

Supplementary Material

Mono- and Bimetallic Zwitterionic Cr(0) and W(0) Metal Allenyls

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S1. Synthesis of compounds **1d**, **1e** and **1i**

S2. UV-vis spectra

S3. Computational details

S1. General procedure for the synthesis of compounds 1d (M = Cr, R = 2-thienyl), 1e (M = Cr, R = 4-Br) and 1i (M = Cr, R = 4-CF₃):

To a solution of the corresponding alkynyl benzene (1 mmol) in dry ether (7 mL) at -78° C, were added dropwise *n*-buthyllitium (1.6 M in hexanes; 1.1 mmol). The mixture was stirred at -78° C for 1h. After this time, the reaction was warmed at 0° C and then was added 1 mmol of hexacarbonyl chromium. The mixture was allowed to reach room temperature and stirred for 1 h, afterwards 2 mL of dry THF were added and the mixture was let to stir at room temperature overnight. Then, 2 mmol of Et₃OBF₄ were added in one portion at -78°C. The solution was stirred at this temperature for 30 min and then allowed to reach room temperature for an additional hour. The residue was

filtered through celite and the solvents were removed under reduced pressure. The crude product was submitted to flash column (SiO₂, hexane)

Compound 1d: Following the general procedure, from 500 mg of 1-bromo-4-ethynylbenzene (2.76 mmol), 1.73 mL (3.04 mmol) of BuLi, 607 mg (2.76 mmol) of hexacarbonyl chromium and 1.05 g (5.52 mmol) of BF₄Et₃O. **1d** (200 mg; 17% yield) was obtained as a dark solid. ¹H NMR (300 MHz, CDCl₃) δ 7.66–7.56 (m, 2H), 7.50–7.39 (m, 2H), 4.75 (q, *J* = 7.1 Hz, 2H), 1.70–1.45 (m, 3H).

Synthesis of 1e: Following the general procedure, from 770 mg (4.52 mmol) of 4-ethynyl- α,α,α -trifluorotoluene, 3.1 mL (4.98 mmol) of BuLi, 994 mg (4.52 mmol) of hexacarbonyl chromium and 1.70 g (9.00 mmol) of BF₄Et₃O. **1e** (200 mg; 8% yield) was obtained as a dark solid. ¹H NMR (300 MHz, CDCl₃) δ 7.76–7.62 (m, 4H), 4.78 (q, *J* = 7.1 Hz, 2H), 1.61 (t, *J* = 7.1 Hz, 3H).

Synthesis of 1i: Following the general procedure, from 700 mg (6.47 mmol) of 2-ethynylthiophene, 4.04 mL (9.24 mmol) of BuLi, 1.42 g (6.47 mmol) of hexacarbonyl chromium and 2.46 g (12.9 mmol) of BF₄Et₃O. **1i** (560 mg; 24% yield) was obtained as a dark solid. ¹H NMR (300 MHz, CDCl₃) δ 7.82 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.43 (dt, *J* = 5.0, 3.0 Hz, 1H), 7.24 (dd, *J* = 5.0, 1.2 Hz, 1H), 4.74 (q, *J* = 7.1 Hz, 2H), 1.58 (t, *J* = 7.1 Hz, 3H).

S2. UV-vis spectra

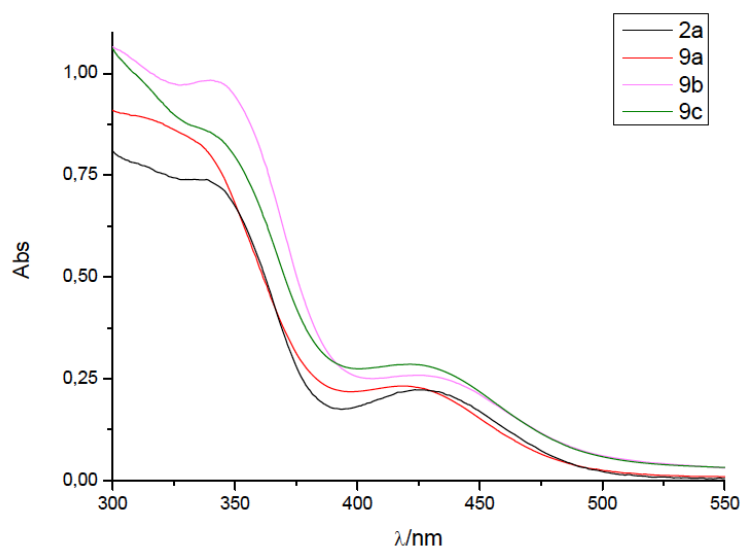


Figure S1. Room temperature UV-vis spectra of complexes **9a-c** measured in diethyl ether solution (concentration $\text{ca. } 1 \times 10^{-4} \text{ mol L}^{-1}$). Compound **2a** is included for comparison.

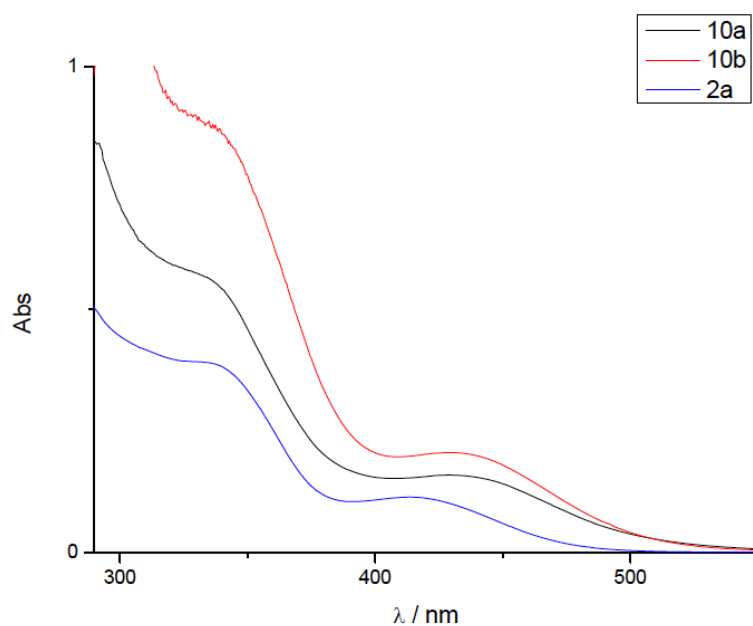


Figure S2. Room temperature UV-vis spectra, of compound **10** measured in THF solution (concentration $\text{ca. } 1 \times 10^{-4} \text{ mol L}^{-1}$). Compound **2a** is included for comparison.

S3. Computational details

Computed Cartesian coordinates and total energies of all species discussed in the text. Cartesian coordinates (in Å) and free energies (in a. u.) of all the stationary points

discussed in the text. All calculations have been performed B3LYP/def2-SVP level with the Gaussian 09 program

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2b E = -4451.800886

C	-3.599657	-1.769095	-1.651113
C	-2.376141	-1.191081	-2.031652
C	-2.306188	0.067284	-2.666949
C	-3.495964	0.781961	-2.825841
C	-4.733696	0.270901	-2.407880
C	-4.763065	-1.008589	-1.845421
N	-1.147143	-1.949002	-1.909452
C	-0.112522	-1.757721	-1.041514
N	0.868160	-2.621050	-1.429651
C	0.453575	-3.338649	-2.538395
C	-0.802426	-2.919104	-2.839915
C	0.023133	-0.814920	0.101264
C	0.971280	0.124205	-0.005981
C	1.874924	1.071635	0.208395
Cr	1.337164	3.174136	-0.271725
C	1.047453	3.284914	1.599475
O	0.872272	3.300317	2.738865
C	2.170898	-2.823753	-0.825656
C	2.293272	-3.741027	0.234078
C	3.577117	-3.974295	0.743254
C	4.711094	-3.339564	0.222598
C	4.541030	-2.452684	-0.848241
C	3.282964	-2.174767	-1.394761
C	1.102072	-4.456666	0.819133
C	6.077956	-3.583583	0.811975
C	3.142630	-1.212203	-2.545365
C	-1.006031	0.601430	-3.206792
C	-5.990946	1.090441	-2.553450
C	-3.733700	-3.164237	-1.086455
O	3.057211	0.581364	0.708722
C	4.139727	1.430944	1.046188
C	5.180211	0.592542	1.767916
C	-0.481426	2.752865	-0.532990
O	-1.616261	2.632105	-0.719222
C	1.758515	2.684786	-2.047651
O	2.025682	2.338963	-3.116637
C	3.050684	3.977290	-0.103414
O	4.026094	4.590816	-0.049174
C	0.797711	4.912383	-0.664191
O	0.451741	5.987736	-0.911751
H	4.572282	1.882202	0.136525
H	3.796058	2.253245	1.694694

H	6.042405	1.217441	2.049592
H	4.756376	0.148399	2.682091
H	5.537543	-0.226707	1.125154
H	1.094049	-4.079797	-3.006736
H	-1.483270	-3.205328	-3.635651
H	3.690513	-4.681789	1.569357
H	5.415357	-1.955748	-1.277647
H	-3.452257	1.768551	-3.293763
H	1.425919	-5.299388	1.445845
H	0.432698	-4.853979	0.039390
H	0.500763	-3.782134	1.449452
H	6.127535	-4.547832	1.339381
H	6.332664	-2.795506	1.541869
H	6.860612	-3.572973	0.037819
H	2.547071	-0.333901	-2.251709
H	2.644960	-1.672318	-3.414831
H	4.127291	-0.855020	-2.876361
H	-0.605717	-0.053692	-3.999450
H	-0.235660	0.674546	-2.426665
H	-1.140955	1.602083	-3.636671
H	-6.060426	1.837591	-1.744227
H	-6.894024	0.464339	-2.504146
H	-6.004284	1.643411	-3.505410
H	-2.781591	-3.707863	-1.043534
H	-4.429226	-3.758972	-1.700411
H	-4.149791	-3.134753	-0.067182
H	-5.723168	-1.440098	-1.547316
C	-0.650838	-1.147344	1.389246
C	-1.604403	-2.188483	1.653475
C	-1.788562	-2.294758	3.068531
C	-0.967781	-1.304326	3.688524
C	-0.285379	-0.588456	2.659936
H	-2.093469	-2.808870	0.909204
H	-2.448523	-2.996744	3.576600
H	-0.891257	-1.109915	4.757456
H	0.416044	0.231481	2.798461
C	-3.506217	0.840385	1.254703
C	-4.329155	-0.132490	1.901894
C	-4.172081	0.023175	3.313910
C	-3.251171	1.092588	3.537689
C	-2.841389	1.596496	2.266151
H	-3.383355	0.974676	0.183063
H	-4.961707	-0.867092	1.405818
H	-4.655777	-0.577359	4.083462
H	-2.903731	1.447097	4.507125
H	-2.127010	2.399147	2.097997
Fe	-2.344345	-0.414474	2.440069

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2c E = -2055.564117

C	-1.252844	2.873183	-1.605269
C	-0.157971	2.994072	-0.725373
C	-0.219693	3.779875	0.439425
C	-1.424366	4.439644	0.716235
C	-2.540750	4.334732	-0.118812
C	-2.432417	3.545664	-1.271655
N	1.096819	2.371748	-1.098692
C	1.740575	1.319495	-0.509963
N	2.919807	1.163335	-1.187571
C	2.996467	2.108893	-2.202045
C	1.866432	2.856424	-2.145574
C	1.232024	0.500573	0.593016
C	-0.090706	0.301095	0.692057
C	-1.373883	0.088018	0.929581
W	-2.351782	-1.656917	-0.206207
C	-3.591774	-2.226753	1.384638
O	-4.295717	-2.594759	2.227220
C	3.957309	0.174248	-0.986154
C	5.215953	0.608684	-0.525744
C	6.222736	-0.352502	-0.373050
C	6.012439	-1.704448	-0.668461
C	4.754104	-2.086232	-1.149831
C	3.709274	-1.170898	-1.324368
C	5.517389	2.056427	-0.218591
C	7.098996	-2.727997	-0.452812
C	2.380747	-1.631810	-1.859269
C	0.942391	3.911473	1.389265
C	-3.836024	5.036317	0.206052
C	-1.178137	2.070681	-2.879913
C	2.186689	-0.025276	1.629696
C	3.149617	0.818069	2.212890
C	3.979723	0.364411	3.240961
C	3.862775	-0.946526	3.710630
C	2.904714	-1.793347	3.144294
C	2.074523	-1.338501	2.117716
O	-1.970201	1.030297	1.735814
C	-3.240604	0.773197	2.317246
C	-3.630273	1.986001	3.141735
C	-3.320892	-3.166730	-1.243932
O	-3.866674	-4.009663	-1.828720
C	-0.931495	-3.029606	0.464093
O	-0.136322	-3.800642	0.810462
C	-1.225241	-1.422184	-1.935408
O	-0.624899	-1.342880	-2.930315
C	-3.735687	-0.269329	-0.945510
O	-4.496407	0.492404	-1.376558
H	-3.989743	0.573054	1.533001
H	-3.188847	-0.121703	2.960545
H	-4.603799	1.815701	3.627783
H	-2.880826	2.181431	3.924538

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H	1.535320	3.696546	-2.747419
H	3.845952	2.146611	-2.876259
H	-1.486209	5.053646	1.618899
H	-3.297207	3.439537	-1.932193
H	4.573616	-3.133711	-1.406725
H	0.829937	4.804468	2.020282
H	1.906870	3.988072	0.863176
H	0.996978	3.035700	2.056468
H	-3.742419	5.672346	1.098262
H	-4.641534	4.306723	0.393665
H	-4.168993	5.670805	-0.631611
H	-0.589076	1.152600	-2.764370
H	-0.721969	2.654051	-3.698845
H	-2.185183	1.780752	-3.210053
H	1.969801	-0.945902	-2.613764
H	1.628530	-1.705801	-1.058347
H	2.468757	-2.625118	-2.320114
H	6.974163	-3.227459	0.523714
H	8.098795	-2.268971	-0.462141
H	7.072338	-3.513468	-1.223528
H	5.839264	2.602917	-1.122117
H	6.334762	2.132601	0.512669
H	4.648252	2.591552	0.187767
H	3.235219	1.854223	1.878068
H	4.712610	1.043713	3.684776
H	4.508118	-1.303447	4.517303
H	2.798550	-2.820225	3.503524
H	1.329326	-2.010274	1.692322
H	7.201227	-0.030493	-0.005584

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2d E = -3354.295313

C	4.479660	1.290188	0.491799
C	3.637818	1.041212	-0.607177
C	3.992187	0.136820	-1.638266
C	5.199760	-0.559591	-1.497814
C	6.051260	-0.363299	-0.401893
C	5.680289	0.575494	0.570303
N	2.400426	1.788965	-0.719997
C	1.123400	1.474755	-0.310788
N	0.331868	2.509615	-0.716702
C	1.095091	3.456653	-1.383992
C	2.373509	3.012779	-1.391890
C	0.619578	0.398564	0.474499
C	-0.733538	0.164702	0.541006
C	-1.902852	-0.365928	0.787708
Cr	-2.146239	-2.159521	-0.655536
C	-0.551910	-2.981381	-0.004435

O	0.352994	-3.613223	0.293438
C	-1.063728	2.707452	-0.405617
C	-1.430451	3.093399	0.898366
C	-2.790593	3.319394	1.158992
C	-3.766253	3.191345	0.166038
C	-3.344209	2.841216	-1.125078
C	-1.999621	2.605853	-1.430442
C	-0.423811	3.232070	2.011088
C	-5.226951	3.442773	0.456744
C	-1.577727	2.237883	-2.819109
C	3.114411	-0.080206	-2.851995
C	7.323646	-1.160494	-0.254274
C	4.108591	2.298524	1.550425
O	-2.667794	-0.025688	1.843155
C	-4.066902	-0.116762	1.700477
C	-4.716503	0.160309	3.049771
C	-1.002840	-1.342047	-1.911029
O	-0.285556	-1.011424	-2.765866
C	-3.712059	-1.420850	-1.449953
O	-4.654214	-0.958617	-1.938922
C	-3.044662	-3.076031	0.759145
O	-3.570697	-3.664377	1.586560
C	-2.341312	-3.597373	-1.812528
O	-2.380657	-4.534580	-2.488848
H	-4.476142	0.617124	0.952272
H	-4.393408	-1.103751	1.323857
H	-5.811994	0.122621	2.982447
H	-4.388579	-0.593613	3.781809
H	-4.423937	1.155043	3.419234
H	0.649256	4.364752	-1.776669
H	3.278787	3.440977	-1.809256
H	-3.089669	3.606971	2.171986
H	-4.086311	2.737345	-1.921261
H	5.485635	-1.272182	-2.277036
H	-0.812088	3.883042	2.808323
H	0.532834	3.651170	1.661897
H	-0.208976	2.245876	2.457692
H	-5.409005	3.591404	1.531690
H	-5.849511	2.598316	0.119485
H	-5.588838	4.341901	-0.072909
H	-0.858890	1.407367	-2.784249
H	-1.095365	3.075918	-3.349965
H	-2.448126	1.921030	-3.409171
H	3.004779	0.860043	-3.424099
H	2.093097	-0.386772	-2.584844
H	3.541592	-0.834943	-3.531884
H	7.154865	-2.042914	0.388066
H	8.122527	-0.565972	0.216153
H	7.690817	-1.524886	-1.225665
H	4.030398	3.316543	1.133001

H	4.862573	2.320771	2.349627
H	3.137127	2.058245	2.010330
H	6.339967	0.751021	1.424887
C	1.416591	-0.745682	1.134784
C	2.361681	-1.690602	0.858663
S	3.154098	-2.310731	2.291135
C	2.195038	-1.248133	3.293601
C	1.386592	-0.515483	2.570120
H	2.546462	-2.150459	-0.111178
H	2.466721	-1.202184	4.361647
H	0.789861	0.278472	3.015744

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2e E = -5606.837104

C	3.741366	-2.424135	-0.022914
C	2.673625	-2.250837	0.878136
C	2.866668	-1.764801	2.184286
C	4.164438	-1.384464	2.549823
C	5.247463	-1.488174	1.668150
C	5.015721	-2.024175	0.393958
N	1.351757	-2.687574	0.487299
C	0.282431	-1.938297	0.063297
N	-0.762411	-2.818072	-0.062691
C	-0.339853	-4.096227	0.279237
C	0.968857	-4.018385	0.616591
C	0.261508	-0.520825	-0.251302
C	-0.907985	0.134843	-0.405548
C	-1.903386	0.961643	-0.615851
Cr	-2.464757	2.154815	1.187361
C	-0.775199	3.021977	1.082026
O	0.238607	3.564821	1.036732
C	-2.117999	-2.584866	-0.513657
C	-2.380939	-2.447819	-1.887422
C	-3.721163	-2.338552	-2.285263
C	-4.775967	-2.361590	-1.367596
C	-4.466686	-2.510017	-0.007704
C	-3.151030	-2.631721	0.445929
C	-1.283323	-2.364818	-2.916388
C	-6.212116	-2.227822	-1.809895
C	-2.865109	-2.806584	1.917388
C	1.729188	-1.663671	3.168278
C	6.624775	-1.018721	2.064989
C	3.540064	-3.042566	-1.383992
C	1.547123	0.205792	-0.581495
C	2.189675	1.037298	0.348471
C	3.324894	1.772739	0.002241
C	3.831225	1.678958	-1.296113
C	3.203012	0.876195	-2.250660
C	2.065491	0.151283	-1.886456
O	-2.398585	1.014112	-1.891737

C	-3.737273	1.413183	-2.152198
C	-3.907142	1.505924	-3.657510
C	-1.717805	0.865051	2.335164
O	-1.244685	0.115359	3.080221
C	-4.117191	1.223540	1.137952
O	-5.121252	0.656583	1.112378
C	-3.153166	3.604329	0.158848
O	-3.551635	4.545825	-0.372146
C	-2.974720	3.119616	2.696190
O	-3.295747	3.706860	3.638782
H	-4.436195	0.672388	-1.724583
H	-3.952322	2.383872	-1.684268
H	-4.935020	1.814461	-3.905626
H	-3.211020	2.246145	-4.081710
H	-3.710053	0.535380	-4.139315
H	-1.018836	-4.941898	0.235979
H	1.671420	-4.776114	0.948974
H	-3.940430	-2.228020	-3.350952
H	-5.276259	-2.519567	0.726732
H	4.329837	-0.995484	3.558335
H	-1.648346	-2.680629	-3.904375
H	-0.413618	-2.987748	-2.658516
H	-0.936988	-1.321307	-3.005328
H	-6.294345	-2.111349	-2.900375
H	-6.687288	-1.353157	-1.335900
H	-6.803891	-3.111442	-1.518000
H	-2.083506	-2.118217	2.269801
H	-2.528762	-3.831067	2.152119
H	-3.770444	-2.615268	2.509927
H	1.214021	-2.630577	3.292366
H	0.963019	-0.938183	2.854581
H	2.095789	-1.351490	4.155918
H	6.828493	-0.018597	1.644731
H	7.407499	-1.693806	1.685481
H	6.731464	-0.946582	3.157394
H	3.350586	-4.127338	-1.310335
H	4.432440	-2.904455	-2.010010
H	2.684069	-2.600195	-1.913594
H	1.557122	-0.453619	-2.641463
H	3.590234	0.826382	-3.269749
Br	5.392591	2.668046	-1.775130
H	3.806089	2.420923	0.736119
H	1.790233	1.124392	1.359973
H	5.852620	-2.133794	-0.301463

83

2f E = -3072.820579

C	-4.437588	-1.500648	0.263952
C	-3.473775	-1.282322	-0.738304
C	-3.743631	-0.508100	-1.881713

C	-5.000406	0.104396	-1.968804
C	-5.974640	-0.048906	-0.974463
C	-5.676125	-0.863703	0.125727
N	-2.213070	-1.986857	-0.658235
C	-0.985872	-1.549414	-0.223032
N	-0.117357	-2.585523	-0.460752
C	-0.801033	-3.645897	-1.041785
C	-2.098029	-3.279113	-1.161352
C	-0.658747	-0.285816	0.408685
C	0.630129	0.095094	0.543600
C	1.790338	0.660144	0.764774
Cr	2.327946	2.201288	-0.764547
C	0.912753	3.276299	-0.079431
O	0.070890	3.948007	0.324526
C	1.286670	-2.713405	-0.133378
C	1.663228	-3.035658	1.182328
C	3.019955	-3.290426	1.426316
C	3.983672	-3.231881	0.413990
C	3.562264	-2.906357	-0.883491
C	2.222017	-2.651349	-1.186296
C	0.672177	-3.067322	2.316934
C	5.438673	-3.517548	0.694128
C	1.806323	-2.318332	-2.597854
C	-2.732654	-0.351368	-2.988676
C	-7.304698	0.655741	-1.074421
C	-4.164703	-2.404211	1.439992
C	-1.734483	0.565563	1.046003
C	-2.319568	1.647568	0.370971
C	-3.236342	2.482886	1.010056
C	-3.601630	2.275677	2.349537
C	-3.010340	1.198761	3.026902
C	-2.089649	0.363415	2.389687
O	2.450569	0.320011	1.915771
C	3.869892	0.318456	1.967948
C	4.280469	0.063977	3.406455
C	1.144425	1.456150	-2.020974
O	0.412034	1.045940	-2.819063
C	3.704131	1.013706	-1.302682
O	4.533197	0.284654	-1.638003
C	3.478242	3.139064	0.431802
O	4.157253	3.795749	1.091463
C	2.806265	3.463085	-2.046377
O	3.104695	4.236810	-2.852350
H	4.263231	-0.471347	1.303097
H	4.274024	1.278597	1.617342
H	5.378568	0.049287	3.492399
H	3.891380	0.854774	4.066556
H	3.890505	-0.902424	3.763059
H	-0.290467	-4.568052	-1.300638
H	-2.959135	-3.803297	-1.563787

H	3.327981	-3.541035	2.445344
H	4.301812	-2.836221	-1.685338
H	-5.223575	0.714604	-2.848503
H	1.051048	-3.673933	3.151954
H	-0.304097	-3.474945	2.013241
H	0.503745	-2.044672	2.694319
H	5.630467	-3.635559	1.770573
H	6.081496	-2.704952	0.318982
H	5.765626	-4.443511	0.191051
H	1.136012	-1.447378	-2.634000
H	1.274492	-3.158036	-3.077739
H	2.686636	-2.089798	-3.214222
H	-2.406330	-1.329197	-3.380076
H	-1.823813	0.174011	-2.657811
H	-3.158180	0.218209	-3.826525
H	-7.284366	1.607716	-0.515734
H	-8.118409	0.048052	-0.649568
H	-7.560928	0.893741	-2.117592
H	-3.983396	-3.444668	1.122220
H	-5.017562	-2.410002	2.132832
H	-3.277674	-2.076014	2.002481
H	-1.620040	-0.448309	2.951725
H	-3.263030	1.017573	4.076036
H	-3.667591	3.322776	0.457819
H	-2.040241	1.848161	-0.665108
H	-6.431496	-1.014918	0.902001
C	-4.559216	3.209284	3.049228
H	-5.318659	3.605134	2.357037
H	-5.080528	2.709421	3.880116
H	-4.025297	4.077662	3.473819

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2g E = -3147.964471

C	-4.241023	-1.886048	0.070256
C	-3.224270	-1.620378	-0.866459
C	-3.458314	-0.869820	-2.033237
C	-4.738092	-0.329304	-2.211661
C	-5.767663	-0.529561	-1.283698
C	-5.500291	-1.319098	-0.157548
N	-1.931961	-2.245231	-0.687967
C	-0.759065	-1.707494	-0.218624
N	0.182417	-2.696509	-0.349852
C	-0.402620	-3.828953	-0.901539
C	-1.711628	-3.552945	-1.108315
C	-0.549224	-0.386024	0.345315
C	0.701285	0.105078	0.476684
C	1.809013	0.769306	0.699234
Cr	2.355137	2.224627	-0.902833
C	0.804652	3.226916	-0.448856
O	-0.125933	3.854702	-0.193387

C	1.571723	-2.710496	0.055596
C	1.895488	-2.908242	1.409370
C	3.250401	-3.048811	1.740743
C	4.262906	-2.997190	0.777174
C	3.893536	-2.797906	-0.560935
C	2.558478	-2.660342	-0.950333
C	0.849537	-2.927671	2.493990
C	5.716364	-3.154337	1.151167
C	2.203578	-2.463936	-2.403403
C	-2.384297	-0.663659	-3.069878
C	-7.123972	0.100965	-1.480112
C	-4.003426	-2.769477	1.269167
C	-1.711259	0.382207	0.932661
C	-2.310580	1.455512	0.263005
C	-3.313277	2.227423	0.858471
C	-3.741247	1.931361	2.161019
C	-3.143965	0.863486	2.852351
C	-2.143026	0.111604	2.245752
O	2.424877	0.556958	1.906330
C	3.836135	0.640250	2.035757
C	4.171166	0.630176	3.515933
C	1.353011	1.282562	-2.184103
O	0.730160	0.745504	-2.999676
C	3.858078	1.115329	-1.232828
O	4.761710	0.430619	-1.446763
C	3.307973	3.332220	0.322842
O	3.863382	4.078695	1.001945
C	2.855729	3.422247	-2.236864
O	3.169331	4.156889	-3.073199
H	4.303793	-0.219339	1.522698
H	4.217816	1.554860	1.560845
H	5.262418	0.675413	3.659620
H	3.718096	1.496643	4.022227
H	3.794586	-0.284647	4.000211
H	0.176179	-4.729633	-1.080055
H	-2.514844	-4.152457	-1.525106
H	3.516790	-3.201317	2.790414
H	4.670625	-2.735613	-1.327238
H	-4.933886	0.261789	-3.110772
H	1.215719	-3.463098	3.381726
H	-0.087003	-3.405557	2.168637
H	0.609936	-1.895491	2.800188
H	5.851329	-3.227082	2.240203
H	6.312549	-2.300895	0.789226
H	6.148026	-4.062157	0.696772
H	1.467082	-1.659771	-2.542405
H	1.776262	-3.379192	-2.848468
H	3.098240	-2.202011	-2.985006
H	-1.977509	-1.623959	-3.427945
H	-1.530447	-0.087506	-2.682883

H	-2.781237	-0.123581	-3.940545
H	-7.188143	1.063068	-0.942256
H	-7.929899	-0.540849	-1.092426
H	-7.326855	0.305596	-2.541995
H	-3.811414	-3.814572	0.972846
H	-4.878221	-2.767444	1.934093
H	-3.135610	-2.433333	1.855516
H	-1.662898	-0.690495	2.812415
H	-3.469861	0.658795	3.874314
H	-3.737597	3.062868	0.301783
H	-1.979303	1.713047	-0.744376
H	-6.296856	-1.505753	0.568118
O	-4.702797	2.617033	2.831677
C	-5.295225	3.742602	2.225451
H	-4.549397	4.521674	1.985670
H	-5.836928	3.476183	1.299092
H	-6.013379	4.148425	2.950931

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2h E = -3167.357511

C	-3.994729	-2.181504	0.069419
C	-2.958659	-1.987267	-0.862823
C	-3.191165	-1.439579	-2.138269
C	-4.494156	-1.024316	-2.438832
C	-5.547317	-1.155782	-1.524791
C	-5.278126	-1.747602	-0.284045
N	-1.639598	-2.497117	-0.557756
C	-0.519919	-1.833188	-0.119124
N	0.485036	-2.768345	-0.109237
C	-0.009254	-3.992307	-0.541523
C	-1.323914	-3.827271	-0.816909
C	-0.414044	-0.449307	0.304508
C	0.800669	0.124235	0.447604
C	1.855122	0.876245	0.642551
Cr	2.357081	2.202656	-1.083160
C	0.741240	3.152249	-0.749212
O	-0.222960	3.752047	-0.563742
C	1.860082	-2.647213	0.324629
C	2.159290	-2.683351	1.697882
C	3.511323	-2.701065	2.068265
C	4.543636	-2.683081	1.124538
C	4.198339	-2.648285	-0.234288
C	2.867998	-2.638294	-0.661356
C	1.086552	-2.654285	2.755563
C	5.993718	-2.703332	1.541814
C	2.537260	-2.614233	-2.133141
C	-2.089473	-1.316087	-3.159509
C	-6.930609	-0.657095	-1.861831
C	-3.746253	-2.843839	1.400770
C	-1.645485	0.318118	0.724926

C	-2.300960	1.213818	-0.133131
C	-3.367757	1.998549	0.295180
C	-3.843236	1.926168	1.628104
C	-3.169621	1.037585	2.501565
C	-2.100048	0.264292	2.052188
O	2.439088	0.827453	1.883442
C	3.838792	1.008141	2.036543
C	4.138218	1.086518	3.522360
C	1.442086	1.082822	-2.284883
O	0.870869	0.433791	-3.055678
C	3.933295	1.166110	-1.266067
O	4.886913	0.527267	-1.384692
C	3.214013	3.481692	0.040644
O	3.710109	4.325756	0.648141
C	2.816275	3.292339	-2.519797
O	3.105601	3.959047	-3.419707
H	4.373390	0.159122	1.574011
H	4.172535	1.924746	1.529466
H	5.219356	1.219572	3.686602
H	3.610351	1.937677	3.979941
H	3.818557	0.167816	4.039075
H	0.630253	-4.867570	-0.597044
H	-2.073707	-4.521148	-1.183828
H	3.759743	-2.727437	3.133008
H	4.989848	-2.614763	-0.987434
H	-4.689555	-0.590436	-3.423597
H	1.463487	-3.054715	3.707619
H	0.195408	-3.233317	2.469378
H	0.765884	-1.613770	2.931663
H	6.103523	-2.658116	2.635144
H	6.541703	-1.851038	1.107998
H	6.496449	-3.619996	1.189834
H	1.778341	-1.854704	-2.370127
H	2.146487	-3.585644	-2.482175
H	3.434344	-2.387383	-2.725623
H	-1.601546	-2.286574	-3.348987
H	-1.296246	-0.623073	-2.840582
H	-2.485371	-0.948860	-4.116541
H	-7.043325	0.402836	-1.573624
H	-7.708530	-1.224217	-1.328526
H	-7.134265	-0.723665	-2.941423
H	-3.348811	-3.865545	1.283618
H	-4.676081	-2.910507	1.982638
H	-3.016416	-2.275417	1.997215
H	-1.584546	-0.382395	2.767929
H	-3.463588	0.960402	3.547750
H	-3.820906	2.686620	-0.416972
H	-1.956122	1.318154	-1.163830
H	-6.092182	-1.881384	0.433842
N	-4.908393	2.700625	2.059620

C	-5.464820	3.710389	1.183380
H	-6.297326	4.214827	1.691265
H	-4.725083	4.481963	0.893858
H	-5.864017	3.270276	0.252022
C	-5.289732	2.687246	3.455640
H	-5.561090	1.671693	3.794842
H	-4.488615	3.056660	4.126313
H	-6.170343	3.327148	3.599364

83

2i E = -3370.343740

C	-3.708888	-2.323250	0.111532
C	-2.710151	-2.164453	-0.869194
C	-2.988955	-1.648219	-2.146949
C	-4.296856	-1.210537	-2.397904
C	-5.304104	-1.281262	-1.428326
C	-4.992623	-1.858510	-0.188601
N	-1.369844	-2.624129	-0.581213
C	-0.284247	-1.904922	-0.142635
N	0.761702	-2.792396	-0.113936
C	0.324717	-4.043513	-0.530572
C	-0.994530	-3.942354	-0.816133
C	-0.244489	-0.514679	0.271446
C	0.931274	0.117934	0.473106
C	1.935981	0.922086	0.715785
Cr	2.398012	2.236881	-1.036314
C	0.746145	3.127047	-0.713495
O	-0.243035	3.683476	-0.526221
C	2.131566	-2.596493	0.310602
C	2.439537	-2.582537	1.681911
C	3.792588	-2.510679	2.043062
C	4.816932	-2.455649	1.092673
C	4.462947	-2.481462	-0.264254
C	3.132440	-2.558712	-0.682703
C	1.376828	-2.588878	2.750241
C	6.267495	-2.369959	1.498791
C	2.794965	-2.595050	-2.153104
C	-1.927916	-1.558368	-3.214789
C	-6.687030	-0.737821	-1.685049
C	-3.421807	-2.991900	1.432512
C	-1.522219	0.219428	0.613186
C	-2.183488	1.021538	-0.330357
C	-3.342543	1.717483	0.006185
C	-3.861390	1.628019	1.303292
C	-3.188077	0.873796	2.269881
C	-2.025937	0.182516	1.924158
O	2.478623	0.893385	1.970139
C	3.827342	1.281031	2.198327
C	4.082847	1.205069	3.692418

C	1.531482	1.060335	-2.221755
O	0.984806	0.383114	-2.986027
C	4.024463	1.271399	-1.178268
O	5.015303	0.687677	-1.264723
C	3.214435	3.594374	0.023638
O	3.688757	4.489287	0.572543
C	2.810285	3.303217	-2.506190
O	3.069666	3.953315	-3.425989
H	4.506186	0.603926	1.650038
H	4.005395	2.302402	1.833976
H	5.118044	1.507378	3.916375
H	3.400587	1.876117	4.237135
H	3.930570	0.181718	4.069573
H	1.003512	-4.889541	-0.569498
H	-1.710922	-4.675672	-1.172989
H	4.047530	-2.495677	3.106449
H	5.247629	-2.426264	-1.023153
H	-4.528160	-0.790995	-3.380866
H	1.768754	-3.003948	3.690072
H	0.490106	-3.173246	2.462462
H	1.048247	-1.555507	2.952588
H	6.383073	-2.323700	2.591442
H	6.743686	-1.474697	1.066398
H	6.835757	-3.242421	1.135081
H	2.007110	-1.872622	-2.411347
H	2.440364	-3.591055	-2.469359
H	3.680714	-2.354407	-2.757108
H	-1.447751	-2.534561	-3.393087
H	-1.122741	-0.855104	-2.949951
H	-2.362453	-1.221224	-4.166100
H	-6.884296	0.123032	-1.024598
H	-7.462082	-1.492028	-1.472485
H	-6.809094	-0.405304	-2.725980
H	-3.275401	-4.078614	1.306584
H	-4.256953	-2.849011	2.132063
H	-2.512254	-2.596852	1.907435
H	-1.493175	-0.391046	2.686158
H	-3.570624	0.831232	3.291270
H	-3.844046	2.336305	-0.740166
H	-1.782095	1.101869	-1.341510
H	-5.772905	-1.940995	0.573108
C	-5.173424	2.291437	1.626142
F	-5.315002	3.471088	1.000107
F	-6.220857	1.521533	1.234679
F	-5.329044	2.506712	2.942785

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3a E = -3034.738027

C	4.596853	1.112862	0.426153
C	3.642784	0.892325	-0.586825

C	3.890375	-0.012302	-1.641037
C	5.086007	-0.739172	-1.621297
C	6.037575	-0.579750	-0.605205
C	5.776904	0.358978	0.399651
N	2.452682	1.698022	-0.626273
C	1.168897	1.381483	-0.288625
N	0.341535	2.371398	-0.728187
C	1.073480	3.362396	-1.531261
C	2.534899	3.042536	-1.216079
C	0.752387	0.223905	0.461065
C	-0.567431	-0.080212	0.584562
C	-1.756936	-0.545786	0.839522
Cr	-2.281973	-2.233267	-0.541031
C	-0.924450	-3.304508	0.260296
O	-0.128287	-3.989529	0.728596
C	-1.042399	2.625117	-0.430176
C	-1.400753	3.150430	0.829377
C	-2.735952	3.518533	1.038459
C	-3.709819	3.391923	0.041237
C	-3.317177	2.869418	-1.197603
C	-1.997427	2.486638	-1.459765
C	-0.404330	3.287439	1.952103
C	-5.137542	3.820812	0.277816
C	-1.635198	1.938172	-2.818083
C	2.908007	-0.192162	-2.770299
C	7.296348	-1.411004	-0.582025
C	4.393475	2.148478	1.504406
C	1.739891	-0.586024	1.273539
C	2.271291	-1.794377	0.796900
C	3.101018	-2.578876	1.601165
C	3.414411	-2.169420	2.900549
C	2.884332	-0.973512	3.393017
C	2.051252	-0.193121	2.586621
O	-2.455880	-0.050929	1.901612
C	-3.876453	0.014033	1.882593
C	-4.337772	0.430275	3.266817
C	-1.060006	-1.669481	-1.857940
O	-0.309786	-1.375912	-2.688724
C	-3.612145	-1.074689	-1.237111
O	-4.415098	-0.372101	-1.674981
C	-3.471102	-2.985966	0.745927
O	-4.172664	-3.533394	1.476735
C	-2.803692	-3.607190	-1.683128
O	-3.130531	-4.450998	-2.402308
H	-4.200703	0.748336	1.124154
H	-4.307694	-0.959413	1.609817
H	-5.436347	0.505515	3.294486
H	-4.021329	-0.307681	4.020261
H	-3.914690	1.408119	3.545196
H	0.840443	3.242319	-2.602952

H	2.977157	3.752096	-0.494673
H	-3.019937	3.920380	2.015414
H	-4.064950	2.738868	-1.984644
H	5.280601	-1.448572	-2.430843
H	-0.758737	4.004575	2.706331
H	0.583057	3.623839	1.599750
H	-0.260751	2.316753	2.455297
H	-5.347568	3.962149	1.348343
H	-5.849370	3.078199	-0.116011
H	-5.354664	4.775905	-0.231506
H	-0.825713	1.198039	-2.763656
H	-1.314524	2.740347	-3.506653
H	-2.504906	1.448524	-3.278870
H	2.655252	0.769004	-3.248456
H	1.957792	-0.635285	-2.436285
H	3.322947	-0.848884	-3.547801
H	7.149700	-2.324475	0.020529
H	8.138693	-0.860138	-0.136276
H	7.590512	-1.730888	-1.593041
H	4.803312	3.127190	1.196705
H	4.911181	1.856897	2.429373
H	3.331794	2.291865	1.745050
H	1.617960	0.727019	2.986778
H	3.107751	-0.652809	4.414164
H	4.058187	-2.787264	3.532018
H	3.494041	-3.521894	1.213172
H	2.020296	-2.130117	-0.210793
H	6.513606	0.511654	1.193939
H	0.781566	4.378892	-1.231639
H	3.174255	3.027110	-2.110041

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3b E = -5608.016394

C	3.630331	-2.408275	-0.143895
C	2.618003	-2.262987	0.826264
C	2.915911	-1.840509	2.138425
C	4.240423	-1.499569	2.438156
C	5.263230	-1.579733	1.484488
C	4.937095	-2.048150	0.205667
N	1.274622	-2.670747	0.517074
C	0.192132	-1.925633	0.147295
N	-0.911955	-2.726517	0.150205
C	-0.601868	-4.059355	0.689212
C	0.925229	-4.092011	0.653704
C	0.206660	-0.538552	-0.237457
C	-0.958127	0.141069	-0.425486
C	-1.937868	0.966712	-0.646917
Cr	-2.270003	2.261883	1.155827
C	-0.587404	3.104247	0.848020

O	0.411654	3.648764	0.683095
C	-2.229057	-2.498405	-0.380162
C	-2.436294	-2.541132	-1.774994
C	-3.750754	-2.462478	-2.253420
C	-4.851138	-2.355091	-1.395541
C	-4.607888	-2.319325	-0.016299
C	-3.315953	-2.394834	0.514371
C	-1.290237	-2.634778	-2.749539
C	-6.261966	-2.285012	-1.927605
C	-3.121004	-2.363497	2.010468
C	1.848326	-1.760912	3.200899
C	6.673219	-1.154989	1.811956
C	3.347813	-2.962019	-1.518893
C	1.492549	0.179217	-0.584160
C	2.200121	0.931752	0.365725
C	3.339756	1.657637	0.015255
C	3.781752	1.638927	-1.309433
C	3.086354	0.919302	-2.283388
C	1.947131	0.200187	-1.913155
O	-2.528787	1.028286	-1.872742
C	-3.914918	1.324520	-1.999293
C	-4.220042	1.485351	-3.476433
C	-1.445222	1.031676	2.318396
O	-0.926740	0.313578	3.063376
C	-3.932425	1.367026	1.334482
O	-4.939962	0.819232	1.455784
C	-3.024380	3.641778	0.075441
O	-3.450464	4.539972	-0.504877
C	-2.632927	3.343838	2.627141
O	-2.864338	4.003971	3.546878
H	-4.504843	0.499496	-1.562620
H	-4.168355	2.242838	-1.450807
H	-5.289627	1.704642	-3.621523
H	-3.634916	2.313244	-3.906026
H	-3.974469	0.566524	-4.031522
H	-1.064564	-4.835598	0.063639
H	1.318478	-4.667547	-0.203024
H	-3.915988	-2.492343	-3.334307
H	-5.450365	-2.216163	0.673314
H	4.478312	-1.160764	3.450571
H	-1.638464	-2.976233	-3.734748
H	-0.503656	-3.325366	-2.407719
H	-0.821925	-1.645684	-2.884708
H	-6.282620	-2.286088	-3.027248
H	-6.774720	-1.373356	-1.579181
H	-6.862569	-3.141765	-1.578541
H	-2.164622	-1.904354	2.294351
H	-3.149578	-3.379600	2.442943
H	-3.924999	-1.787098	2.489798
H	1.335042	-2.727979	3.336256

H	1.068520	-1.021990	2.961837
H	2.283976	-1.481292	4.170421
H	6.883889	-0.154378	1.396396
H	7.414544	-1.845527	1.380071
H	6.841450	-1.105136	2.897893
H	3.446257	-4.062249	-1.529779
H	4.062454	-2.566362	-2.254555
H	2.335744	-2.716182	-1.867255
H	1.392144	-0.346152	-2.679528
H	3.425037	0.926554	-3.320795
Br	5.348308	2.616005	-1.796653
H	3.873824	2.241574	0.766264
H	1.851226	0.960354	1.399277
H	5.724491	-2.134747	-0.548850
H	-0.997059	-4.165314	1.713861
H	1.368304	-4.506889	1.570007

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5a E= -3073.982739

C	-4.482519	-0.343841	-0.050972
C	-3.303187	-0.292590	-0.818663
C	-2.949694	0.871690	-1.537689
C	-3.748765	2.008541	-1.390043
C	-4.894057	2.014607	-0.582252
C	-5.249555	0.825104	0.058618
N	-2.501440	-1.490052	-0.998235
C	-1.219760	-1.581082	-0.553353
N	-0.414385	-2.551147	-1.050153
C	-0.877603	-3.467383	-2.110708
C	-3.100764	-2.444359	-1.948853
C	-0.714588	-0.629047	0.467273
C	0.518341	-0.108232	0.329392
C	1.660670	0.524353	0.547080
Cr	1.964588	2.574208	-0.298092
C	2.146250	3.088226	1.528119
O	2.237707	3.403421	2.631211
C	0.957476	-2.802563	-0.629508
C	1.215096	-3.546784	0.537870
C	2.540999	-3.908411	0.815682
C	3.602150	-3.564308	-0.026403
C	3.306051	-2.833156	-1.183316
C	2.000981	-2.452251	-1.512510
C	0.129188	-3.953298	1.499560
C	5.023816	-3.947908	0.302444
C	1.753794	-1.707459	-2.800101
C	-1.761407	0.901817	-2.463787
C	-5.704825	3.274489	-0.409374
C	-4.991203	-1.600342	0.615269
C	-1.537305	-0.352247	1.696700
C	-1.511816	0.917738	2.301609

C	-2.180073	1.159667	3.501718
C	-2.888308	0.135690	4.140311
C	-2.917817	-1.133566	3.558896
C	-2.252252	-1.370893	2.352184
O	2.516956	-0.192710	1.342748
C	3.864877	0.177376	1.575754
C	4.365014	-0.632196	2.759726
C	0.125833	3.011229	-0.240964
O	-0.969372	3.377909	-0.260483
C	1.736192	1.924296	-2.055765
O	1.597418	1.558716	-3.142720
C	3.835308	2.336614	-0.540346
O	4.963573	2.280879	-0.770653
C	2.245139	4.316561	-0.887606
O	2.419944	5.400936	-1.249277
H	4.474757	-0.029857	0.678605
H	3.943872	1.253397	1.792352
H	5.419302	-0.389986	2.968345
H	3.771318	-0.408917	3.659749
H	4.286311	-1.711604	2.558718
H	-0.273733	-4.380548	-2.032152
H	-4.155736	-2.578869	-1.675340
H	2.742702	-4.487924	1.721217
H	4.116775	-2.550631	-1.861595
H	-3.462602	2.919005	-1.922369
H	0.444399	-4.819243	2.099438
H	-0.808317	-4.219704	0.988284
H	-0.100776	-3.132645	2.197766
H	5.064963	-4.727943	1.077137
H	5.590125	-3.078421	0.678078
H	5.557819	-4.319104	-0.586667
H	0.896282	-1.026813	-2.732128
H	1.572380	-2.403924	-3.638100
H	2.627302	-1.099865	-3.072341
H	-1.794692	0.082757	-3.201698
H	-0.815037	0.805263	-1.913955
H	-1.722783	1.847229	-3.020448
H	-5.176774	3.989773	0.244255
H	-6.685573	3.069367	0.044644
H	-5.870706	3.782656	-1.372625
H	-5.870976	-1.994077	0.075759
H	-5.309522	-1.390362	1.646608
H	-4.238097	-2.395212	0.661506
H	-2.275710	-2.375743	1.927488
H	-3.452732	-1.951140	4.050463
H	-3.404461	0.324279	5.085071
H	-2.143571	2.158759	3.943756
H	-0.953077	1.721061	1.824313
H	-6.155137	0.797678	0.671863
H	-0.679082	-3.026899	-3.102711

H	-3.089819	-1.990898	-2.955943
C	-2.356613	-3.762676	-1.951154
H	-2.535485	-4.311768	-1.012187
H	-2.713442	-4.395372	-2.777858

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5b E = -3113.223385

C	4.416334	-0.110256	0.368661
C	3.436827	0.298139	-0.560348
C	3.267257	-0.400707	-1.779727
C	4.031734	-1.549433	-2.005094
C	4.985538	-2.003641	-1.084097
C	5.170008	-1.257799	0.082121
N	2.675839	1.516519	-0.344553
C	1.307056	1.465309	-0.203511
N	0.546759	2.471073	-0.720775
C	1.118471	3.459893	-1.658377
C	3.524023	2.730721	-0.486589
C	0.691150	0.357020	0.520204
C	-0.621287	0.041194	0.377833
C	-1.784979	-0.514765	0.647859
Cr	-2.195081	-2.374127	-0.518336
C	-1.330795	-3.293392	0.910074
O	-0.833183	-3.856583	1.780562
C	-0.874339	2.682321	-0.472467
C	-1.326815	3.279523	0.718090
C	-2.683294	3.634834	0.811394
C	-3.589142	3.414616	-0.225021
C	-3.110030	2.793814	-1.388853
C	-1.772768	2.425830	-1.538335
C	-0.451028	3.488925	1.925662
C	-5.039611	3.813465	-0.109039
C	-1.332464	1.718325	-2.795641
C	2.336946	0.089115	-2.860971
C	5.773924	-3.262555	-1.347013
C	4.706781	0.626655	1.653698
C	1.417229	-0.347748	1.647027
C	1.787552	-1.698935	1.544596
C	2.300367	-2.388676	2.644960
C	2.457376	-1.740675	3.874824
C	2.098047	-0.395358	3.992193
C	1.584205	0.291871	2.888142
O	-2.551815	0.146430	1.561675
C	-3.842205	-0.316669	1.926256
C	-4.406615	0.643967	2.957285
C	-0.572350	-2.244466	-1.479278
O	0.391514	-2.276277	-2.116394
C	-3.103773	-1.247387	-1.739778
O	-3.683445	-0.562311	-2.464120

C	-3.867133	-2.827523	0.263922
O	-4.879972	-3.220500	0.650117
C	-2.472654	-3.912803	-1.527112
O	-2.634782	-4.864274	-2.163641
H	-4.495251	-0.363744	1.038218
H	-3.774003	-1.332389	2.348688
H	-5.405562	0.309450	3.278575
H	-3.754916	0.690693	3.843795
H	-4.495044	1.659493	2.542014
H	0.291229	3.864215	-2.251335
H	4.434421	2.526370	0.089472
H	-3.032576	4.101523	1.737165
H	-3.804636	2.573173	-2.203972
H	3.885321	-2.097786	-2.939764
H	-0.766542	4.376721	2.493632
H	0.609535	3.604748	1.671745
H	-0.535847	2.618510	2.597658
H	-5.265852	4.241179	0.878774
H	-5.704450	2.947668	-0.263977
H	-5.310483	4.563820	-0.870987
H	-0.835142	0.767613	-2.549728
H	-0.628228	2.311282	-3.401882
H	-2.197998	1.482543	-3.427301
H	2.645376	1.081971	-3.230802
H	1.297001	0.164063	-2.519077
H	2.344124	-0.599001	-3.716331
H	5.154491	-4.158523	-1.168741
H	6.655739	-3.334323	-0.693166
H	6.116650	-3.312809	-2.392696
H	5.659578	1.180698	1.581916
H	4.806769	-0.084885	2.486085
H	3.914014	1.331654	1.926060
H	1.284729	1.336292	2.998064
H	2.205176	0.120657	4.950308
H	2.847215	-2.285006	4.738922
H	2.567308	-3.443472	2.543170
H	1.664337	-2.215407	0.591081
H	5.917376	-1.582928	0.811966
H	1.784231	2.934358	-2.355934
H	3.851596	2.826581	-1.537261
C	1.859363	4.593512	-0.954134
H	2.334707	5.218505	-1.729190
H	1.147059	5.242853	-0.421152
C	2.914904	4.035969	0.007895
H	2.491098	3.872011	1.010928
H	3.731811	4.762275	0.142957

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6a E = -2414.908252

N	2.841544	1.738594	-1.046668
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C	2.061742	1.401165	0.018442
N	1.666162	2.570171	0.593171
C	2.192743	3.634066	-0.115628
C	2.932217	3.115961	-1.133022
C	1.666091	0.054778	0.428867
C	0.378668	-0.119663	0.784324
C	-0.900694	-0.141879	1.071431
Cr	-2.153349	-0.318454	-0.767960
C	-1.640811	-2.149553	-0.778242
O	-1.294104	-3.246887	-0.756572
C	2.686914	-1.035617	0.448689
C	2.318582	-2.369352	0.189697
C	3.261699	-3.395957	0.249537
C	4.595989	-3.119129	0.569138
C	4.975025	-1.801190	0.837943
C	4.030160	-0.772438	0.781445
O	-1.245255	0.099256	2.373492
C	-2.580424	-0.074114	2.827489
C	-2.606250	0.237188	4.312756
C	-0.700029	0.095119	-1.892152
O	0.151308	0.345673	-2.635647
C	-2.430349	1.519289	-0.429689
O	-2.531571	2.640029	-0.168453
C	-3.776050	-0.801148	0.108503
O	-4.805034	-1.114389	0.520418
C	-3.179834	-0.385094	-2.322766
O	-3.810701	-0.416442	-3.290145
H	-3.261209	0.597641	2.277857
H	-2.910125	-1.110285	2.644222
H	-3.626014	0.111786	4.708903
H	-1.932605	-0.435792	4.865538
H	-2.286911	1.274154	4.502558
H	1.994096	4.664930	0.162262
H	3.500587	3.607413	-1.917147
H	4.339435	0.248701	1.025300
H	6.009718	-1.571574	1.106917
H	5.332353	-3.925343	0.614187
H	2.951031	-4.423022	0.040723
H	1.280003	-2.597008	-0.057341
C	3.383601	0.813633	-2.038226
H	4.283613	0.310160	-1.659443
H	2.623094	0.064024	-2.286987
H	3.627446	1.386352	-2.941925
C	0.792507	2.719230	1.754092
H	-0.251747	2.840796	1.433946
H	0.851855	1.825101	2.385282
H	1.115696	3.603817	2.320164

Radical cation derived from 2a E = -3033.350059

C	4.659837	1.068490	0.356360
C	3.698095	0.845203	-0.648080
C	3.893793	-0.074961	-1.692929
C	5.076750	-0.825435	-1.679026
C	6.046924	-0.668187	-0.681146
C	5.819868	0.288112	0.319822
N	2.512148	1.681160	-0.676049
C	1.240177	1.395827	-0.275776
N	0.479489	2.479969	-0.605503
C	1.279627	3.437944	-1.206563
C	2.542447	2.942468	-1.249928
C	0.779050	0.195650	0.436957
C	-0.512278	-0.135049	0.486167
C	-1.735972	-0.612061	0.725938
Cr	-2.406421	-2.175271	-0.556507
C	-0.854310	-3.240372	-0.032586
O	0.038350	-3.887684	0.254186
C	-0.934211	2.716498	-0.388809
C	-1.383757	3.110786	0.884329
C	-2.739087	3.447033	1.015337
C	-3.629360	3.402522	-0.063258
C	-3.132759	3.007011	-1.315431
C	-1.789591	2.673158	-1.511031
C	-0.479840	3.155581	2.089438
C	-5.078213	3.789837	0.095362
C	-1.287691	2.321755	-2.890994
C	2.885725	-0.250018	-2.801771
C	7.306968	-1.495868	-0.676183
C	4.470636	2.116122	1.425093
C	1.738797	-0.599243	1.300061
C	2.363803	-1.766366	0.835286
C	3.179193	-2.519741	1.683087
C	3.377496	-2.119405	3.007861
C	2.751249	-0.964044	3.484228
C	1.933607	-0.211439	2.636950
O	-2.323356	-0.069937	1.831580
C	-3.737387	0.044354	1.985565
C	-4.024946	0.429953	3.423130
C	-1.323717	-1.476890	-1.972937
O	-0.655909	-1.105676	-2.827318
C	-3.956531	-1.087816	-1.030278
O	-4.856032	-0.449116	-1.318250
C	-3.421952	-2.971667	0.894412
O	-3.996362	-3.506081	1.722994
C	-3.020471	-3.584965	-1.766204
O	-3.383291	-4.396454	-2.479278
H	-4.112547	0.812547	1.287705
H	-4.233819	-0.905403	1.738815
H	-5.110044	0.539568	3.573020

H	-3.655656	-0.340930	4.116306
H	-3.542263	1.385071	3.679651
H	0.871626	4.388170	-1.537544
H	3.464305	3.360998	-1.642632
H	-3.103649	3.763930	1.996219
H	-3.811138	2.972197	-2.172545
H	5.247185	-1.547571	-2.481883
H	-0.847922	3.883914	2.825656
H	0.555290	3.426645	1.834622
H	-0.460073	2.168767	2.581707
H	-5.345086	3.952828	1.149214
H	-5.745563	3.014372	-0.313794
H	-5.297777	4.721302	-0.452893
H	-0.567665	1.491602	-2.880545
H	-0.785608	3.181384	-3.367056
H	-2.122625	2.036812	-3.546144
H	2.655652	0.706000	-3.300336
H	1.929107	-0.657583	-2.437487
H	3.266552	-0.938774	-3.568039
H	7.315826	-2.191321	0.179902
H	8.201523	-0.860062	-0.581407
H	7.407096	-2.092038	-1.594210
H	4.478687	3.135528	1.004048
H	5.277330	2.061790	2.168514
H	3.516349	1.988594	1.958673
H	1.426999	0.677291	3.020373
H	2.889402	-0.652491	4.522426
H	4.010923	-2.712989	3.671423
H	3.655481	-3.428438	1.307569
H	2.211387	-2.090633	-0.195176
H	6.574340	0.438448	1.096865

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Radical catión derived from 6a E = -2414.690343

7	2.850630000	1.686690000	-1.190049000
6	2.155854000	1.357971000	-0.074669000
7	1.959886000	2.501544000	0.625034000
6	2.533343000	3.556228000	-0.058391000
6	3.094136000	3.045585000	-1.191173000
6	1.681652000	0.009006000	0.298259000
6	0.391025000	-0.108435000	0.614447000
6	-0.898774000	-0.102093000	0.939512000
24	-2.272095000	-0.265491000	-0.702452000
6	-1.385120000	-1.899162000	-1.263480000
8	-0.857313000	-2.854072000	-1.596341000
6	2.683114000	-1.100657000	0.356136000
6	2.296850000	-2.437002000	0.151428000
6	3.230453000	-3.469402000	0.248379000
6	4.567227000	-3.188694000	0.550821000
6	4.963068000	-1.864858000	0.760894000

6	4.029567000	-0.829692000	0.665568000
8	-1.139736000	0.219317000	2.245733000
6	-2.336852000	-0.174711000	2.919021000
6	-2.229109000	0.268633000	4.364383000
6	-0.982603000	0.670551000	-1.794884000
8	-0.220159000	1.203025000	-2.462894000
6	-3.074658000	1.364344000	-0.020429000
8	-3.523182000	2.328597000	0.391848000
6	-3.610524000	-1.271259000	0.318243000
8	-4.423245000	-1.872363000	0.841951000
6	-3.491049000	-0.274562000	-2.241961000
8	-4.196285000	-0.271700000	-3.135363000
1	-3.214072000	0.291035000	2.438733000
1	-2.448428000	-1.270439000	2.855262000
1	-3.135508000	-0.025545000	4.915034000
1	-1.360535000	-0.197066000	4.853597000
1	-2.125400000	1.362376000	4.433323000
1	2.497305000	4.575765000	0.315666000
1	3.637069000	3.535671000	-1.994813000
1	4.354724000	0.196475000	0.860753000
1	6.001834000	-1.635723000	1.010599000
1	2.912251000	-4.501374000	0.082606000
1	1.258714000	-2.668156000	-0.090163000
1	5.296433000	-3.998603000	0.624803000
6	1.253183000	2.637415000	1.900272000
1	1.203568000	1.665342000	2.402890000
1	1.794435000	3.357991000	2.527439000
1	0.226655000	2.991248000	1.730625000
6	3.258143000	0.766867000	-2.252781000
1	3.350050000	1.334326000	-3.187120000
1	4.218004000	0.292088000	-2.005732000
1	2.495371000	-0.010143000	-2.376590000

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