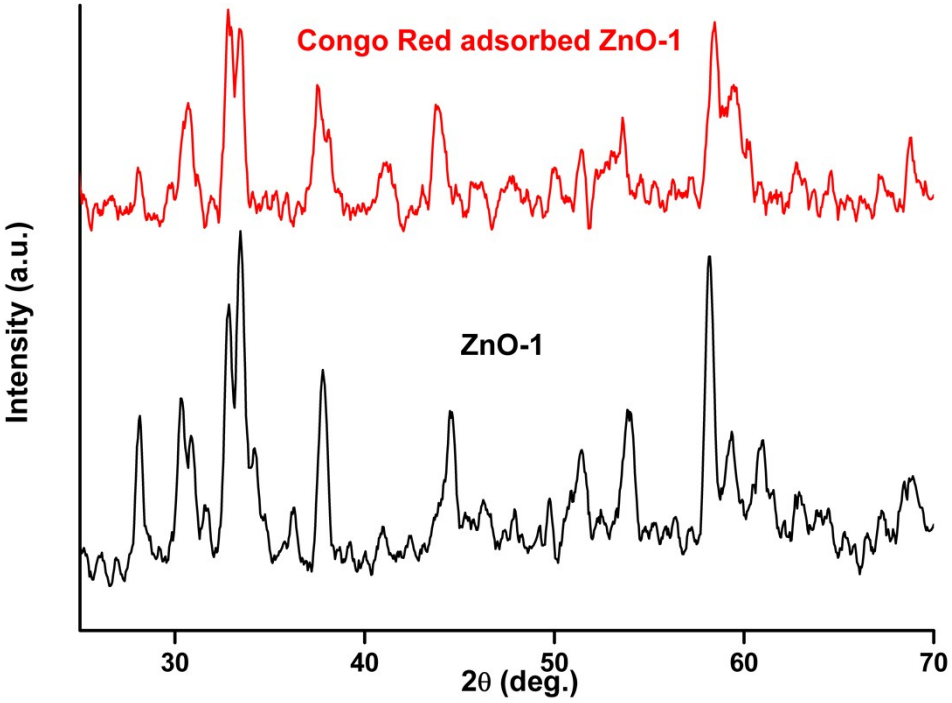

Figure S1. XRD pattern of ZnO-1 material before and after the 7 cycle of use in adsorption of Congo Red.

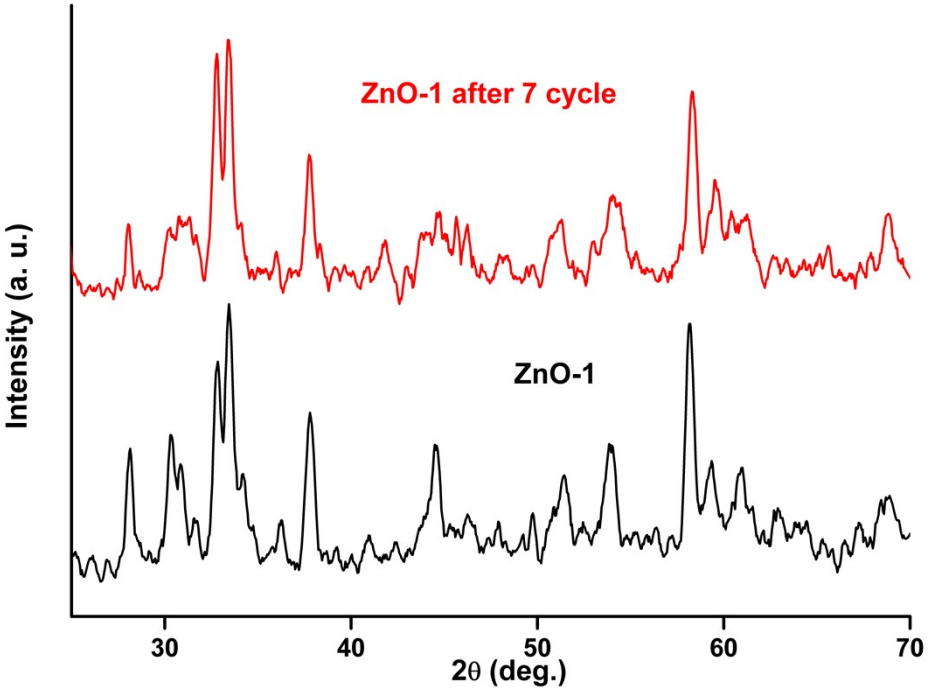

Figure S2. XRD pattern of ZnO-1 material before and after the 7 cycle of use in adsorption of Congo Red.

The Cartesian coordinates of the optimized geometries, Frequency data, and NImag Obtained at the B3LYP/LANL2DZ/6-31G* Level of Theory

Optimized Geometry:

Zn(allyl)Br(PhCHO) Reactant

Cartesian Coordinates (Angstroms):

1	30	0	-1.708411	0.467446	0.128811
2	6	0	-1.366902	2.483731	0.430899
3	6	0	0.058501	2.755325	0.710361
4	6	0	0.995839	3.159444	-0.166314
5	6	0	1.218052	-0.019119	-0.687667
6	8	0	0.210719	-0.428683	-0.094520
7	1	0	-1.717143	2.988996	-0.477135
8	1	0	-2.015115	2.778153	1.262927
9	1	0	0.380790	2.566566	1.737279
10	1	0	2.025678	3.324490	0.137288
11	1	0	0.748525	3.387450	-1.202503
12	35	0	-3.374702	-1.280208	-0.163033
13	1	0	1.114316	0.637107	-1.565012
14	6	0	5.191185	-1.116582	0.337603
15	6	0	4.120741	-1.620722	1.087471
16	6	0	2.817104	-1.265143	0.762695
17	6	0	2.579465	-0.397484	-0.319021
18	6	0	3.656984	0.103330	-1.068832
19	6	0	4.961254	-0.255863	-0.739880
20	1	0	6.208703	-1.397925	0.594768
21	1	0	4.309894	-2.290972	1.920758
22	1	0	1.971396	-1.647945	1.324891
23	1	0	3.465067	0.774914	-1.902178
24	1	0	5.795712	0.131022	-1.317010

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.182147 (Hartree/Particle)
Thermal correction to Energy= 0.197360
Thermal correction to Enthalpy= 0.198305
Thermal correction to Gibbs Free Energy= 0.134295
Sum of electronic and zero-point Energies= -541.515120
Sum of electronic and thermal Energies= -541.499907
Sum of electronic and thermal Enthalpies= -541.498962
Sum of electronic and thermal Free Energies= -541.562972

Zn(allyl)Br(4OMe-C_6H_4-CHO) Reactant

Cartesian Coordinates (Angstroms):

1	30	0	2.488194	0.267432	0.245660
2	6	0	2.878734	2.255395	0.612101
3	6	0	2.144160	3.132119	-0.334769
4	6	0	1.044346	3.861680	-0.080246
5	6	0	-0.560227	0.567657	-0.134866
6	8	0	0.386891	-0.142179	0.243132
7	1	0	2.613492	2.468938	1.654433
8	1	0	3.963466	2.366539	0.502455
9	1	0	2.545929	3.165092	-1.350999
10	1	0	0.575119	4.471871	-0.847544
11	1	0	0.601781	3.900237	0.914219
12	35	0	3.494251	-1.890608	-0.291183
13	1	0	-0.356014	1.567126	-0.551843
14	6	0	-4.645481	-0.570736	0.091873
15	6	0	-3.644128	-1.464303	0.532688
16	6	0	-2.315434	-1.102429	0.463312
17	6	0	-1.947527	0.162875	-0.048703
18	6	0	-2.950790	1.043587	-0.486131
19	6	0	-4.293268	0.690456	-0.420258
20	1	0	-3.952454	-2.430069	0.919287
21	1	0	-1.535643	-1.780618	0.794800
22	1	0	-2.672322	2.018132	-0.880220
23	1	0	-5.050759	1.385284	-0.762279
24	8	0	-5.911276	-1.022936	0.203339
25	6	0	-6.986667	-0.189851	-0.222761
26	1	0	-6.910478	0.040149	-1.292169
27	1	0	-7.894787	-0.764418	-0.037630
28	1	0	-7.019150	0.742273	0.353900

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.215042 (Hartree/Particle)
Thermal correction to Energy= 0.232985
Thermal correction to Enthalpy= 0.233930
Thermal correction to Gibbs Free Energy= 0.162883
Sum of electronic and zero-point Energies= -656.008533
Sum of electronic and thermal Energies= -655.990589
Sum of electronic and thermal Enthalpies= -655.989645
Sum of electronic and thermal Free Energies= -656.060691

Zn(allyl)Br(4Cl-C_6H_4-CHO) Reactant

Cartesian Coordinates (Angstroms):

1	30	0	2.441147	0.382731	-0.167646
2	6	0	2.257930	2.407249	-0.546765
3	6	0	0.849996	2.787791	-0.778821
4	6	0	-0.009356	3.310930	0.115227
5	6	0	-0.480246	0.216540	0.783268
6	8	0	0.453627	-0.318367	0.169952
7	1	0	2.691651	2.917977	0.321167
8	1	0	2.889757	2.606098	-1.418684
9	1	0	0.466542	2.582063	-1.781114
10	1	0	-1.033262	3.553367	-0.154657
11	1	0	0.303297	3.564474	1.127498
12	35	0	3.948940	-1.499179	0.131867
13	1	0	-0.275335	0.887823	1.630471
14	6	0	-4.570317	-0.513072	-0.052115
15	6	0	-3.593746	-1.160416	-0.819764
16	6	0	-2.253790	-0.918524	-0.550451
17	6	0	-1.886228	-0.033843	0.479652
18	6	0	-2.881911	0.602673	1.238812
19	6	0	-4.227315	0.368207	0.977594
20	1	0	-3.890643	-1.841274	-1.609875
21	1	0	-1.475879	-1.411135	-1.124796
22	1	0	-2.598792	1.287672	2.034085
23	1	0	-5.003701	0.855742	1.556534
24	17	0	-6.257650	-0.815984	-0.388589

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172416 (Hartree/Particle)
Thermal correction to Energy= 0.188830
Thermal correction to Enthalpy= 0.189774
Thermal correction to Gibbs Free Energy= 0.122422
Sum of electronic and zero-point Energies= -1001.115936
Sum of electronic and thermal Energies= -1001.099522
Sum of electronic and thermal Enthalpies= -1001.098578
Sum of electronic and thermal Free Energies= -1001.165930

Zn(allyl)Br(PhCHO) TS

Cartesian Coordinates (Angstroms):

1	30	0	1.570788	0.264846	0.145857
2	6	0	1.102536	2.237609	0.884522
3	6	0	0.015798	2.592279	0.044347
4	6	0	-1.299363	2.175994	0.199273
5	6	0	-1.237453	0.204588	-0.718027
6	8	0	-0.224682	-0.428499	-0.249025
7	1	0	0.868558	2.027488	1.930544
8	1	0	2.033706	2.787766	0.750553
9	1	0	0.267044	3.114019	-0.882454
10	1	0	-2.073619	2.619076	-0.419102
11	1	0	-1.627514	1.813255	1.170057
12	35	0	3.629957	-0.949225	-0.181198
13	1	0	-1.157940	0.643335	-1.721527
14	6	0	-5.188848	-1.075102	0.340945
15	6	0	-4.090587	-1.502102	1.093710
16	6	0	-2.805051	-1.082762	0.758537
17	6	0	-2.606829	-0.225406	-0.333792
18	6	0	-3.711715	0.194600	-1.089127
19	6	0	-4.996539	-0.228042	-0.754018
20	1	0	-6.190005	-1.406305	0.602720
21	1	0	-4.237575	-2.169167	1.938761
22	1	0	-1.942206	-1.422592	1.322204
23	1	0	-3.560548	0.850354	-1.944340
24	1	0	-5.846262	0.098297	-1.347247

Frequency Data:
NImag: 1 (-271.5195)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.183189 (Hartree/Particle)
Thermal correction to Energy= 0.196709
Thermal correction to Enthalpy= 0.197653
Thermal correction to Gibbs Free Energy= 0.139609
Sum of electronic and zero-point Energies= -541.509443
Sum of electronic and thermal Energies= -541.495924
Sum of electronic and thermal Enthalpies= -541.494979
Sum of electronic and thermal Free Energies= -541.553024

Zn(allyl)Br(4OMe-C_6H_4-CHO) TS

Cartesian Coordinates (Angstroms):

1	30	0	-2.299783	0.211121	-0.149532
2	6	0	-2.009391	2.207046	-0.937913
3	6	0	-0.956561	2.657301	-0.104727
4	6	0	0.387336	2.322767	-0.240528
5	6	0	0.489843	0.419342	0.721174
6	8	0	-0.462726	-0.317854	0.261809
7	1	0	-1.759438	1.985109	-1.977685
8	1	0	-2.983771	2.678450	-0.813666
9	1	0	-1.248400	3.183070	0.807873
10	1	0	1.123686	2.851777	0.356598
11	1	0	0.741882	1.966858	-1.204835
12	35	0	-4.271422	-1.140527	0.186649
13	1	0	0.361304	0.865720	1.716666
14	6	0	4.551909	-0.604642	-0.220346
15	6	0	3.494062	-1.127434	-0.985739
16	6	0	2.183809	-0.791612	-0.686889

17	6	0	1.891222	0.077250	0.379793
18	6	0	2.950811	0.588709	1.137172
19	6	0	4.274741	0.257764	0.849994
20	1	0	3.732837	-1.802065	-1.801866
21	1	0	1.364522	-1.209676	-1.262739
22	1	0	2.742299	1.254264	1.972578
23	1	0	5.071858	0.665638	1.460588
24	8	0	5.798823	-0.998650	-0.593122
25	6	0	6.911776	-0.521895	0.149013
26	1	0	6.859903	-0.838122	1.198940
27	1	0	7.793201	-0.964107	-0.318183
28	1	0	6.987261	0.572369	0.103462

Frequency Data:
NImag: 1 (- -302.0053)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.216059 (Hartree/Particle)
Thermal correction to Energy= 0.232157
Thermal correction to Enthalpy= 0.233102
Thermal correction to Gibbs Free Energy= 0.168999
Sum of electronic and zero-point Energies= -655.998937
Sum of electronic and thermal Energies= -655.982839
Sum of electronic and thermal Enthalpies= -655.981895
Sum of electronic and thermal Free Energies= -656.045998

Zn(allyl)Br(4Cl-C_6H_4-CHO) TS

Cartesian Coordinates (Angstroms):

1	30	0	-2.284620	0.213676	-0.177784
2	6	0	-1.965196	2.170041	-1.023691
3	6	0	-0.948107	2.681990	-0.175029
4	6	0	0.404685	2.390435	-0.262006
5	6	0	0.483483	0.463473	0.793083
6	8	0	-0.445814	-0.283906	0.326545
7	1	0	-1.672538	1.921610	-2.046353
8	1	0	-2.946712	2.639262	-0.957450
9	1	0	-1.282329	3.236181	0.705500
10	1	0	1.109696	2.941546	0.352409
11	1	0	0.803041	1.992754	-1.191942
12	35	0	-4.217481	-1.187204	0.161892
13	1	0	0.322294	0.962068	1.757720
14	6	0	4.560908	-0.495749	-0.044189
15	6	0	3.548134	-1.085509	-0.804485
16	6	0	2.221081	-0.764328	-0.534366
17	6	0	1.899541	0.143977	0.484902
18	6	0	2.932914	0.717261	1.240239
19	6	0	4.264437	0.403367	0.982375
20	1	0	3.800189	-1.790244	-1.589643
21	1	0	1.418799	-1.226096	-1.100374
22	1	0	2.694392	1.413121	2.041522
23	1	0	5.064175	0.843086	1.568386
24	17	0	6.234980	-0.898230	-0.377990

Frequency Data:
NImag: 1 (-260.0175)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.
Zero-point correction= 0.173359 (Hartree/Particle)
Thermal correction to Energy= 0.188168
Thermal correction to Enthalpy= 0.189112
Thermal correction to Gibbs Free Energy= 0.127303
Sum of electronic and zero-point Energies= -1001.111137
Sum of electronic and thermal Energies= -1001.096328
Sum of electronic and thermal Enthalpies= -1001.095384
Sum of electronic and thermal Free Energies= -1001.157193

Zn(allyl)Br(4Cl-C_6H_4-CHO)(H_2O) React

Cartesian Coordinates (Angstroms):

1	30	0	1.437680	0.617418	0.008054
2	6	0	1.060716	2.266397	-1.209767
3	6	0	-0.384838	2.375549	-1.451811
4	6	0	-1.271622	3.125786	-0.764615
5	6	0	-1.349498	0.938443	1.289280
6	8	0	-0.128598	0.748252	1.396411
7	1	0	1.464709	3.138491	-0.682217
8	1	0	1.626955	2.101954	-2.132157
9	1	0	-0.779818	1.733935	-2.243108
10	1	0	-2.327552	3.130610	-1.019119
11	1	0	-0.951988	3.811325	0.018534
12	1	0	-1.786974	1.827692	1.770433
13	6	0	-4.175525	-1.721177	-0.457456
14	6	0	-2.822343	-2.076879	-0.431905
15	6	0	-1.883236	-1.216872	0.129417
16	6	0	-2.299887	0.015791	0.664844
17	6	0	-3.662146	0.363006	0.643471
18	6	0	-4.596851	-0.501534	0.082466
19	1	0	-4.904167	-2.397898	-0.895695
20	1	0	-2.500618	-3.027836	-0.846086
21	1	0	-0.834546	-1.497408	0.163277
22	1	0	-3.977860	1.315800	1.062256
23	1	0	-5.648442	-0.230374	0.063905
24	35	0	2.123533	-1.803169	-0.319385
25	1	0	3.902647	1.287207	1.065143
26	1	0	3.422905	-0.168253	1.339077
27	8	0	3.147607	0.770758	1.392222

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.206889 (Hartree/Particle)
Thermal correction to Energy= 0.224776
Thermal correction to Enthalpy= 0.225720
Thermal correction to Gibbs Free Energy= 0.157791
Sum of electronic and zero-point Energies= -617.926693
Sum of electronic and thermal Energies= -617.908806
Sum of electronic and thermal Enthalpies= -617.907862
Sum of electronic and thermal Free Energies= -617.975792

Zn(allyl)Br(4Cl-C_6H_4-CHO)(H_2O) TS

Cartesian Coordinates (Angstroms):

1	30	0	-1.469805	0.418496	-0.028063
2	6	0	-0.974408	2.017199	-1.377714
3	6	0	0.188994	2.579300	-0.785324
4	6	0	1.477036	2.085799	-0.893194
5	6	0	1.433813	0.510999	0.711283
6	8	0	0.343608	-0.143398	0.608205
7	1	0	-0.833024	1.468958	-2.311749
8	1	0	-1.870643	2.638758	-1.378884
9	1	0	0.026072	3.388903	-0.069370
10	1	0	2.310298	2.661135	-0.502410
11	1	0	1.717695	1.386155	-1.689319
12	35	0	-3.315755	-1.245369	-0.213875
13	1	0	1.504125	1.304255	1.468561
14	6	0	5.158165	-1.368891	-0.260317
15	6	0	3.954227	-1.941246	-0.682888
16	6	0	2.741194	-1.328206	-0.377837
17	6	0	2.722384	-0.128630	0.350364
18	6	0	3.933406	0.437724	0.776476
19	6	0	5.145377	-0.178996	0.473251
20	1	0	6.102655	-1.850920	-0.497512
21	1	0	3.962748	-2.870514	-1.246023
22	1	0	1.798564	-1.770613	-0.683761
23	1	0	3.921481	1.362603	1.349818
24	1	0	6.078526	0.264000	0.810241
25	8	0	-2.181305	0.909704	2.001555
26	1	0	-1.568068	0.459896	2.608426
27	1	0	-2.984419	0.349665	1.986831

Frequency Data:
NImag: 1 (-226.0996)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.207772 (Hartree/Particle)
Thermal correction to Energy= 0.224237
Thermal correction to Enthalpy= 0.225181
Thermal correction to Gibbs Free Energy= 0.160310
Sum of electronic and zero-point Energies= -617.922713
Sum of electronic and thermal Energies= -617.906248
Sum of electronic and thermal Enthalpies= -617.905304
Sum of electronic and thermal Free Energies= -617.970174

Zn(allyl)Br(4Cl-C_6H_4-CHO)(NH_3) React

Cartesian Coordinates (Angstroms):

1	30	0	1.506016	0.600069	-0.021090

2	6	0	1.066376	2.161873	-1.349291
3	6	0	-0.380910	2.243852	-1.564521
4	6	0	-1.261683	3.037695	-0.915911
5	6	0	-1.319415	1.027453	1.233900
6	8	0	-0.100209	0.837385	1.371519
7	1	0	1.479242	3.073940	-0.901708
8	1	0	1.614042	1.922809	-2.266607
9	1	0	-0.789671	1.538971	-2.292469
10	1	0	-2.322394	3.016181	-1.148258
11	1	0	-0.931309	3.788371	-0.199586
12	1	0	-1.761691	1.941739	1.661221
13	6	0	-4.150980	-1.723710	-0.360468
14	6	0	-2.796428	-2.072672	-0.330622
15	6	0	-1.854453	-1.183790	0.179486
16	6	0	-2.269766	0.072582	0.657371
17	6	0	-3.633573	0.413922	0.630545
18	6	0	-4.570963	-0.479978	0.122796
19	1	0	-4.881345	-2.423176	-0.758389
20	1	0	-2.474201	-3.040756	-0.702711
21	1	0	-0.804309	-1.459313	0.210861
22	1	0	-3.948926	1.385561	1.004137
23	1	0	-5.623570	-0.212680	0.101061
24	35	0	2.085265	-1.835848	-0.341653
25	7	0	2.943921	0.903492	1.623519
26	1	0	3.691371	1.583650	1.492525
27	1	0	2.442372	1.145122	2.477767
28	1	0	3.370635	-0.014701	1.756213

Frequency Data:

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.220583 (Hartree/Particle)
Thermal correction to Energy= 0.238624
Thermal correction to Enthalpy= 0.239568
Thermal correction to Gibbs Free Energy= 0.171353
Sum of electronic and zero-point Energies= -598.059391
Sum of electronic and thermal Energies= -598.041350
Sum of electronic and thermal Enthalpies= -598.040405
Sum of electronic and thermal Free Energies= -598.108620

Zn(allyl)Br(4Cl-C_6H_4-CHO)(NH_3) React

Cartesian Coordinates (Angstroms):

1	30	0	-1.504879	0.433017	0.050514
2	6	0	-1.014887	1.891369	-1.484407
3	6	0	0.172044	2.506811	-1.005257
4	6	0	1.453707	1.996617	-1.099121
5	6	0	1.437237	0.582142	0.677758
6	8	0	0.349483	-0.074275	0.642964
7	1	0	-0.910987	1.231166	-2.347898
8	1	0	-1.904459	2.520850	-1.537740
9	1	0	0.041738	3.399607	-0.386898

10	1	0	2.302547	2.602671	-0.798526
11	1	0	1.665469	1.205013	-1.812769
12	35	0	-3.208940	-1.364906	-0.223322
13	1	0	1.515738	1.452412	1.345565
14	6	0	5.157655	-1.368799	-0.162379
15	6	0	3.950250	-1.984441	-0.507043
16	6	0	2.738664	-1.349171	-0.244581
17	6	0	2.724469	-0.083919	0.362524
18	6	0	3.938921	0.525659	0.712119
19	6	0	5.149590	-0.112838	0.451306
20	1	0	6.101010	-1.868025	-0.366480
21	1	0	3.954918	-2.964639	-0.976124
22	1	0	1.793557	-1.822206	-0.491394
23	1	0	3.930743	1.502859	1.191166
24	1	0	6.085483	0.365115	0.727794
25	7	0	-2.364199	1.192936	1.944950
26	1	0	-2.643217	2.171473	2.007212
27	1	0	-3.204475	0.619197	2.041355
28	1	0	-1.761170	0.988770	2.741719

Frequency Data:

NImag: 1 (-214.0602)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.220934 (Hartree/Particle)

Thermal correction to Energy= 0.237797

Thermal correction to Enthalpy= 0.238741

Thermal correction to Gibbs Free Energy= 0.172823

Sum of electronic and zero-point Energies= -598.053466

Sum of electronic and thermal Energies= -598.036603

Sum of electronic and thermal Enthalpies= -598.035659

Sum of electronic and thermal Free Energies= -598.101577