

ELECTRONIC SUPPLEMENTARY INFORMATION

**Stabilisation of dianion dimers trapped inside cyanostar
macrocycles**

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Table S1. Interaction electronic energies (kcal mol⁻¹) for 2:2 anion:cyanostar minima in dichloromethane. Note: E_{int}^* refers to the interaction energy of anionic dimers in dichloromethane solution.^(a)

$$E_{\text{int}}^{(1)} = E_{\text{complex}} - E_{\text{PP:CS,a}} - E_{\text{PP:CS,b}} \quad (1)$$

$$E_{\text{int}}^{(2)} = E_{\text{complex}} - E_{\text{PP,a}} - E_{\text{CS,a}} - E_{\text{PP,b}} - E_{\text{CS,b}} \quad (2)$$

$$E_{\text{int}}^{(3)} = E_{\text{complex}} - E_{\text{PP:PP}} - E_{\text{CS:CS}} \quad (3)$$

$$E_{\text{int}}^{(\text{PH})} = E_{\text{PH:PH}} - E_{\text{PH,a}} - E_{\text{PH,b}} \quad (4)$$

$$E_{\text{int}}^{(\text{CS})} = E_{\text{CS:CS}} - E_{\text{CS,a}} - E_{\text{CS,b}} \quad (5)$$

$$E_{\text{int}}^{(\text{PHCS})} = E_{\text{CS:PH}} - E_{\text{CS,a}} - E_{\text{PH,a}} \quad (6)$$

Anion	$E_{\text{int}}^{(1)}$	$E_{\text{int}}^{(2)}$	$E_{\text{int}}^{(3)}$	$E_{\text{int}}^{(\text{PH})}$	$E_{\text{int}}^{(\text{CS})}$	$E_{\text{int}}^{(\text{PHCS})}$	E_{int}^*
CH ₃ PO ₃ H ⁻	-25.7	-37.6	-16.3	-12.6	-8.7	-6.0	-11.7
H ₂ BO ₃ ⁻	-25.9	-38.8	-20.1	-10.9	-7.8	-6.5	-11.0
HCO ₃ ⁻	-22.8	-36.5	-16.9	-10.0	-9.7	-6.8	-8.7
HSO ₄ ⁻	-23.7	-35.1	-16.2	-9.2	-9.7	-5.7	-8.2
HSeO ₄ ⁻	-21.6	-29.3	-11.7	-9.2	-8.4	-3.8	-9.6
H ₂ PO ₄ ⁻	-26.7	-38.6	-16.4	-13.1	-9.1	-6.0	-12.0
H ₂ AsO ₄ ⁻	-24.9	-33.9	-13.0	-11.7	-9.2	-4.5	-11.8

^(a) $E_{\text{int}}^{(\text{PHCS})}$ cross terms ($E_{\text{CS:PH}} - E_{\text{CS,a}} - E_{\text{PH,b}}$) are minor quantities and have been omitted for clarity.

OPTIMISED CARTESIAN COORDINATES

2:2 phosphonate:cyanostar in dichloromethane

N	2.29829915	-7.89921010	-1.57995918
N	7.74296310	-0.53633343	-1.42805747
N	2.36638461	6.91151178	-2.95061368
N	-6.39205574	4.23408988	-1.46547885
N	-6.52750251	-4.97427358	-1.76144059
C	4.16346669	-5.07150001	-2.31172731
C	3.14237713	-4.12161609	-2.10521718
C	3.49519298	-2.76196100	-1.99481790
C	4.83508407	-2.34899381	-2.06769442
C	5.82505784	-3.32595151	-2.25404205
C	5.50238215	-4.68440292	-2.37636012
C	5.22302396	-0.91405429	-1.95176069
C	4.33037089	0.10770965	-2.08607108
C	4.48353955	1.55881924	-2.00923000
C	3.28621062	2.29994358	-2.05107528
C	3.28993689	3.70115743	-2.01048833
C	4.52662689	4.36117648	-1.94308946

C	5.73629792	3.65161074	-1.90890229
C	5.70644469	2.25555562	-1.94011221
C	2.02303362	4.48409395	-2.08046965
C	0.80420943	3.96805750	-1.74902000
C	-0.53998905	4.53890444	-1.83963164
C	-1.61450822	3.63037424	-1.76417865
C	-2.94248214	4.06536511	-1.90256386
C	-3.18187633	5.43950831	-2.05952468
C	-2.13383926	6.36940338	-2.09093715
C	-0.81878571	5.91117881	-1.99418971
C	-4.08623359	3.10835045	-1.89562874
C	-3.93263826	1.76441682	-2.07176559
C	-4.90913816	0.67685241	-2.11721506
C	-4.38736390	-0.62956990	-2.02390325
C	-5.22465473	-1.75430635	-2.05733923
C	-6.60846690	-1.54587518	-2.18984819
C	-7.15374940	-0.26003700	-2.29195403
C	-6.29919018	0.84431024	-2.26334867
C	-4.69008086	-3.14100137	-1.93674652
C	-3.35791498	-3.43857891	-1.93109663
C	-2.64087789	-4.70044202	-1.75414361
C	-1.24266656	-4.61461711	-1.89359238
C	-0.41594663	-5.73030938	-1.70946154
C	-1.01922163	-6.95498836	-1.38430316
C	-2.40862949	-7.07047343	-1.23086262
C	-3.21324652	-5.94488686	-1.42069472
C	1.06580696	-5.62211775	-1.82816169
C	1.71868380	-4.43403803	-1.99028497
C	6.59221335	-5.70648895	-2.55667515
C	-3.01422153	-8.38758274	-0.82412632
C	-8.64262375	-0.06749798	-2.39917208
C	-2.42934390	7.84047569	-2.20365204
C	7.04419137	4.39329360	-1.83894390
C	1.77205637	-6.85655407	-1.70444942
C	6.60269571	-0.68036255	-1.67033794
C	2.17691981	5.82086432	-2.55746666
C	-5.36617211	3.70038808	-1.67231811
C	-5.67965675	-4.16398232	-1.83149329
H	3.92656464	-6.12059742	-2.43322998
H	6.86865467	-3.03145566	-2.31560197
H	4.55904810	5.44670731	-1.91920522
H	6.64887540	1.72276947	-1.93317634
H	-4.20002458	5.80445799	-2.15971925
H	-0.01747568	6.63853046	-2.01315263
H	-7.28355223	-2.39578853	-2.21649482
H	-6.73100255	1.83196244	-2.36753523
H	-0.40801788	-7.84023651	-1.23536093
H	-4.28287582	-6.05070723	-1.29054654
H	7.11324841	-5.88635576	-1.60786431
H	6.18701500	-6.66238270	-2.90002701
H	7.34208817	-5.36782332	-3.27909107
H	-2.95369603	-8.52062981	0.26392472
H	-4.06959086	-8.44427008	-1.10553065
H	-2.48707752	-9.22868773	-1.28518350
H	-9.13202958	-0.95702659	-2.80570181

H	-9.07790023	0.12617721	-1.41025876
H	-8.88921769	0.78692517	-3.03655513
H	-1.55891270	8.39197187	-2.57016718
H	-3.26920489	8.02786536	-2.87990299
H	-2.69705466	8.25629848	-1.22378455
H	7.16871170	4.87111042	-0.85960713
H	7.89038546	3.71816702	-1.99266767
H	7.09162685	5.18287475	-2.59660476
H	2.70400253	-2.03592848	-1.83034644
H	1.08650220	-3.54961438	-2.01640576
H	-0.83113052	-3.64099194	-2.14117980
H	-2.67652622	-2.60175754	-2.07734409
H	-3.31394550	-0.73209196	-1.90200231
H	-2.90778865	1.41135176	-2.16113921
H	-1.39686095	2.57907475	-1.58664727
H	0.81138083	2.94340665	-1.38479632
H	2.35629842	1.74891672	-2.13197195
H	3.30115382	-0.19043796	-2.26476272
N	6.39205574	-4.23408988	1.46547885
N	6.52750251	4.97427358	1.76144059
N	-2.29829915	7.89921010	1.57995918
N	-7.74296310	0.53633343	1.42805747
N	-2.36638461	-6.91151178	2.95061368
C	6.29919018	-0.84431024	2.26334867
C	4.90913816	-0.67685241	2.11721506
C	4.38736390	0.62956990	2.02390325
C	5.22465473	1.75430635	2.05733923
C	6.60846690	1.54587518	2.18984819
C	7.15374940	0.26003700	2.29195403
C	4.69008086	3.14100137	1.93674652
C	3.35791498	3.43857891	1.93109663
C	2.64087789	4.70044202	1.75414361
C	1.24266656	4.61461711	1.89359238
C	0.41594663	5.73030938	1.70946154
C	1.01922163	6.95498836	1.38430316
C	2.40862949	7.07047343	1.23086262
C	3.21324652	5.94488686	1.42069472
C	-1.06580696	5.62211775	1.82816169
C	-1.71868380	4.43403803	1.99028497
C	-3.14237713	4.12161609	2.10521718
C	-3.49519298	2.76196100	1.99481790
C	-4.83508407	2.34899381	2.06769442
C	-5.82505784	3.32595151	2.25404205
C	-5.50238215	4.68440292	2.37636012
C	-4.16346669	5.07150001	2.31172731
C	-5.22302396	0.91405429	1.95176069
C	-4.33037089	-0.10770965	2.08607108
C	-4.48353955	-1.55881924	2.00923000
C	-3.28621062	-2.29994358	2.05107528
C	-3.28993689	-3.70115743	2.01048833
C	-4.52662689	-4.36117648	1.94308946
C	-5.73629792	-3.65161074	1.90890229
C	-5.70644469	-2.25555562	1.94011221
C	-2.02303362	-4.48409395	2.08046965
C	-0.80420943	-3.96805750	1.74902000

C	0.53998905	-4.53890444	1.83963164
C	1.61450822	-3.63037424	1.76417865
C	2.94248214	-4.06536511	1.90256386
C	3.18187633	-5.43950831	2.05952468
C	2.13383926	-6.36940338	2.09093715
C	0.81878571	-5.91117881	1.99418971
C	4.08623359	-3.10835045	1.89562874
C	3.93263826	-1.76441682	2.07176559
C	8.64262375	0.06749798	2.39917208
C	2.42934390	-7.84047569	2.20365204
C	-7.04419137	-4.39329360	1.83894390
C	-6.59221335	5.70648895	2.55667515
C	3.01422153	8.38758274	0.82412632
C	5.36617211	-3.70038808	1.67231811
C	5.67965675	4.16398232	1.83149329
C	-1.77205637	6.85655407	1.70444942
C	-6.60269571	0.68036255	1.67033794
C	-2.17691981	-5.82086432	2.55746666
H	6.73100255	-1.83196244	2.36753523
H	7.28355223	2.39578853	2.21649482
H	0.40801788	7.84023651	1.23536093
H	4.28287582	6.05070723	1.29054654
H	-6.86865467	3.03145566	2.31560197
H	-3.92656464	6.12059742	2.43322998
H	-4.55904810	-5.44670731	1.91920522
H	-6.64887540	-1.72276947	1.93317634
H	4.20002458	-5.80445799	2.15971925
H	0.01747568	-6.63853046	2.01315263
H	9.13202958	0.95702659	2.80570181
H	8.88921769	-0.78692517	3.03655513
H	9.07790023	-0.12617721	1.41025876
H	3.26920489	-8.02786536	2.87990299
H	1.55891270	-8.39197187	2.57016718
H	2.69705466	-8.25629848	1.22378455
H	-7.16871170	-4.87111042	0.85960713
H	-7.09162685	-5.18287475	2.59660476
H	-7.89038546	-3.71816702	1.99266767
H	-7.11324841	5.88635576	1.60786431
H	-7.34208817	5.36782332	3.27909107
H	-6.18701500	6.66238270	2.90002701
H	2.48707752	9.22868773	1.28518350
H	4.06959086	8.44427008	1.10553065
H	2.95369603	8.52062981	-0.26392472
H	3.31394550	0.73209196	1.90200231
H	2.90778865	-1.41135176	2.16113921
H	1.39686095	-2.57907475	1.58664727
H	-0.81138083	-2.94340665	1.38479632
H	-2.35629842	-1.74891672	2.13197195
H	-3.30115382	0.19043796	2.26476272
H	-2.70400253	2.03592848	1.83034644
H	-1.08650220	3.54961438	2.01640576
H	0.83113052	3.64099194	2.14117980
H	2.67652622	2.60175754	2.07734409
P	-0.27000633	-0.29212252	-2.13479534
P	0.27000633	0.29212252	2.13479534

O	-1.23553527	0.38709119	-1.15314969
O	1.21613907	-0.25814643	-1.47324757
O	-0.62749986	-1.70605961	-2.56530884
O	1.23553527	-0.38709119	1.15314969
O	-1.21613907	0.25814643	1.47324757
O	0.62749986	1.70605961	2.56530884
C	-0.06987230	0.71148956	-3.63229338
C	0.06987230	-0.71148956	3.63229338
H	-1.18791133	0.28968092	0.46428558
H	1.18791133	-0.28968092	-0.46428558
H	0.71809224	0.28386801	-4.26139361
H	-1.01092318	0.68701865	-4.19188352
H	0.17782001	1.75252012	-3.41207442
H	1.01092318	-0.68701865	4.19188352
H	-0.71809224	-0.28386801	4.26139361
H	-0.17782001	-1.75252012	3.41207442

2:2 phosphonate:cyanostar in water

N	2.57581288	-7.83939989	-1.47441569
N	7.64857798	-0.27712642	-1.37819959
N	1.98294433	6.92693710	-3.09146529
N	-6.62589434	3.85088293	-1.34368753
N	-6.38366006	-5.31075215	-1.63599108
C	4.28702513	-4.95614139	-2.37370264
C	3.23296687	-4.05119207	-2.13344350
C	3.53066237	-2.67840511	-2.02733146
C	4.84941744	-2.20975089	-2.13277815
C	5.87552506	-3.14157898	-2.35034671
C	5.60641171	-4.51250447	-2.47542552
C	5.17353940	-0.75915300	-2.01542108
C	4.24347628	0.22138849	-2.19413061
C	4.33265896	1.67830293	-2.12078282
C	3.10525087	2.36842613	-2.15923128
C	3.05069976	3.76904498	-2.12241710
C	4.25958161	4.48026322	-2.06661179
C	5.49842513	3.82181481	-2.04036764
C	5.52608746	2.42521453	-2.06405996
C	1.75146557	4.49902458	-2.18691914
C	0.55817083	3.93713916	-1.83753478
C	-0.81087878	4.44869581	-1.91817877
C	-1.84373700	3.49487619	-1.81837171
C	-3.19130213	3.86848789	-1.94187396
C	-3.49533813	5.22829686	-2.11046856
C	-2.48965960	6.20338027	-2.16772795
C	-1.15358407	5.80532376	-2.08338794
C	-4.28804528	2.85818828	-1.90676454
C	-4.07740705	1.52685380	-2.11309408
C	-5.00359702	0.39523710	-2.13535304
C	-4.42897920	-0.88550938	-2.00603501
C	-5.21965559	-2.04401230	-2.01778000
C	-6.60972790	-1.89541890	-2.16768509
C	-7.20609618	-0.63633709	-2.31127979
C	-6.39684479	0.50279597	-2.30095095
C	-4.62847754	-3.40446062	-1.86384376
C	-3.28486518	-3.64542794	-1.86041481

C	-2.51127687	-4.86997730	-1.66013756
C	-1.12011873	-4.72785175	-1.82402985
C	-0.24278901	-5.80186719	-1.62538132
C	-0.78710113	-7.04246524	-1.25945133
C	-2.16799241	-7.21370716	-1.08025005
C	-3.02366549	-6.12892640	-1.28509019
C	1.23073704	-5.63331803	-1.77353185
C	1.82767808	-4.42328196	-1.98011823
C	6.73166332	-5.48311288	-2.71295740
C	-2.70815168	-8.54577978	-0.63339516
C	-8.69933304	-0.50856474	-2.45046528
C	-2.85193380	7.65796484	-2.29719904
C	6.77541224	4.61710494	-1.99558923
C	1.99606064	-6.82928254	-1.62496067
C	6.52827887	-0.46744826	-1.67514180
C	1.84453219	5.83491201	-2.68173777
C	-5.58464821	3.37919195	-1.61382152
C	-5.57329438	-4.46547703	-1.72930744
H	4.08990048	-6.01318825	-2.49890084
H	6.90394389	-2.80255332	-2.43776950
H	4.24733082	5.56629678	-2.04731119
H	6.48975984	1.93131336	-2.06876992
H	-4.53002947	5.54604043	-2.20376563
H	-0.38653664	6.56823090	-2.12211945
H	-7.24996210	-2.77221277	-2.18171068
H	-6.86351332	1.47002129	-2.44405269
H	-0.13675800	-7.89735881	-1.09903593
H	-4.08539374	-6.27795283	-1.13335193
H	7.40548605	-5.51735017	-1.84846260
H	6.35337972	-6.49421430	-2.88555165
H	7.33421794	-5.18887719	-3.57936375
H	-2.59385381	-8.66446828	0.45188333
H	-3.77218654	-8.64184831	-0.86658762
H	-2.17268423	-9.37323176	-1.10920420
H	-9.14773595	-1.44114768	-2.80381089
H	-9.15915190	-0.26624083	-1.48369200
H	-8.96680572	0.29179704	-3.14696917
H	-2.01224941	8.24239322	-2.68373161
H	-3.70865606	7.79688464	-2.96370508
H	-3.12449937	8.07608088	-1.31968520
H	6.86507264	5.16116914	-1.04794207
H	7.64886298	3.96704356	-2.09432805
H	6.80639497	5.35894088	-2.80099032
H	2.71557390	-1.98511354	-1.84008293
H	1.15669812	-3.56868815	-2.01284194
H	-0.75560576	-3.74407437	-2.10222399
H	-2.64190931	-2.78356909	-2.03395193
H	-3.35275811	-0.94234487	-1.87925208
H	-3.04168974	1.22826525	-2.24985339
H	-1.57935768	2.45555304	-1.63530179
H	0.61269975	2.91738380	-1.46389024
H	2.19933603	1.77890243	-2.23688632
H	3.23627382	-0.12394863	-2.41009692
N	6.62589434	-3.85088293	1.34368753
N	6.38366006	5.31075215	1.63599108

N	-2.57581288	7.83939989	1.47441569
N	-7.64857798	0.27712642	1.37819959
N	-1.98294433	-6.92693710	3.09146529
C	6.39684479	-0.50279597	2.30095095
C	5.00359702	-0.39523710	2.13535304
C	4.42897920	0.88550938	2.00603501
C	5.21965559	2.04401230	2.01778000
C	6.60972790	1.89541890	2.16768509
C	7.20609618	0.63633709	2.31127979
C	4.62847754	3.40446062	1.86384376
C	3.28486518	3.64542794	1.86041481
C	2.51127687	4.86997730	1.66013756
C	1.12011873	4.72785175	1.82402985
C	0.24278901	5.80186719	1.62538132
C	0.78710113	7.04246524	1.25945133
C	2.16799241	7.21370716	1.08025005
C	3.02366549	6.12892640	1.28509019
C	-1.23073704	5.63331803	1.77353185
C	-1.82767808	4.42328196	1.98011823
C	-3.23296687	4.05119207	2.13344350
C	-3.53066237	2.67840511	2.02733146
C	-4.84941744	2.20975089	2.13277815
C	-5.87552506	3.14157898	2.35034671
C	-5.60641171	4.51250447	2.47542552
C	-4.28702513	4.95614139	2.37370264
C	-5.17353940	0.75915300	2.01542108
C	-4.24347628	-0.22138849	2.19413061
C	-4.33265896	-1.67830293	2.12078282
C	-3.10525087	-2.36842613	2.15923128
C	-3.05069976	-3.76904498	2.12241710
C	-4.25958161	-4.48026322	2.06661179
C	-5.49842513	-3.82181481	2.04036764
C	-5.52608746	-2.42521453	2.06405996
C	-1.75146557	-4.49902458	2.18691914
C	-0.55817083	-3.93713916	1.83753478
C	0.81087878	-4.44869581	1.91817877
C	1.84373700	-3.49487619	1.81837171
C	3.19130213	-3.86848789	1.94187396
C	3.49533813	-5.22829686	2.11046856
C	2.48965960	-6.20338027	2.16772795
C	1.15358407	-5.80532376	2.08338794
C	4.28804528	-2.85818828	1.90676454
C	4.07740705	-1.52685380	2.11309408
C	8.69933304	0.50856474	2.45046528
C	2.85193380	-7.65796484	2.29719904
C	-6.77541224	-4.61710494	1.99558923
C	-6.73166332	5.48311288	2.71295740
C	2.70815168	8.54577978	0.63339516
C	5.58464821	-3.37919195	1.61382152
C	5.57329438	4.46547703	1.72930744
C	-1.99606064	6.82928254	1.62496067
C	-6.52827887	0.46744826	1.67514180
C	-1.84453219	-5.83491201	2.68173777
H	6.86351332	-1.47002129	2.44405269
H	7.24996210	2.77221277	2.18171068

H	0.13675800	7.89735881	1.09903593
H	4.08539374	6.27795283	1.13335193
H	-6.90394389	2.80255332	2.43776950
H	-4.08990048	6.01318825	2.49890084
H	-4.24733082	-5.56629678	2.04731119
H	-6.48975984	-1.93131336	2.06876992
H	4.53002947	-5.54604043	2.20376563
H	0.38653664	-6.56823090	2.12211945
H	9.14773595	1.44114768	2.80381089
H	8.96680572	-0.29179704	3.14696917
H	9.15915190	0.26624083	1.48369200
H	3.70865606	-7.79688464	2.96370508
H	2.01224941	-8.24239322	2.68373161
H	3.12449937	-8.07608088	1.31968520
H	-6.86507264	-5.16116914	1.04794207
H	-6.80639497	-5.35894088	2.80099032
H	-7.64886298	-3.96704356	2.09432805
H	-7.40548605	5.51735017	1.84846260
H	-7.33421794	5.18887719	3.57936375
H	-6.35337972	6.49421430	2.88555165
H	2.17268423	9.37323176	1.10920420
H	3.77218654	8.64184831	0.86658762
H	2.59385381	8.66446828	-0.45188333
H	3.35275811	0.94234487	1.87925208
H	3.04168974	-1.22826525	2.24985339
H	1.57935768	-2.45555304	1.63530179
H	-0.61269975	-2.91738380	1.46389024
H	-2.19933603	-1.77890243	2.23688632
H	-3.23627382	0.12394863	2.41009692
H	-2.71557390	1.98511354	1.84008293
H	-1.15669812	3.56868815	2.01284194
H	0.75560576	3.74407437	2.10222399
H	2.64190931	2.78356909	2.03395193
P	-0.35366046	-0.35599227	-2.12325137
P	0.35366046	0.35599227	2.12325137
O	-1.28917798	0.30293955	-1.09927273
O	1.15703876	-0.29349653	-1.52433146
O	-0.70045778	-1.78057846	-2.53115944
O	1.28917798	-0.30293955	1.09927273
O	-1.15703876	0.29349653	1.52433146
O	0.70045778	1.78057846	2.53115944
C	-0.24423380	0.63674650	-3.63661885
C	0.24423380	-0.63674650	3.63661885
H	-1.16731940	0.27390679	0.51524648
H	1.16731940	-0.27390679	-0.51524648
H	0.52409465	0.21977942	-4.29652792
H	-1.20936137	0.58645375	-4.15191208
H	-0.00895340	1.68501684	-3.43913674
H	1.20936137	-0.58645375	4.15191208
H	-0.52409465	-0.21977942	4.29652792
H	0.00895340	-1.68501684	3.43913674

phosphonate:phosphonate dianion in dichloromethane

P	0.08774961	-2.17896092	0.07188846
P	-0.08774961	2.17896092	-0.07188846

O	-0.74974954	-3.44520896	0.11452414
O	-0.02453415	-1.22151208	1.26814401
O	-0.32604874	-1.37469860	-1.28549301
O	0.02453415	1.22151208	-1.26814401
O	0.74974954	3.44520896	-0.11452414
O	0.32604874	1.37469860	1.28549301
C	1.84412735	-2.57848360	-0.18314411
C	-1.84412735	2.57848360	0.18314411
H	-0.17323094	-0.37925763	-1.22400282
H	0.17323094	0.37925763	1.22400282
H	2.23274021	-3.12208936	0.68457009
H	1.97235876	-3.20024327	-1.07502829
H	2.42259711	-1.65671213	-0.30718788
H	-2.23274021	3.12208936	-0.68457009
H	-2.42259711	1.65671213	0.30718788
H	-1.97235876	3.20024327	1.07502829
2:2 complex $\text{H}_2\text{BO}_3^-:\text{CS}$ in dichloromethane			
N	-3.58275159	-7.01104591	-1.59215431
N	5.46253813	-5.03480537	-2.93506564
N	6.31803104	3.96674472	-3.31431750
N	-1.98050183	7.79000698	-1.92992017
N	-7.98327509	1.13861366	-2.78035015
C	-0.20175260	-6.23314181	-2.09628152
C	-0.35876842	-4.83773256	-2.22177974
C	0.78913553	-4.02954538	-2.31840205
C	2.07502979	-4.58506839	-2.27424125
C	2.19649518	-5.97728297	-2.15139940
C	1.07017934	-6.80771805	-2.05867326
C	3.29113447	-3.72992698	-2.34345492
C	3.26310024	-2.38323749	-2.13537866
C	4.34305036	-1.39950651	-2.11874116
C	3.95911395	-0.04969889	-2.22019665
C	4.91108321	0.97774733	-2.20178214
C	6.26739468	0.63796833	-2.08223432
C	6.67620155	-0.69608785	-1.95632935
C	5.71068552	-1.70548016	-1.97889137
C	4.50383895	2.40503739	-2.29881538
C	3.27208332	2.83523474	-1.91117155
C	2.65902047	4.15919410	-1.94087685
C	1.25911103	4.18302399	-1.81998516
C	0.54856602	5.39106146	-1.85969314
C	1.27311301	6.58575141	-1.99280236
C	2.67298593	6.59153635	-2.07944939
C	3.35911234	5.37566847	-2.06203517
C	-0.93613450	5.41312070	-1.75996942
C	-1.68628789	4.28223366	-1.62580573
C	-3.13197153	4.10753733	-1.51601595
C	-3.61781261	2.81248796	-1.78096006
C	-4.98631169	2.52525666	-1.71199471
C	-5.87376823	3.55741191	-1.36714351
C	-5.41585166	4.84758512	-1.07312830
C	-4.04607557	5.11435368	-1.15309501
C	-5.50491000	1.15892904	-1.99294141
C	-4.74070157	0.04011999	-1.84428116
C	-5.02279815	-1.36904038	-2.09921479

C	-3.93674331	-2.25289512	-1.96006496
C	-4.07834905	-3.62472167	-2.20819249
C	-5.34434980	-4.11602106	-2.55768556
C	-6.45007508	-3.26327626	-2.68126099
C	-6.27977710	-1.89643401	-2.45787646
C	-2.91822237	-4.55137403	-2.10943917
C	-1.63376351	-4.13032788	-2.28227887
C	1.24180462	-8.29466465	-1.90038730
C	-7.79580975	-3.82085851	-3.05965630
C	-6.37968044	5.91764598	-0.63753702
C	3.42069303	7.89606916	-2.15271180
C	8.13020523	-1.03102059	-1.75988569
C	-3.25175935	-5.90894950	-1.82748112
C	4.50099263	-4.42009852	-2.65704813
C	5.48364993	3.28574031	-2.84594947
C	-1.53657660	6.70558157	-1.84832283
C	-6.86205642	1.11291813	-2.43088659
H	-1.06324660	-6.88667849	-2.04291086
H	3.18104790	-6.43472969	-2.12175671
H	7.01963700	1.42151198	-2.06822087
H	6.03752509	-2.73094349	-1.86026165
H	0.74931434	7.53706072	-2.01793718
H	4.44108255	5.38915842	-2.11634764
H	-6.93884341	3.35359978	-1.30378271
H	-3.69942559	6.11141482	-0.91119262
H	-5.47764407	-5.17780923	-2.74612139
H	-7.14445122	-1.25240243	-2.55127614
H	1.50161728	-8.54621300	-0.86428674
H	0.32113128	-8.82839632	-2.15169044
H	2.04718670	-8.67163766	-2.53884682
H	-8.10226997	-4.61473674	-2.36930152
H	-8.56421853	-3.04343239	-3.04894384
H	-7.77155092	-4.25855779	-4.06460147
H	-7.37585497	5.75302655	-1.05893993
H	-6.47963288	5.92224295	0.45559632
H	-6.03363354	6.91049119	-0.93991608
H	4.42270897	7.75694741	-2.56831127
H	2.88803352	8.62706900	-2.76915105
H	3.53494269	8.33345740	-1.15255150
H	8.40543531	-0.96102618	-0.69965882
H	8.35031195	-2.05017991	-2.09020571
H	8.77456122	-0.33926768	-2.31122393
H	0.64844489	-2.95754930	-2.42313095
H	-1.51758837	-3.07263882	-2.50519044
H	-2.98298651	-1.84923958	-1.63525731
H	-3.73151466	0.21191821	-1.47919222
H	-2.90518431	2.04446456	-2.06623344
H	-1.14778033	3.33225916	-1.59889867
H	0.74169074	3.23393242	-1.69423136
H	2.60671732	2.06520845	-1.52817476
H	2.90486052	0.17832987	-2.34456981
H	2.28238459	-1.94528895	-1.95265172
N	1.98050183	-7.79000698	1.92992017
N	7.98327509	-1.13861366	2.78035015
N	3.58275159	7.01104591	1.59215431

N	-5.46253813	5.03480537	2.93506564
N	-6.31803104	-3.96674472	3.31431750
C	4.04607557	-5.11435368	1.15309501
C	3.13197153	-4.10753733	1.51601595
C	3.61781261	-2.81248796	1.78096006
C	4.98631169	-2.52525666	1.71199471
C	5.87376823	-3.55741191	1.36714351
C	5.41585166	-4.84758512	1.07312830
C	5.50491000	-1.15892904	1.99294141
C	4.74070157	-0.04011999	1.84428116
C	5.02279815	1.36904038	2.09921479
C	3.93674331	2.25289512	1.96006496
C	4.07834905	3.62472167	2.20819249
C	5.34434980	4.11602106	2.55768556
C	6.45007508	3.26327626	2.68126099
C	6.27977710	1.89643401	2.45787646
C	2.91822237	4.55137403	2.10943917
C	1.63376351	4.13032788	2.28227887
C	0.35876842	4.83773256	2.22177974
C	-0.78913553	4.02954538	2.31840205
C	-2.07502979	4.58506839	2.27424125
C	-2.19649518	5.97728297	2.15139940
C	-1.07017934	6.80771805	2.05867326
C	0.20175260	6.23314181	2.09628152
C	-3.29113447	3.72992698	2.34345492
C	-3.26310024	2.38323749	2.13537866
C	-4.34305036	1.39950651	2.11874116
C	-3.95911395	0.04969889	2.22019665
C	-4.91108321	-0.97774733	2.20178214
C	-6.26739468	-0.63796833	2.08223432
C	-6.67620155	0.69608785	1.95632935
C	-5.71068552	1.70548016	1.97889137
C	-4.50383895	-2.40503739	2.29881538
C	-3.27208332	-2.83523474	1.91117155
C	-2.65902047	-4.15919410	1.94087685
C	-1.25911103	-4.18302399	1.81998516
C	-0.54856602	-5.39106146	1.85969314
C	-1.27311301	-6.58575141	1.99280236
C	-2.67298593	-6.59153635	2.07944939
C	-3.35911234	-5.37566847	2.06203517
C	0.93613450	-5.41312070	1.75996942
C	1.68628789	-4.28223366	1.62580573
C	6.37968044	-5.91764598	0.63753702
C	-3.42069303	-7.89606916	2.15271180
C	-8.13020523	1.03102059	1.75988569
C	-1.24180462	8.29466465	1.90038730
C	7.79580975	3.82085851	3.05965630
C	1.53657660	-6.70558157	1.84832283
C	6.86205642	-1.11291813	2.43088659
C	3.25175935	5.90894950	1.82748112
C	-4.50099263	4.42009852	2.65704813
C	-5.48364993	-3.28574031	2.84594947
H	3.69942559	-6.11141482	0.91119262
H	6.93884341	-3.35359978	1.30378271
H	5.47764407	5.17780923	2.74612139

H	7.14445122	1.25240243	2.55127614
H	-3.18104790	6.43472969	2.12175671
H	1.06324660	6.88667849	2.04291086
H	-7.01963700	-1.42151198	2.06822087
H	-6.03752509	2.73094349	1.86026165
H	-0.74931434	-7.53706072	2.01793718
H	-4.44108255	-5.38915842	2.11634764
H	7.37585497	-5.75302655	1.05893993
H	6.03363354	-6.91049119	0.93991608
H	6.47963288	-5.92224295	-0.45559632
H	-2.88803352	-8.62706900	2.76915105
H	-4.42270897	-7.75694741	2.56831127
H	-3.53494269	-8.33345740	1.15255150
H	-8.40543531	0.96102618	0.69965882
H	-8.77456122	0.33926768	2.31122393
H	-8.35031195	2.05017991	2.09020571
H	-1.50161728	8.54621300	0.86428674
H	-2.04718670	8.67163766	2.53884682
H	-0.32113128	8.82839632	2.15169044
H	7.77155092	4.25855779	4.06460147
H	8.56421853	3.04343239	3.04894384
H	8.10226997	4.61473674	2.36930152
H	2.90518431	-2.04446456	2.06623344
H	1.14778033	-3.33225916	1.59889867
H	-0.74169074	-3.23393242	1.69423136
H	-2.60671732	-2.06520845	1.52817476
H	-2.90486052	-0.17832987	2.34456981
H	-2.28238459	1.94528895	1.95265172
H	-0.64844489	2.95754930	2.42313095
H	1.51758837	3.07263882	2.50519044
H	2.98298651	1.84923958	1.63525731
H	3.73151466	-0.21191821	1.47919222
B	-0.15113839	0.45180606	-1.86137437
B	0.15113839	-0.45180606	1.86137437
O	-0.36050759	1.40629187	-0.96330260
O	0.16858219	-0.87906386	-1.59760145
O	0.36050759	-1.40629187	0.96330260
O	-0.16858219	0.87906386	1.59760145
O	-0.22996489	0.69378942	-3.26029312
O	0.22996489	-0.69378942	3.26029312
H	-0.23128474	1.05219827	0.60259101
H	0.23128474	-1.05219827	-0.60259101
H	-0.44869156	1.62638983	-3.38954581
H	0.44869156	-1.62638983	3.38954581

2:2 complex $\text{HCO}_3^-:\text{CS}$ in dichloromethane

N	3.68137474	6.77499195	-2.51507425
N	-5.45659234	5.85741290	-1.84266628
N	-7.37876966	-3.10536791	-1.29296171
N	0.53593784	-7.82170825	-2.75525997
N	7.32565837	-1.59990867	-1.25279129
C	0.37503090	6.27995205	-1.55639919
C	0.35256359	4.89225933	-1.79495408
C	-0.88929319	4.23820221	-1.88415513
C	-2.09589607	4.93987459	-1.75699085

C	-2.03663607	6.32418357	-1.53062902
C	-0.81352650	6.99964394	-1.41763925
C	-3.41181605	4.25032981	-1.85679841
C	-3.53478815	2.89333134	-1.91019886
C	-4.69467875	2.02257054	-2.06170423
C	-4.45506372	0.64337134	-1.90527219
C	-5.48622349	-0.29422527	-2.04560541
C	-6.77829506	0.17187934	-2.33511817
C	-7.04662281	1.53779025	-2.49569581
C	-6.00076603	2.45353194	-2.36652951
C	-5.23901641	-1.75399611	-1.88994980
C	-4.00810202	-2.31547378	-2.05756459
C	-3.53631116	-3.68967514	-1.92082146
C	-2.15769344	-3.89152000	-2.12196445
C	-1.58320332	-5.16451171	-2.00445155
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C	-3.79682063	-6.08186730	-1.50706832
C	-4.34488475	-4.80261154	-1.61404871
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C	2.24043283	-4.34314931	-2.11766661
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C	4.22818285	-2.91451350	-2.13148985
C	5.02624651	-4.06455726	-2.22324413
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C	4.19302336	-0.42530136	-2.40325701
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C	3.60535296	1.93816504	-2.32635840
C	3.90665088	3.30593582	-2.24941151
C	5.25691316	3.69101820	-2.25546885
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C	2.83857059	4.33944158	-2.16104599
C	1.52940882	4.03905044	-1.93146280
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H	7.85880558	4.11988515	-2.89803790
H	6.19645796	-6.41430094	-2.97236191
H	5.75629695	-6.77619491	-1.30101093
H	4.79483097	-7.44670540	-2.62539601
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H	-9.04207815	2.04078028	-1.86455089
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H	-8.95844016	1.32984346	-3.47765801
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H	3.15898513	-0.55140690	-2.71230457
H	2.18744253	-2.21042222	-1.93045401
H	0.36673206	-3.38761239	-1.77239009
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C	-4.22818285	2.91451350	2.13148985
C	-5.02624651	4.06455726	2.22324413
C	-4.46124568	5.34694287	2.25446639
C	-4.86065186	1.56837888	2.08338404
C	-4.19302336	0.42530136	2.40325701
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C	2.15769344	3.89152000	2.12196445
C	1.58320332	5.16451171	2.00445155
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C	3.79682063	6.08186730	1.50706832
C	4.34488475	4.80261154	1.61404871
C	0.11928626	5.37271087	2.17514753
C	-0.78356568	4.36340328	2.02076257
C	-5.34779023	6.56240068	2.29697510
C	4.66054380	7.26280534	1.15467211
C	8.44680405	-2.00620178	2.78580460
C	0.78686764	-8.47400960	1.11577300
C	-7.72788197	-3.19615626	2.32599610
C	-0.26928166	6.70745658	2.49520094
C	-6.21622337	1.55389073	1.63494711
C	-3.27461994	-5.68597365	2.34735299
C	4.55191898	-5.10871458	1.86293677
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H	-6.77170087	-0.67130767	2.45971668
H	2.95405190	-6.89627037	1.42985948
H	-1.31370108	-6.80888432	1.45045100
H	7.59446589	0.53586528	2.44778219
H	6.21748336	-3.50376265	2.51550555
H	1.99996332	7.24883170	1.61953642
H	5.41027038	4.68870262	1.46221391
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H	8.44611393	-3.01072131	3.21772519
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H	3.21920064	1.62503286	2.34435127

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H	0.87872474	-3.17011858	2.07049269
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C	-0.05289665	0.42248133	1.94812810
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H	0.02439556	0.96578226	-0.59033740

2:2 complex $\text{HSO}_4^-:\text{CS}$ in dichloromethane

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C	7.02860047	-1.11797605	-1.76070909
C	5.08634836	2.13371815	-2.11282354
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C	1.94826234	4.18364642	-1.94396441
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C	2.20389516	6.56179373	-1.66953156
C	3.59551844	6.42164698	-1.57836677
C	4.15771498	5.14881529	-1.68668940
C	-0.11898527	5.64078095	-1.87747030
C	-1.00124777	4.62434388	-2.10142590
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C	-3.31797784	5.70024788	-2.00854188
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H	2.36521848	-2.45089154	2.26006714
H	0.56209327	-3.64752469	2.28633851
H	-1.33844117	-3.29606416	2.06757214
H	-3.04319172	-1.90545299	1.79856517
H	-3.34272554	-0.00132713	2.27173645
H	-2.57752339	2.03328146	2.21526475
H	-0.84436760	2.89810495	1.83234725
H	1.31500122	2.79667661	1.74678044
S	-0.08243823	0.48287169	-1.99852495
S	0.08243823	-0.48287169	1.99852495
O	-1.14087327	0.80212993	-0.99132712
O	1.31422679	0.65662254	-1.21075408
O	-0.15533627	-0.91424684	-2.46402911
O	1.14087327	-0.80212993	0.99132712
O	-1.31422679	-0.65662254	1.21075408
O	0.15533627	0.91424684	2.46402911
O	0.00297622	1.48195541	-3.07463456
O	-0.00297622	-1.48195541	3.07463456
H	-1.28636368	-0.11922805	0.36170566
H	1.28636368	0.11922805	-0.36170566

2:2 complex $\text{HSeO}_4^-:\text{CS}$ in dichloromethane

N	2.74505657	-6.23719055	-2.24054831
N	7.99128487	1.17263855	-1.40271310
N	2.47592998	8.63770866	-2.04720192
N	-6.09869309	5.38608320	-0.27218674
N	-6.18196397	-3.56374870	-2.54523850
C	4.54498663	-3.32913517	-2.77710482
C	3.49945501	-2.43314149	-2.48712552
C	3.81767142	-1.08447709	-2.23015469

C	5.14248724	-0.62960396	-2.24475425
C	6.16201222	-1.55726324	-2.51900113
C	5.87614404	-2.90164791	-2.78487694
C	5.47980848	0.79493673	-1.96315062
C	4.55519599	1.79803912	-1.99813984
C	4.64093300	3.22294565	-1.68695067
C	3.44180839	3.95724250	-1.80672337
C	3.39527892	5.32463188	-1.50569871
C	4.57868580	5.96517413	-1.10352703
C	5.78278626	5.26285299	-0.97826425
C	5.80556748	3.89687403	-1.27249322
C	2.12598472	6.10067601	-1.59496431
C	0.90336566	5.51646832	-1.44698478
C	-0.45324131	6.05620991	-1.50005900
C	-1.49451991	5.11001459	-1.43575009
C	-2.83830216	5.50363233	-1.47044718
C	-3.13621559	6.87230005	-1.54271943
C	-2.12067086	7.83798033	-1.59681813
C	-0.78734343	7.42337538	-1.57938411
C	-3.93661443	4.49865976	-1.41333692
C	-3.79498553	3.22596144	-1.87863394
C	-4.73408169	2.10486650	-1.89349420
C	-4.18302501	0.82641717	-2.09206628
C	-4.98534594	-0.32435920	-2.09171625
C	-6.37082303	-0.16453786	-1.93187588
C	-6.95197894	1.10057193	-1.76417240
C	-6.12977131	2.22789680	-1.74453446
C	-4.40393281	-1.68927783	-2.24268016
C	-3.06268928	-1.94035325	-2.21192721
C	-2.29265872	-3.17937574	-2.30108438
C	-0.89157450	-3.02978226	-2.29834988
C	-0.03526329	-4.13843127	-2.37193015
C	-0.61205508	-5.41696770	-2.43445147
C	-2.00219529	-5.59820477	-2.42709979
C	-2.83409614	-4.47919138	-2.36720334
C	1.44774401	-3.98658558	-2.38812915
C	2.07869972	-2.77848012	-2.44574432
C	6.98344562	-3.88291720	-3.06122054
C	-2.58404123	-6.98589737	-2.45458250
C	-8.44156009	1.22860125	-1.59281479
C	-2.47354840	9.29958657	-1.66162012
C	7.02982477	5.95678087	-0.50008918
C	2.18297892	-5.20876241	-2.31503685
C	6.85055608	1.03402241	-1.64676783
C	2.28850358	7.49690404	-1.83889653
C	-5.14023906	4.95934608	-0.79995929
C	-5.35917387	-2.73672913	-2.40933492
H	4.33746062	-4.36580252	-3.01112667
H	7.19824500	-1.23286242	-2.53853089
H	4.56318146	7.02533590	-0.86717960
H	6.74592478	3.36982199	-1.17427738
H	-4.17205333	7.20045718	-1.56243682
H	-0.01377300	8.18040187	-1.60945354
H	-7.02070004	-1.03430975	-1.93482325
H	-6.59164673	3.20157096	-1.63662907

H	0.02275598	-6.29636288	-2.48950217
H	-3.90486440	-4.63723209	-2.36243484
H	7.13398851	-4.54433249	-2.19893716
H	6.74565839	-4.51907055	-3.92030551
H	7.92856385	-3.37143911	-3.26202834
H	-2.61589536	-7.41333693	-1.44403728
H	-3.60705480	-6.97942375	-2.84139136
H	-1.98290406	-7.65796199	-3.07469850
H	-8.97952367	0.65644865	-2.35632044
H	-8.75390612	0.83846348	-0.61642886
H	-8.76027136	2.27239467	-1.65532727
H	-1.58329783	9.91427372	-1.81881430
H	-3.17832201	9.50025271	-2.47596735
H	-2.95191813	9.62911960	-0.73154646
H	7.22376734	5.71844364	0.55322032
H	7.90632033	5.63691169	-1.07262976
H	6.93905059	7.04334168	-0.58487089
H	3.00796823	-0.40482900	-1.99114615
H	1.43251456	-1.90387171	-2.46028538
H	-0.49117661	-2.02266467	-2.24995388
H	-2.42824271	-1.06783448	-2.08816340
H	-3.11010719	0.75704397	-2.22102233
H	-2.81827947	2.98499782	-2.29149133
H	-1.23180556	4.06127330	-1.35100573
H	0.92192224	4.44437801	-1.27324281
H	2.54900188	3.44309763	-2.15172435
H	3.55447607	1.49485804	-2.28818395
N	6.09869309	-5.38608320	0.27218674
N	6.18196397	3.56374870	2.54523850
N	-2.74505657	6.23719055	2.24054831
N	-7.99128487	-1.17263855	1.40271310
N	-2.47592998	-8.63770866	2.04720192
C	6.12977131	-2.22789680	1.74453446
C	4.73408169	-2.10486650	1.89349420
C	4.18302501	-0.82641717	2.09206628
C	4.98534594	0.32435920	2.09171625
C	6.37082303	0.16453786	1.93187588
C	6.95197894	-1.10057193	1.76417240
C	4.40393281	1.68927783	2.24268016
C	3.06268928	1.94035325	2.21192721
C	2.29265872	3.17937574	2.30108438
C	0.89157450	3.02978226	2.29834988
C	0.03526329	4.13843127	2.37193015
C	0.61205508	5.41696770	2.43445147
C	2.00219529	5.59820477	2.42709979
C	2.83409614	4.47919138	2.36720334
C	-1.44774401	3.98658558	2.38812915
C	-2.07869972	2.77848012	2.44574432
C	-3.49945501	2.43314149	2.48712552
C	-3.81767142	1.08447709	2.23015469
C	-5.14248724	0.62960396	2.24475425
C	-6.16201222	1.55726324	2.51900113
C	-5.87614404	2.90164791	2.78487694
C	-4.54498663	3.32913517	2.77710482
C	-5.47980848	-0.79493673	1.96315062

C	-4.55519599	-1.79803912	1.99813984
C	-4.64093300	-3.22294565	1.68695067
C	-3.44180839	-3.95724250	1.80672337
C	-3.39527892	-5.32463188	1.50569871
C	-4.57868580	-5.96517413	1.10352703
C	-5.78278626	-5.26285299	0.97826425
C	-5.80556748	-3.89687403	1.27249322
C	-2.12598472	-6.10067601	1.59496431
C	-0.90336566	-5.51646832	1.44698478
C	0.45324131	-6.05620991	1.50005900
C	1.49451991	-5.11001459	1.43575009
C	2.83830216	-5.50363233	1.47044718
C	3.13621559	-6.87230005	1.54271943
C	2.12067086	-7.83798033	1.59681813
C	0.78734343	-7.42337538	1.57938411
C	3.93661443	-4.49865976	1.41333692
C	3.79498553	-3.22596144	1.87863394
C	8.44156009	-1.22860125	1.59281479
C	2.47354840	-9.29958657	1.66162012
C	-7.02982477	-5.95678087	0.50008918
C	-6.98344562	3.88291720	3.06122054
C	2.58404123	6.98589737	2.45458250
C	5.14023906	-4.95934608	0.79995929
C	5.35917387	2.73672913	2.40933492
C	-2.18297892	5.20876241	2.31503685
C	-6.85055608	-1.03402241	1.64676783
C	-2.28850358	-7.49690404	1.83889653
H	6.59164673	-3.20157096	1.63662907
H	7.02070004	1.03430975	1.93482325
H	-0.02275598	6.29636288	2.48950217
H	3.90486440	4.63723209	2.36243484
H	-7.19824500	1.23286242	2.53853089
H	-4.33746062	4.36580252	3.01112667
H	-4.56318146	-7.02533590	0.86717960
H	-6.74592478	-3.36982199	1.17427738
H	4.17205333	-7.20045718	1.56243682
H	0.01377300	-8.18040187	1.60945354
H	8.97952367	-0.65644865	2.35632044
H	8.76027136	-2.27239467	1.65532727
H	8.75390612	-0.83846348	0.61642886
H	3.17832201	-9.50025271	2.47596735
H	1.58329783	-9.91427372	1.81881430
H	2.95191813	-9.62911960	0.73154646
H	-7.22376734	-5.71844364	-0.55322032
H	-6.93905059	-7.04334168	0.58487089
H	-7.90632033	-5.63691169	1.07262976
H	-7.13398851	4.54433249	2.19893716
H	-7.92856385	3.37143911	3.26202834
H	-6.74565839	4.51907055	3.92030551
H	1.98290406	7.65796199	3.07469850
H	3.60705480	6.97942375	2.84139136
H	2.61589536	7.41333693	1.44403728
H	3.11010719	-0.75704397	2.22102233
H	2.81827947	-2.98499782	2.29149133
H	1.23180556	-4.06127330	1.35100573

H	-0.92192224	-4.44437801	1.27324281
H	-2.54900188	-3.44309763	2.15172435
H	-3.55447607	-1.49485804	2.28818395
H	-3.00796823	0.40482900	1.99114615
H	-1.43251456	1.90387171	2.46028538
H	0.49117661	2.02266467	2.24995388
H	2.42824271	1.06783448	2.08816340
Se	0.16087729	1.13241227	-1.90059521
Se	-0.16087729	-1.13241227	1.90059521
O	-1.14776192	0.97309890	-0.91940629
O	1.53071881	1.00758091	-0.81149546
O	0.28742233	-0.05899740	-2.99895618
O	1.14776192	-0.97309890	0.91940629
O	-1.53071881	-1.00758091	0.81149546
O	-0.28742233	0.05899740	2.99895618
O	0.31827573	2.61592516	-2.52977552
O	-0.31827573	-2.61592516	2.52977552
H	-1.34081433	-0.28369651	0.13822042
H	1.34081433	0.28369651	-0.13822042

2:2 complex H_2PO_4^- :CS in dichloromethane

N	-5.00923573	6.36307945	-1.11606960
N	-7.00830146	-2.58011133	-2.80941380
N	0.97580327	-7.24606998	-1.54122986
N	7.82657603	-1.07776480	-2.44023024
N	4.00987874	7.30151107	-1.28276066
C	-5.69346755	2.97101722	-1.60377894
C	-4.37529732	2.55585876	-1.88045447
C	-4.12493874	1.18169429	-2.06558514
C	-5.15206416	0.23304436	-1.96308420
C	-6.45234968	0.68378557	-1.68959289
C	-6.73315199	2.04477820	-1.50567636
C	-4.89308892	-1.22340646	-2.13871327
C	-3.66310332	-1.78348127	-1.96123809
C	-3.19736810	-3.16320515	-2.08610783
C	-1.80467563	-3.35193318	-2.01070949
C	-1.23130719	-4.62456931	-2.13827662
C	-2.08312343	-5.72734135	-2.30181982
C	-3.47660529	-5.57398532	-2.35052496
C	-4.02332922	-4.29281966	-2.25295898
C	0.24556513	-4.81441898	-2.10615826
C	1.12837273	-3.79976240	-2.32907724
C	2.59025231	-3.78255458	-2.33848457
C	3.19564215	-2.51354089	-2.26372521
C	4.59081664	-2.36986882	-2.26573386
C	5.37647208	-3.53030432	-2.36012440
C	4.80134775	-4.80481488	-2.44548221
C	3.40922306	-4.92319442	-2.44146356
C	5.24003352	-1.03228438	-2.16407885
C	4.54181330	0.12068277	-1.95777416
C	4.98258405	1.50299977	-1.78460260
C	3.97373122	2.48152950	-1.87221239
C	4.25649875	3.84191742	-1.68414411
C	5.58234107	4.20910580	-1.40082670
C	6.60299292	3.25558795	-1.29015770

C	6.29817544	1.90674079	-1.48729003
C	3.18641058	4.87736872	-1.74639823
C	1.87362157	4.57813135	-1.96286641
C	0.68877652	5.42851379	-2.04594691
C	-0.54864492	4.76910508	-1.91503797
C	-1.75831641	5.47474994	-1.97085104
C	-1.71280401	6.86369494	-2.16848346
C	-0.49580559	7.54377785	-2.31776075
C	0.69744770	6.82059018	-2.25920828
C	-3.06820221	4.78107841	-1.81807518
C	-3.21904714	3.43910164	-2.00890852
C	-8.13576005	2.48907860	-1.19013096
C	-0.48296286	9.03506901	-2.52327746
C	7.99887448	3.67593776	-0.91630153
C	5.67302762	-6.02984583	-2.51184419
C	-4.36715200	-6.78012092	-2.48312480
C	-4.15296525	5.62565924	-1.43643447
C	-6.03625049	-1.99455458	-2.50576774
C	0.67685305	-6.14131048	-1.80445295
C	6.66031825	-1.02909006	-2.30835973
C	3.61443654	6.21813189	-1.50583036
H	-5.92880611	4.01937241	-1.47112140
H	-7.26670593	-0.03074217	-1.61200101
H	-1.66546681	-6.72587804	-2.39491018
H	-5.10052766	-4.19180088	-2.28758610
H	6.45969897	-3.45224482	-2.36894315
H	2.97532211	-5.91076835	-2.53803687
H	5.83511076	5.25392683	-1.24534857
H	7.09134515	1.17708699	-1.37971309
H	-2.63642545	7.43331008	-2.21909049
H	1.63131645	7.35163179	-2.39805725
H	-8.40986366	2.20985120	-0.16526987
H	-8.23730370	3.57388072	-1.28096854
H	-8.86171419	2.01616312	-1.86000429
H	-0.66089778	9.55948694	-1.57595131
H	0.48101335	9.37330327	-2.91308722
H	-1.26746061	9.34762987	-3.21985952
H	8.18667051	4.71849982	-1.18864387
H	8.15068930	3.58394020	0.16698820
H	8.74898236	3.04791602	-1.40648174
H	5.21921787	-6.80867436	-3.13248719
H	6.66165553	-5.79521613	-2.91697038
H	5.81549793	-6.45086780	-1.50819826
H	-4.47184960	-7.29052614	-1.51730674
H	-5.36853585	-6.49903199	-2.82107365
H	-3.95312206	-7.50462774	-3.19183150
H	-3.11000725	0.87503628	-2.29523066
H	-2.31590625	2.90561511	-2.29076606
H	-0.54071693	3.69742946	-1.74645342
H	1.63300211	3.52407616	-2.08819396
H	2.96502873	2.14824979	-2.09486565
H	3.46029184	0.01938838	-1.88731853
H	2.54751977	-1.64704105	-2.17832064
H	0.68799118	-2.82418164	-2.52177057
H	-1.18060106	-2.47848781	-1.85986866

H	-2.87254577	-1.09049932	-1.68416950
N	-7.82657603	1.07776480	2.44023024
N	-4.00987874	-7.30151107	1.28276066
N	5.00923573	-6.36307945	1.11606960
N	7.00830146	2.58011133	2.80941380
N	-0.97580327	7.24606998	1.54122986
C	-6.29817544	-1.90674079	1.48729003
C	-4.98258405	-1.50299977	1.78460260
C	-3.97373122	-2.48152950	1.87221239
C	-4.25649875	-3.84191742	1.68414411
C	-5.58234107	-4.20910580	1.40082670
C	-6.60299292	-3.25558795	1.29015770
C	-3.18641058	-4.87736872	1.74639823
C	-1.87362157	-4.57813135	1.96286641
C	-0.68877652	-5.42851379	2.04594691
C	0.54864492	-4.76910508	1.91503797
C	1.75831641	-5.47474994	1.97085104
C	1.71280401	-6.86369494	2.16848346
C	0.49580559	-7.54377785	2.31776075
C	-0.69744770	-6.82059018	2.25920828
C	3.06820221	-4.78107841	1.81807518
C	3.21904714	-3.43910164	2.00890852
C	4.37529732	-2.55585876	1.88045447
C	4.12493874	-1.18169429	2.06558514
C	5.15206416	-0.23304436	1.96308420
C	6.45234968	-0.68378557	1.68959289
C	6.73315199	-2.04477820	1.50567636
C	5.69346755	-2.97101722	1.60377894
C	4.89308892	1.22340646	2.13871327
C	3.66310332	1.78348127	1.96123809
C	3.19736810	3.16320515	2.08610783
C	1.80467563	3.35193318	2.01070949
C	1.23130719	4.62456931	2.13827662
C	2.08312343	5.72734135	2.30181982
C	3.47660529	5.57398532	2.35052496
C	4.02332922	4.29281966	2.25295898
C	-0.24556513	4.81441898	2.10615826
C	-1.12837273	3.79976240	2.32907724
C	-2.59025231	3.78255458	2.33848457
C	-3.19564215	2.51354089	2.26372521
C	-4.59081664	2.36986882	2.26573386
C	-5.37647208	3.53030432	2.36012440
C	-4.80134775	4.80481488	2.44548221
C	-3.40922306	4.92319442	2.44146356
C	-5.24003352	1.03228438	2.16407885
C	-4.54181330	-0.12068277	1.95777416
C	-7.99887448	-3.67593776	0.91630153
C	-5.67302762	6.02984583	2.51184419
C	4.36715200	6.78012092	2.48312480
C	8.13576005	-2.48907860	1.19013096
C	0.48296286	-9.03506901	2.52327746
C	-6.66031825	1.02909006	2.30835973
C	-3.61443654	-6.21813189	1.50583036
C	4.15296525	-5.62565924	1.43643447
C	6.03625049	1.99455458	2.50576774

C	-0.67685305	6.14131048	1.80445295
H	-7.09134515	-1.17708699	1.37971309
H	-5.83511076	-5.25392683	1.24534857
H	2.63642545	-7.43331008	2.21909049
H	-1.63131645	-7.35163179	2.39805725
H	7.26670593	0.03074217	1.61200101
H	5.92880611	-4.01937241	1.47112140
H	1.66546681	6.72587804	2.39491018
H	5.10052766	4.19180088	2.28758610
H	-6.45969897	3.45224482	2.36894315
H	-2.97532211	5.91076835	2.53803687
H	-8.18667051	-4.71849982	1.18864387
H	-8.74898236	-3.04791602	1.40648174
H	-8.15068930	-3.58394020	-0.16698820
H	-6.66165553	5.79521613	2.91697038
H	-5.21921787	6.80867436	3.13248719
H	-5.81549793	6.45086780	1.50819826
H	4.47184960	7.29052614	1.51730674
H	3.95312206	7.50462774	3.19183150
H	5.36853585	6.49903199	2.82107365
H	8.40986366	-2.20985120	0.16526987
H	8.86171419	-2.01616312	1.86000429
H	8.23730370	-3.57388072	1.28096854
H	1.26746061	-9.34762987	3.21985952
H	-0.48101335	-9.37330327	2.91308722
H	0.66089778	-9.55948694	1.57595131
H	-2.96502873	-2.14824979	2.09486565
H	-3.46029184	-0.01938838	1.88731853
H	-2.54751977	1.64704105	2.17832064
H	-0.68799118	2.82418164	2.52177057
H	1.18060106	2.47848781	1.85986866
H	2.87254577	1.09049932	1.68416950
H	3.11000725	-0.87503628	2.29523066
H	2.31590625	-2.90561511	2.29076606
H	0.54071693	-3.69742946	1.74645342
H	-1.63300211	-3.52407616	2.08819396
P	0.37118858	0.68410602	-1.96530563
P	-0.37118858	-0.68410602	1.96530563
O	1.40919009	0.00885238	-1.07887448
O	-0.78316907	1.34819849	-1.06085960
O	0.82353511	1.71193454	-2.96956064
O	-1.40919009	-0.00885238	1.07887448
O	0.78316907	-1.34819849	1.06085960
O	-0.82353511	-1.71193454	2.96956064
O	-0.36024183	-0.56458065	-2.73972375
O	0.36024183	0.56458065	2.73972375
H	1.00325807	-0.80338663	0.23802711
H	-1.00325807	0.80338663	-0.23802711
H	-1.03471061	-0.25031709	-3.36364829
H	1.03471061	0.25031709	3.36364829

2:2 complex H_2AsO_4^- :CS in dichloromethane

N	3.88700026	-7.48336909	-1.71646846
N	7.59049805	1.02960251	-1.21003626
N	0.79354831	7.05959657	-3.23154590

N	-7.17630824	2.48761441	-1.69215226
N	-5.31470153	-6.38483207	-1.14092362
C	5.20308990	-4.25437683	-1.97210160
C	3.99277029	-3.55234927	-1.80032224
C	4.03001138	-2.14418455	-1.75873103
C	5.23502642	-1.44091650	-1.88929374
C	6.42205393	-2.17293913	-2.04313329
C	6.41757772	-3.57479363	-2.08352792
C	5.27179159	0.04872839	-1.86366123
C	4.18218936	0.82200162	-2.13536420
C	4.00891800	2.27310558	-2.17538104
C	2.68167242	2.73402478	-2.25807261
C	2.38577140	4.10289359	-2.32897132
C	3.45331883	5.01381676	-2.33495369
C	4.78732775	4.58350916	-2.27363309
C	5.05650457	3.21601674	-2.19095352
C	0.98068012	4.59113521	-2.43219681
C	-0.10670914	3.80972436	-2.16976836
C	-1.54049677	4.08789739	-2.24140516
C	-2.39058865	2.96772225	-2.16783304
C	-3.78565164	3.10330020	-2.24220200
C	-4.32319210	4.39466766	-2.35725852
C	-3.50174155	5.53047919	-2.39946267
C	-2.11574663	5.36981991	-2.35183126
C	-4.68739619	1.91679245	-2.19113397
C	-4.24080508	0.63687763	-2.33711929
C	-4.95085889	-0.64115541	-2.30442138
C	-4.16336978	-1.78474388	-2.06517191
C	-4.73262758	-3.06478447	-2.01177691
C	-6.11902357	-3.18192384	-2.20804431
C	-6.92532133	-2.06388840	-2.45597404
C	-6.33431502	-0.79857811	-2.50958978
C	-3.91029598	-4.27727698	-1.73361671
C	-2.54668048	-4.28606621	-1.79837396
C	-1.55984076	-5.31837994	-1.48387272
C	-0.21239039	-4.96187903	-1.70130081
C	0.83356808	-5.84408738	-1.39794466
C	0.51105789	-7.11384152	-0.89310966
C	-0.81799572	-7.49798046	-0.67115124
C	-1.84430097	-6.59767132	-0.96621447
C	2.26103503	-5.45737328	-1.58594819
C	2.67147022	-4.15713469	-1.63713974
C	7.71299277	-4.32889532	-2.22419939
C	-1.12774658	-8.84846473	-0.08393575
C	-8.41171321	-2.22291062	-2.63285010
C	-4.11284260	6.90437032	-2.46768661
C	5.90661888	5.58899393	-2.30390591
C	3.17480673	-6.55025265	-1.66791828
C	6.53495316	0.61524463	-1.51583569
C	0.84590665	5.94512199	-2.86441342
C	-6.06170219	2.20450406	-1.93108882
C	-4.65677031	-5.44530275	-1.39550527
H	5.21620693	-5.33608480	-2.01287777
H	7.37121894	-1.65315594	-2.13737639
H	3.25396047	6.07944102	-2.40001890

H	6.09032503	2.89548781	-2.17203887
H	-5.39968506	4.53127859	-2.41236297
H	-1.49576104	6.25701293	-2.37334401
H	-6.58853107	-4.16069620	-2.17720874
H	-6.95995322	0.05829145	-2.73006426
H	1.30262105	-7.81935416	-0.65698300
H	-2.86476156	-6.90977944	-0.78506395
H	8.26516122	-4.33128647	-1.27604303
H	7.53754989	-5.36967118	-2.50999827
H	8.36183420	-3.86820487	-2.97629377
H	-1.07364523	-8.81308127	1.01185965
H	-2.13474425	-9.17860464	-0.35439462
H	-0.41135247	-9.60319904	-0.42281765
H	-8.66382227	-3.21394626	-3.02099559
H	-8.92865057	-2.10326163	-1.67199442
H	-8.81402198	-1.46839384	-3.31542584
H	-3.38557406	7.64452123	-2.81314876
H	-4.97463191	6.92345266	-3.14237744
H	-4.46472201	7.22223482	-1.47801116
H	5.94241141	6.16132801	-1.36908709
H	6.87423429	5.09665282	-2.43307335
H	5.77354331	6.30576040	-3.12151413
H	3.09555525	-1.61669061	-1.59819191
H	1.88680863	-3.41537871	-1.50996968
H	-0.01430570	-3.98245375	-2.12775110
H	-2.08039352	-3.36400625	-2.14261486
H	-3.10103636	-1.64344382	-1.90123938
H	-3.16680176	0.51978817	-2.45314926
H	-1.93904895	1.98883227	-2.03032331
H	0.10837165	2.78615501	-1.87578618
H	1.89054510	1.99388018	-2.30388167
H	3.26742118	0.27943936	-2.36136680
N	7.17630824	-2.48761441	1.69215226
N	5.31470153	6.38483207	1.14092362
N	-3.88700026	7.48336909	1.71646846
N	-7.59049805	-1.02960251	1.21003626
N	-0.79354831	-7.05959657	3.23154590
C	6.33431502	0.79857811	2.50958978
C	4.95085889	0.64115541	2.30442138
C	4.16336978	1.78474388	2.06517191
C	4.73262758	3.06478447	2.01177691
C	6.11902357	3.18192384	2.20804431
C	6.92532133	2.06388840	2.45597404
C	3.91029598	4.27727698	1.73361671
C	2.54668048	4.28606621	1.79837396
C	1.55984076	5.31837994	1.48387272
C	0.21239039	4.96187903	1.70130081
C	-0.83356808	5.84408738	1.39794466
C	-0.51105789	7.11384152	0.89310966
C	0.81799572	7.49798046	0.67115124
C	1.84430097	6.59767132	0.96621447
C	-2.26103503	5.45737328	1.58594819
C	-2.67147022	4.15713469	1.63713974
C	-3.99277029	3.55234927	1.80032224
C	-4.03001138	2.14418455	1.75873103

C	-5.23502642	1.44091650	1.88929374
C	-6.42205393	2.17293913	2.04313329
C	-6.41757772	3.57479363	2.08352792
C	-5.20308990	4.25437683	1.97210160
C	-5.27179159	-0.04872839	1.86366123
C	-4.18218936	-0.82200162	2.13536420
C	-4.00891800	-2.27310558	2.17538104
C	-2.68167242	-2.73402478	2.25807261
C	-2.38577140	-4.10289359	2.32897132
C	-3.45331883	-5.01381676	2.33495369
C	-4.78732775	-4.58350916	2.27363309
C	-5.05650457	-3.21601674	2.19095352
C	-0.98068012	-4.59113521	2.43219681
C	0.10670914	-3.80972436	2.16976836
C	1.54049677	-4.08789739	2.24140516
C	2.39058865	-2.96772225	2.16783304
C	3.78565164	-3.10330020	2.24220200
C	4.32319210	-4.39466766	2.35725852
C	3.50174155	-5.53047919	2.39946267
C	2.11574663	-5.36981991	2.35183126
C	4.68739619	-1.91679245	2.19113397
C	4.24080508	-0.63687763	2.33711929
C	8.41171321	2.22291062	2.63285010
C	4.11284260	-6.90437032	2.46768661
C	-5.90661888	-5.58899393	2.30390591
C	-7.71299277	4.32889532	2.22419939
C	1.12774658	8.84846473	0.08393575
C	6.06170219	-2.20450406	1.93108882
C	4.65677031	5.44530275	1.39550527
C	-3.17480673	6.55025265	1.66791828
C	-6.53495316	-0.61524463	1.51583569
C	-0.84590665	-5.94512199	2.86441342
H	6.95995322	-0.05829145	2.73006426
H	6.58853107	4.16069620	2.17720874
H	-1.30262105	7.81935416	0.65698300
H	2.86476156	6.90977944	0.78506395
H	-7.37121894	1.65315594	2.13737639
H	-5.21620693	5.33608480	2.01287777
H	-3.25396047	-6.07944102	2.40001890
H	-6.09032503	-2.89548781	2.17203887
H	5.39968506	-4.53127859	2.41236297
H	1.49576104	-6.25701293	2.37334401
H	8.66382227	3.21394626	3.02099559
H	8.81402198	1.46839384	3.31542584
H	8.92865057	2.10326163	1.67199442
H	4.97463191	-6.92345266	3.14237744
H	3.38557406	-7.64452123	2.81314876
H	4.46472201	-7.22223482	1.47801116
H	-5.94241141	-6.16132801	1.36908709
H	-5.77354331	-6.30576040	3.12151413
H	-6.87423429	-5.09665282	2.43307335
H	-8.26516122	4.33128647	1.27604303
H	-8.36183420	3.86820487	2.97629377
H	-7.53754989	5.36967118	2.50999827
H	0.41135247	9.60319904	0.42281765

H	2.13474425	9.17860464	0.35439462
H	1.07364523	8.81308127	-1.01185965
H	3.10103636	1.64344382	1.90123938
H	3.16680176	-0.51978817	2.45314926
H	1.93904895	-1.98883227	2.03032331
H	-0.10837165	-2.78615501	1.87578618
H	-1.89054510	-1.99388018	2.30388167
H	-3.26742118	-0.27943936	2.36136680
H	-3.09555525	1.61669061	1.59819191
H	-1.88680863	3.41537871	1.50996968
H	0.01430570	3.98245375	2.12775110
H	2.08039352	3.36400625	2.14261486
As	-0.18847222	-0.81940841	-2.08401501
As	0.18847222	0.81940841	2.08401501
O	-1.32421227	0.05859116	-1.25452796
O	0.99164014	-1.42459411	-0.94947352
O	-0.63695788	-2.05523694	-3.07296429
O	1.32421227	-0.05859116	1.25452796
O	-0.99164014	1.42459411	0.94947352
O	0.63695788	2.05523694	3.07296429
O	0.68762050	0.37276205	-3.06784247
O	-0.68762050	-0.37276205	3.06784247
H	-1.04145362	0.85157737	0.11756764
H	1.04145362	-0.85157737	-0.11756764
H	1.19200686	-0.09179223	-3.75724341
H	-1.19200686	0.09179223	3.75724341

$\text{H}_2\text{BO}_3^-:\text{H}_2\text{BO}_3^-$ dianion in dichloromethane

B	0.02737586	-1.91999314	0.00000000
B	-0.02737586	1.91999314	0.00000000
O	1.17414841	-1.25227443	0.00000000
O	-1.25445841	-1.36863439	0.00000000
O	-1.17414841	1.25227443	0.00000000
O	1.25445841	1.36863439	0.00000000
O	-0.01277570	-3.34548713	0.00000000
O	0.01277570	3.34548713	0.00000000
H	1.18324900	0.35794721	0.00000000
H	-1.18324900	-0.35794721	0.00000000
H	0.90086351	-3.65756221	0.00000000
H	-0.90086351	3.65756221	0.00000000

$\text{HCO}_3^-:\text{HCO}_3^-$ dianion in dichloromethane

C	0.04965758	-2.00854773	0.00000000
C	-0.04965758	2.00854773	0.00000000
O	1.03711041	-1.21122111	0.00000000
O	-1.19649060	-1.44278522	0.00000000
O	0.09119739	-3.25452838	0.00000000
O	-1.03711041	1.21122111	0.00000000
O	1.19649060	1.44278522	0.00000000
O	-0.09119739	3.25452838	0.00000000
H	1.08138269	0.44782849	0.00000000
H	-1.08138269	-0.44782849	0.00000000

$\text{HSO}_4^-:\text{HSO}_4^-$ dianion in dichloromethane

S	0.05048703	-2.12164514	0.05680528
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S	-0.05048703	2.12164514	-0.05680528
O	0.76980085	-1.19266377	0.98075863
O	-1.31154292	-1.35324646	-0.36313610
O	0.80401724	-2.38204628	-1.18480871
O	-0.76980085	1.19266377	-0.98075863
O	1.31154292	1.35324646	0.36313610
O	-0.80401724	2.38204628	1.18480871
O	-0.43986430	-3.33510625	0.73205813
O	0.43986430	3.33510625	-0.73205813
H	1.10497930	0.39859047	0.58959223
H	-1.10497930	-0.39859047	-0.58959223

HSeO₄⁻:HSeO₄⁻ dianion in dichloromethane

Se	-0.03673175	-2.22892060	-0.08014592
Se	0.03673175	2.22892060	0.08014592
O	-0.72781258	-1.23169222	-1.18988330
O	1.28351621	-1.31017223	0.62093901
O	-1.04737469	-2.61642760	1.13406562
O	0.72781258	1.23169222	1.18988330
O	-1.28351621	1.31017223	-0.62093901
O	1.04737469	2.61642760	-1.13406562
O	0.71907520	-3.50214963	-0.74529775
O	-0.71907520	3.50214963	0.74529775
H	-0.99541603	0.35580464	-0.76435179
H	0.99541603	-0.35580464	0.76435179

H₂PO₄⁻:H₂PO₄⁻ dianion in dichloromethane

P	-0.08225676	-2.08419028	-0.27250834
P	0.08225676	2.08419028	0.27250834
O	0.68080773	-1.12224662	-1.17110919
O	-1.31668600	-1.32469009	0.44189195
O	-0.60635248	-3.37787414	-0.84264302
O	-0.68080773	1.12224662	1.17110919
O	1.31668600	1.32469009	-0.44189195
O	0.60635248	3.37787414	0.84264302
O	0.96978311	-2.39496154	0.95660794
O	-0.96978311	2.39496154	-0.95660794
H	1.07409974	0.38105383	-0.70454392
H	-1.07409974	-0.38105383	0.70454392
H	0.60419641	-3.05084796	1.57118586
H	-0.60419641	3.05084796	-1.57118586

H₂AsO₄⁻:H₂AsO₄⁻ dianion in dichloromethane

As	0.06419245	-2.21449526	-0.26441335
As	-0.06419245	2.21449526	0.26441335
O	1.24230531	-1.16261469	-0.77429237
O	-1.43548915	-1.36136988	0.04382185
O	-0.31264840	-3.56538637	-1.12741296
O	-1.24230531	1.16261469	0.77429237
O	1.43548915	1.36136988	-0.04382185
O	0.31264840	3.56538637	1.12741296
O	0.61187970	-2.69231225	1.36513457
O	-0.61187970	2.69231225	-1.36513457
H	1.27900429	0.39657696	-0.29530072
H	-1.27900429	-0.39657696	0.29530072
H	0.01899288	-3.38272842	1.70645721

H	-0.01899288	3.38272842	-1.70645721
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