$[Mn(CO)_4S_2CNMe(CH_2CO_2H)]$, a new CO-Releasing Molecule (CO-RM) Supplementary information

Sian H. Crook,[1] Brian E. Mann,[1,*] Anthony J. H. M. Meijer,[1] Harry Adams,[1] Philip Sawle,[2] David Scapens,[1] and Roberto Motterlini[3,†]

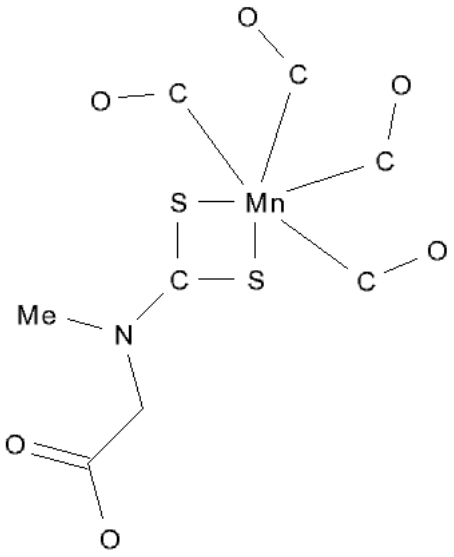
[1]*Department of Chemistry, University of Sheffield, Sheffield S3 7HF, United Kingdom*
[2]*Vascular Biology Unit, Department of Surgical Research, Northwick Park Institute for Medical Research, Harrow, Middlesex, United Kingdom*
[3]*Department of Drug Discovery and Development, Italian Institute of Technology, Via Morego, 30, 16163 Genova, Italy*

(Dated: August 3, 2010)

Contents

1. $[MN(CO)_4S_2CNME(CH_2CO_2)]^-$ MINIMUM ENERGY W/O SOLVENT

General Information



SMILES : CN(CC(=O)[O])[C]1S[Mn](S1)([C][O])([C][O])([C][O])[C][O]
Formula : $C_8H_5MnNO_6S_2^{1-}$
Charge : -1
Multiplicity : 1
Energy : -2761.78948073 a.u.

Cartesian Co-ordinates (XYZ format)

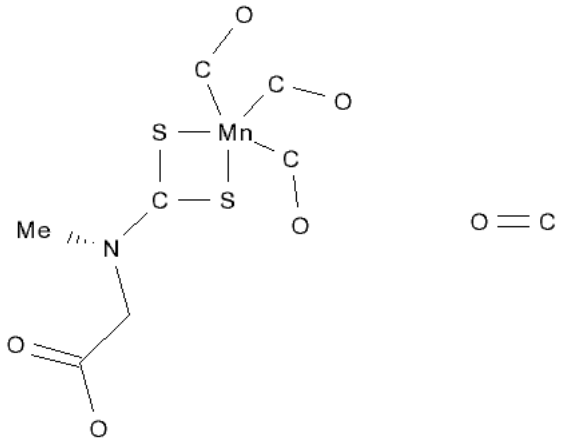
23

Mn	-1.21869433	0.18611202	-1.31881690
S	-1.22042859	0.19067258	1.12182772
S	1.11461532	0.20064883	-0.60765284
N	1.31496954	0.22767906	2.09267092
O	-1.02832377	-2.80606604	-1.07800949
O	-0.64593089	0.18577419	-4.22068167
O	-4.16000271	0.17135771	-1.62847757
O	-1.04732347	3.17377806	-1.07829034
O	2.83142352	-1.85052514	3.29063630
O	4.75592566	-0.96554923	2.47036314
C	-1.10813761	-1.67433703	-1.18250668
C	-0.87266964	0.18474525	-3.09371066
C	-3.01576829	0.17558193	-1.51317179
C	-1.12504065	2.04045820	-1.18681490

C	0.52893162	0.20261328	1.03626764
C	2.78726220	0.22222397	2.01115942
H	3.14798474	1.12397575	2.51688480
H	3.08674169	0.27606860	0.96830082
C	3.53545761	-1.03014922	2.67230964
C	0.78303754	0.23335451	3.45831585
H	-0.28028592	0.00744888	3.45032024
H	0.94186378	1.22293878	3.90193224
H	1.33469701	-0.53522950	4.00207186

2. $[MN(CO)_4S_2CNME(CH_2CO_2)]^-$ TRANSITION STATE CO RELEASE W/O SOLVENT

General Information



SMILES : CN(CC(=O)[O])[C]1S[Mn](S1)([C][O])([C][O])[C][O].[C]=O
Formula : $C_8H_5MnNO_6S_2^{1-}$
Charge : -1
Multiplicity : 1
Energy : -2761.75529322 a.u.

Cartesian Co-ordinates (XYZ format)

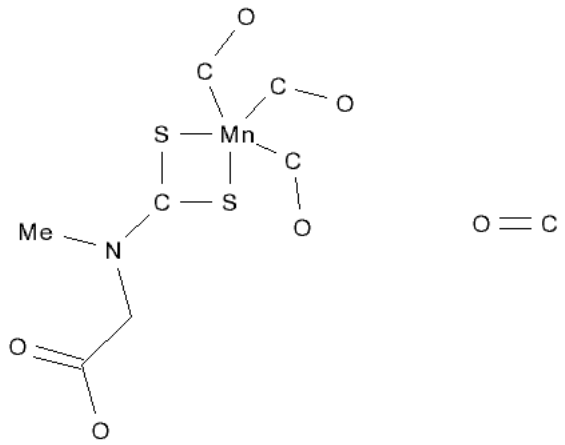
23

Mn	-1.06909180	0.60839063	-1.13366175
S	-1.19870746	0.84347105	1.20821464
S	1.15107989	1.02824295	-0.49067089
N	1.31683052	0.43946320	2.14675283
O	-0.15398793	-3.65004039	-0.09062310
O	-0.25203303	-0.27231872	-3.83589172
O	-3.76439857	-0.59753269	-1.29222929
O	-1.94222832	3.25543427	-2.00767303
O	1.87170100	-2.22455478	1.79252553

O	4.11343288	-1.86250174	1.90205574
C	-0.16007103	-2.53040838	-0.22876157
C	-0.57798612	0.07928002	-2.79096293
C	-2.72032213	-0.11688326	-1.24223280
C	-1.61868787	2.19516563	-1.69351280
C	0.54850006	0.75291473	1.12323117
C	2.71865106	0.03759195	1.98801744
H	3.27943826	0.40124509	2.85100603
H	3.12684107	0.48978385	1.08734453
C	2.91708803	-1.54893887	1.88001800
C	0.73618644	0.08337241	3.44344211
H	-0.21532841	0.59028608	3.58545375
H	1.43678355	0.38507450	4.22437811
H	0.60374767	-1.00027287	3.46464634

3. $[MN(CO)_4S_2CNME(CH_2CO_2)]^-$ DISSOCIATED W/O SOLVENT

General Information



SMILES : CN(CC(=O)[O])[C]1S[Mn](S1)([C][O])([C][O])[C][O].[C]=O
Formula : $C_8H_5MnNO_6S_2^{1-}$
Charge : -1
Multiplicity : 1
Energy : -2761.75262981 a.u.

Cartesian Co-ordinates (XYZ format)

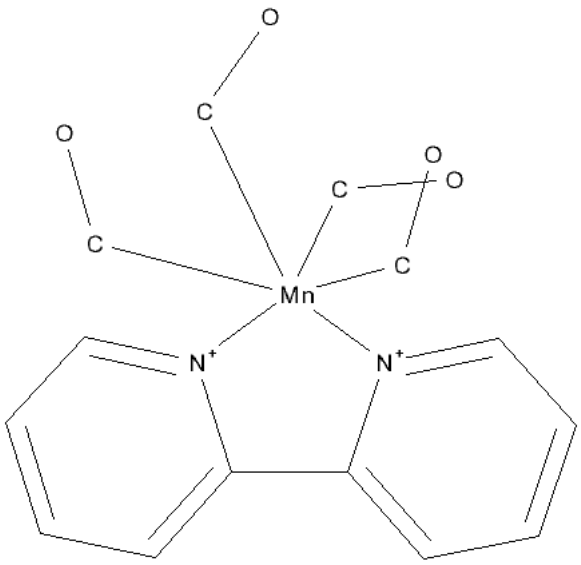
23

Mn	-1.22132659	1.19017339	-1.23847818
S	-1.19452310	1.32316196	1.10645497
S	1.00088561	0.70988679	-0.67691439
N	1.30461776	0.73609346	2.02141595

O	0.66446030	-8.31519604	-0.81753606
O	-0.84880579	0.17150928	-3.98845720
O	-4.16792393	0.96508986	-1.29865849
O	-1.17627287	4.00468969	-2.02100682
O	2.03186655	-1.78242731	3.05881429
O	4.16930151	-1.51038706	2.33540392
C	-0.00968857	-8.65625954	0.01834652
C	-0.99763441	0.58545625	-2.92559147
C	-3.02228999	1.07390201	-1.28765023
C	-1.22330570	2.88713527	-1.74544251
C	0.50651002	0.89608133	0.99353832
C	2.69386363	0.26512286	1.91026330
H	3.32633543	0.97268665	2.45331860
H	2.98931456	0.26274827	0.86524451
C	2.98458648	-1.19987679	2.51221466
C	0.83261347	0.87455463	3.40367413
H	-0.19177739	1.23561108	3.41913939
H	1.48580575	1.58467638	3.91897917
H	0.92042738	-0.11441962	3.85811830

4. [MN(CO)BIPY]$^+$ MINIMUM ENERGY W/O SOLVENT

General Information



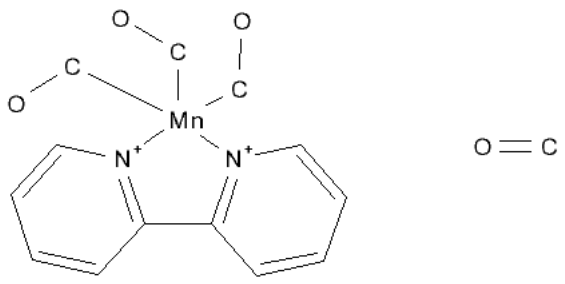
SMILES : c1cc[n+]2c(c1)-c3cccc[n+]3[Mn]2([C][O])([C][O])([C][O])[C][O]
Formula : $C_{14}H_8MnN_2O_4^+$
Charge : 1
Multiplicity : 1
Energy : -2099.83616687 a.u.

Cartesian Co-ordinates (XYZ format)

Mn	0.06927738	-0.03099836	0.03775196
O	0.44537309	0.06855744	3.04009461
C	0.31139228	0.03006504	1.91572297
O	2.46551991	1.69485688	-0.37468466
C	1.55823958	1.02436054	-0.21801810
O	1.69824994	-2.52216220	-0.13816719
C	1.08742559	-1.56303489	-0.07293031
O	-0.46187183	-0.10194018	-2.94183946
C	-0.25625309	-0.07657204	-1.82795596
C	-2.57116127	1.22117269	0.40132475
C	-0.95443183	2.86544752	0.11073347
C	-3.56370234	2.19417286	0.52326167
C	-2.83502483	-0.22823068	0.48270723
C	-1.89346814	3.88036180	0.22349842
H	0.08823077	3.10121703	-0.05321535
C	-3.22403431	3.53754735	0.43381253
H	-4.59339523	1.90978122	0.68658829
C	-4.10346794	-0.77116573	0.69005132
H	-1.57807159	4.91252995	0.14663790
H	-3.98598099	4.30148506	0.52692616
C	-1.90516043	-2.35685301	0.40351078
C	-4.25926542	-2.14948821	0.75332272
H	-4.96411896	-0.12722671	0.80160332
C	-3.13845134	-2.95855594	0.60727847
H	-1.01526380	-2.96016669	0.28638828
H	-5.23900223	-2.58212233	0.91387063
H	-3.20736670	-4.03757238	0.64885014
N	-1.27440774	1.56288922	0.19596593
N	-1.74536157	-1.02387083	0.34091058

5. [MN(CO)BIPY]$^+$ TRANSITION STATE CO RELEASE W/O SOLVENT

General Information



SMILES	:	[C]=O.c1cc[n+]2c(c1)-c3cccc[n+]3[Mn]2([C][O])([C][O])[C][O]
Formula	:	$C_{14}H_8MnN_2O_4^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-2099.79336031 a.u.

Cartesian Co-ordinates (XYZ format)

29

Mn	-1.16194558	0.00195449	1.31953633
O	1.26728249	-0.02316000	-4.87183142
C	1.38269663	-0.01699607	-3.75298500
O	-3.26139116	2.10869598	1.45585668
C	-2.46027327	1.29841709	1.42274773
O	-3.25726652	-2.10770679	1.47309911
C	-2.45773578	-1.29615879	1.43336773
O	-0.68792307	0.01432160	4.22126675
C	-0.91096956	0.00951456	3.10311675
C	1.47753441	0.73865676	0.33293030
C	0.26574305	2.65323782	0.85859704
C	2.55250931	1.51255691	-0.09664045
C	1.47898221	-0.73764694	0.33899248
C	1.30346978	3.48037720	0.45439413
H	-0.65349191	3.07500172	1.24116266
C	2.46659136	2.89869905	-0.03570189
H	3.45051551	1.04452932	-0.47358888
C	2.55547833	-1.51293945	-0.08421751
H	1.19189739	4.55420017	0.52562296
H	3.29681158	3.51177335	-0.36423680
C	0.27095783	-2.65022278	0.88040107
C	2.47228241	-2.89870095	-0.01189009
H	3.45256948	-1.04625988	-0.46499801
C	1.31030846	-3.47861552	0.48299527
H	-0.64744598	-3.07063198	1.26643860
H	3.30370617	-3.51282310	-0.33538595
H	1.20084846	-4.55203390	0.56305420
N	0.33721483	1.31042612	0.80019295
N	0.33978540	-1.30779934	0.81095183

6. [MN(CO)BIPY]$^+$ CO DISSOCIATED W/O SOLVENT

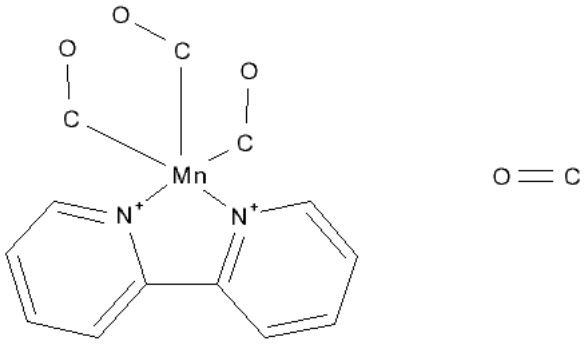
General Information

SMILES	:	[C]=O.c1cc[n+]2c(c1)-c3cccc[n+]3[Mn]2([C][O])([C][O])[C][O]
Formula	:	$C_{14}H_8MnN_2O_4^+$
Charge	:	1
Multiplicity	:	1
Energy	:	-2099.79234146 a.u.

Cartesian Co-ordinates (XYZ format)

29

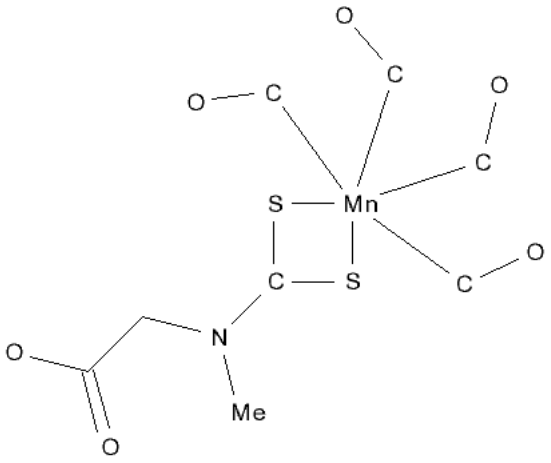
Mn	0.91258073	1.17305756	0.07463979
O	-10.10190678	-0.29209691	-0.49055874



C	-8.99005795	-0.11807857	-0.44567126
O	0.59450871	3.29187202	-1.99309611
C	0.73357278	2.48818111	-1.19691122
O	0.39200419	3.17508030	2.21622658
C	0.60853434	2.41635203	1.39365220
O	3.83200788	1.48902285	0.22585581
C	2.69637585	1.40588176	0.16799323
C	0.72258097	-1.61507356	-0.75118655
C	0.98857558	-0.25234357	-2.61719108
C	0.64924783	-2.74505758	-1.56175911
C	0.64788657	-1.65553737	0.72310507
C	0.92914116	-1.33780754	-3.47931814
H	1.12259698	0.74807888	-3.00504255
C	0.75317603	-2.60690975	-2.94137812
H	0.51635206	-3.72586727	-1.12774050
C	0.49208626	-2.82754898	1.45891511
H	1.01960206	-1.18067718	-4.54596138
H	0.69981253	-3.47822881	-3.58246493
C	0.72518778	-0.39833257	2.67839193
C	0.45641872	-2.76552343	2.84748769
H	0.40198922	-3.78227901	0.96050280
C	0.57877898	-1.52885890	3.46926689
H	0.82009518	0.57853454	3.13214397
H	0.33693594	-3.67003536	3.43111086
H	0.56165576	-1.43073177	4.54661226
N	0.88479751	-0.37437534	-1.28088832
N	0.75602037	-0.44651368	1.33375072

7. $[MN(CO)_4S_2CNME(CH_2CO_2)]^-$ MINIMUM ENERGY STRUCTURE W/ WATER SOLVENT

General Information



SMILES : CN(CC(=O)[O])[C]1S[Mn](S1)([C][O])([C][O])([C][O])[C][O]
Formula : $C_8H_5MnNO_6S_2^{1-}$
Charge : -1
Multiplicity : 1
Energy : -2761.87135384 a.u.

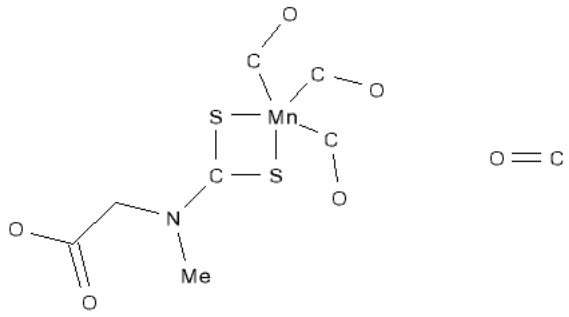
Cartesian Co-ordinates (XYZ format)

23

Mn	-1.70970666	-0.11688242	-0.02101470
S	-0.07603597	1.47870934	0.86420244
S	0.45403987	-0.66224104	-1.02575207
N	2.38119531	1.03632426	-0.18204875
O	-0.86785752	-1.90454030	2.24484611
O	-3.23099756	-2.26336265	-1.37815440
O	-4.03615522	0.95826977	1.46091974
O	-2.04543495	1.80781460	-2.30397677
O	3.64887047	-0.98311871	1.20201027
O	4.99122047	-1.47554028	-0.54946393
C	-1.20860553	-1.23479843	1.38861716
C	-2.64964199	-1.42916536	-0.84819460
C	-3.14043021	0.53537011	0.88332546
C	-1.94238150	1.07308316	-1.43914080
C	1.11006665	0.67008621	-0.11992647
C	3.38563895	0.22453137	-0.87262821
H	4.14916134	0.89649296	-1.26706982
H	2.92079258	-0.28270653	-1.71720815
C	4.07690716	-0.85640293	0.03528447
C	2.90940189	2.10493922	0.66911894
H	2.13704085	2.84234619	0.87508023
H	3.73535752	2.58665490	0.14635399
H	3.27382374	1.67661190	1.60543597

8. $[MN(CO)_4S_2CNME(CH_2CO_2)]^-$ TRANSITION STATE W/ WATER SOLVENT

General Information



SMILES : CN(CC(=O)[O])[C]1S[Mn](S1)([C][O])([C][O])[C][O].[C]=O
Formula : $C_8H_5MnNO_6S_2^{1-}$
Charge : -1
Multiplicity : 1
Energy : -2761.83661290 a.u.

Cartesian Co-ordinates (XYZ format)

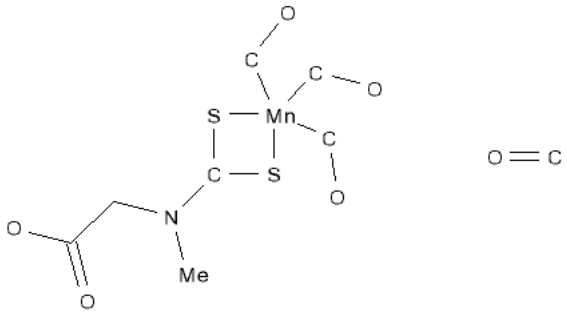
23

Mn	1.85682797	0.11779650	-0.03446650
S	0.46484062	-1.05385423	1.48305678
S	-0.12335733	-0.32206690	-1.26107192
N	-1.94992077	-1.53192055	0.32962701
O	3.79188704	0.89490467	2.06650019
O	2.85499072	2.10596895	-1.98604429
O	-2.55617023	3.94218349	0.67188203
O	3.51785398	-2.05948496	-1.05101204
O	-3.57514095	0.68856531	0.39833140
O	-4.72983170	0.02430788	-1.42907107
C	-1.63617980	3.29504895	0.59984976
C	2.48316646	1.32401514	-1.23207760
C	3.05168986	0.58986384	1.24357414
C	2.90071344	-1.17398739	-0.65220171
C	-0.73047078	-1.05213106	0.20504287
C	-2.96228671	-1.36525941	-0.71795833
H	-3.61199641	-2.24123120	-0.69741559
H	-2.47334981	-1.33034611	-1.68964803

C	-3.84484196	-0.07329839	-0.55478638
C	-2.46026897	-2.05527592	1.60060775
H	-1.64059377	-2.26260710	2.28209233
H	-3.01287174	-2.97463322	1.40312350
H	-3.12910867	-1.31045210	2.03519654

9. $[MN(CO)_4S_2CNME(CH_2CO_2)]^-$ DISSOCIATED W/ WATER SOLVENT

General Information



SMILES : CN(CC(=O)[O])[C]1S[Mn](S1)([C][O])([C][O])[C][O].[C]=O
Formula : $C_8H_5MnNO_6S_2^{1-}$
Charge : -1
Multiplicity : 1
Energy : -2761.83561666 a.u.

Cartesian Co-ordinates (XYZ format)

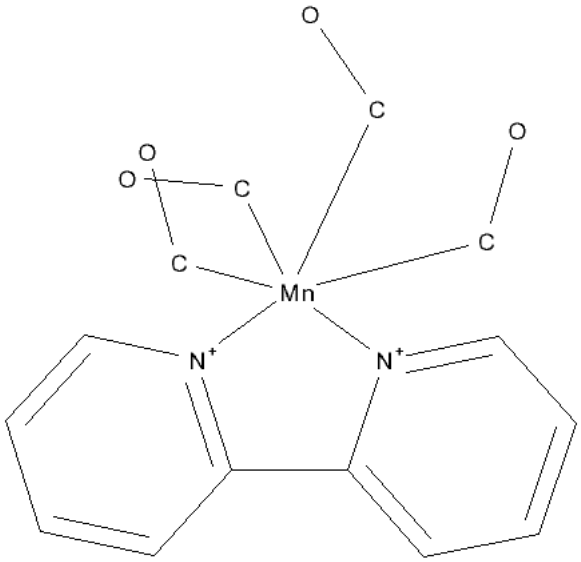
23

Mn	1.77827847	0.90114880	-0.06654660
S	1.14962018	-0.77185053	1.50057936
S	0.43309659	-0.59802908	-1.30517364
N	-0.52011520	-2.55373216	0.30787966
O	-6.74311876	4.80286026	0.85487813
O	1.78926992	2.94119239	-2.21212292
O	2.75469470	2.76263881	2.01829839
O	4.44042253	-0.10126520	-0.72938645
O	-3.09206343	-1.58918166	0.16652763
O	-3.58855915	-2.88280010	-1.62074220
C	-7.64819050	4.15008593	0.69896388
C	1.79646230	2.15294480	-1.37744308
C	2.39142299	2.04154444	1.20207453

C	3.40874529	0.33726758	-0.46997425
C	0.23604733	-1.48274767	0.18969364
C	-1.38938475	-3.01817346	-0.77791697
H	-1.44663846	-4.10576200	-0.71891814
H	-0.94282252	-2.75463009	-1.73489571
C	-2.84631491	-2.42588067	-0.72703958
C	-0.73642898	-3.21718955	1.59742844
H	0.04141319	-2.93849039	2.30229783
H	-0.71810430	-4.29623842	1.44134951
H	-1.71374953	-2.91814613	1.98032248

10. [MN(CO)BIPY]$^+$ CO MINIMUM ENERGY STRUCTURE W/ WATER SOLVENT

General Information



SMILES : c1cc[n+]2c(c1)-c3cccc[n+]3[Mn]2([C][O])([C][O])([C][O])[C][O]
Formula : $C_{14}H_8MnN_2O_4^+$
Charge : 1
Multiplicity : 1
Energy : -2099.90426184 a.u.

Cartesian Co-ordinates (XYZ format)

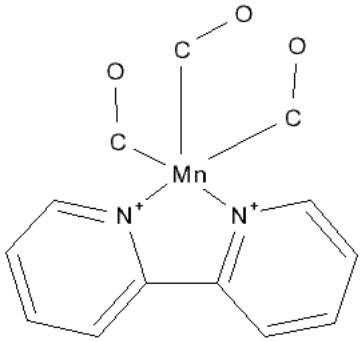
29

Mn	1.10770988	-0.00033145	0.00010430
O	1.02839696	-0.00007575	-3.02361584
C	1.06125677	-0.00018217	-1.88979495
O	3.19782615	-2.12113237	0.00057730
C	2.39790964	-1.30665123	0.00038380
O	3.19911599	2.11918974	0.00068602
C	2.39861274	1.30528474	0.00047076
O	1.02705824	-0.00035234	3.02379942

C	1.06040156	-0.00036173	1.88999319
C	-1.73874223	-0.73643452	-0.00016789
C	-0.42738351	-2.65542126	-0.00049177
C	-2.90105724	-1.50698400	-0.00003355
C	-1.73833621	0.73733407	-0.00019894
C	-1.54419863	-3.47781301	-0.00044077
H	0.56530935	-3.08219004	-0.00067418
C	-2.80437326	-2.89186025	-0.00016100
H	-3.87249660	-1.03496122	0.00018913
C	-2.90022922	1.50851941	-0.00033332
H	-1.41626596	-4.55167341	-0.00059138
H	-3.69956398	-3.50047636	-0.00005195
C	-0.42592856	2.65560246	-0.00026150
C	-2.80279016	2.89334249	-0.00040118
H	-3.87192440	1.03702366	-0.00041175
C	-1.54229391	3.47860456	-0.00036932
H	0.56699830	3.08182740	-0.00026178
H	-3.69764829	3.50244689	-0.00049281
H	-1.41377354	4.55239487	-0.00043890
N	-0.51215023	-1.31497335	-0.00031741
N	-0.51142681	1.31520045	-0.00016155

11. [MN(CO)BIPY]$^+$ CO DISSOCIATION W/ WATER SOLVENT

General Information



SMILES : [C]=O.c1cc[n+]2c(c1)-c3cccc[n+]3[Mn]2([C][O])([C][O])[C][O]
Formula : $C_{14}H_8MnN_2O_4^+$
Charge : 1
Multiplicity : 1
Energy : -2099.86851758 a.u.

Cartesian Co-ordinates (XYZ format)

29

Mn	-0.94366896	-1.09387684	-0.00823910
O	10.17200089	-0.60716504	0.01059725
C	9.04784012	-0.68188721	-0.00415450
O	-0.80757087	-3.19735384	-2.11213231
C	-0.86644804	-2.38717175	-1.30807006
O	-0.83128148	-3.22246170	2.07197475
C	-0.88006663	-2.40321231	1.27647233
O	-3.87820053	-1.06252933	-0.01966635
C	-2.73450184	-1.10803699	-0.01559976
C	-0.46754381	1.68325233	-0.72523564
C	-0.78495622	0.41599262	-2.64856887
C	-0.24797794	2.82730794	-1.48842597
C	-0.45506448	1.66853368	0.75001830
C	-0.57852429	1.51756883	-3.46609211
H	-1.00117087	-0.55166018	-3.07836723
C	-0.30291745	2.74420905	-2.87456942
H	-0.04064062	3.77508688	-1.01348162
C	-0.19929941	2.79259014	1.53115690
H	-0.63542283	1.40450585	-4.54008532
H	-0.13521668	3.62630105	-3.47935510
C	-0.77080989	0.37203425	2.65379500
C	-0.23846209	2.68539119	2.91617322
H	0.02763889	3.74266100	1.07027555
C	-0.53503031	1.45459998	3.48857975
H	-1.00016630	-0.59890801	3.06889486
H	-0.04245648	3.55212212	3.53449130
H	-0.58277255	1.32337391	4.56094408
N	-0.72984380	0.48554972	-1.30731106
N	-0.72903693	0.46430582	1.31341398

* Electronic address: b.mann@sheffield.ac.uk
† Electronic address: roberto.motterlini@iit.it