

Supporting Information

Potassium Fluoride Activation for the Nucleophilic Fluorination Reaction Using 18-crown-6, [2.2.2]-Cryptand, Pentaethylene Glycol and Comparison with the New Hydro-crown Scaffold: A Theoretical Analysis

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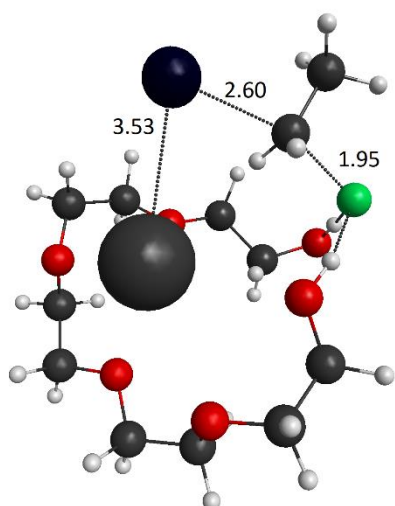
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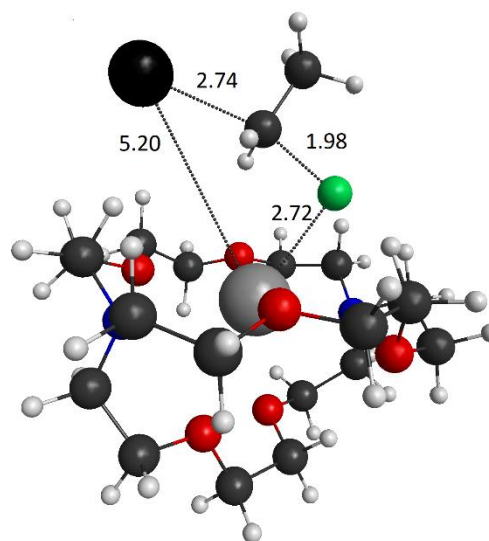
Table S1: Electronic energies and thermodynamics data for the reaction steps of the investigated systems.^a

Catalyst	Process	PBE ^b	M06-2X ^c	$\Delta\Delta G_{\text{solv}}^{\text{d}}$	$\Delta G_{\text{g}}^{\text{e}}$	$\Delta G_{\text{sol}}^{\text{f}}$
	CsF(s) \rightarrow CsF(g)				38.2 ^g	
	CsBr(s) \rightarrow CsBr(g)				(38) ^h	
	KI(s) \rightarrow KI(g)				39.4 ^g	
PentaEG	CsF(g) + Cat \rightarrow CsF-Cat	-37.41	-39.21	-5.31	-29.72	-35.03
	CsF-Cat + EtBr \rightarrow TS1-Cat	10.41	10.69	5.71	20.83	26.54
	CsF-Cat + EtBr \rightarrow CsBr-Cat + EtF	-5.67	-12.62	1.15	-12.95	-11.80
	CsBr(g) + Cat \rightarrow CsBr-Cat	-27.52	-31.84	-5.69	-23.72	-29.41
[2.2.2]-Cryptand	KF(g) + Cat \rightarrow KF-Cat	-39.98	-43.36	-13.60	-31.47	-45.07
	KF-Cat + EtI \rightarrow TS1-Cat	-1.37	-1.54	8.36	8.62	16.98
	KF-Cat + EtI \rightarrow KI-Cat + EtF	-17.93	-27.58	4.14	-27.12	-22.98
	KI(g) + Cat \rightarrow KI-Cat	-42.65	-47.53	-7.83	-36.51	-44.34

a – Units in kcal mol⁻¹, 1 mol L⁻¹ standard state, 298.15 K. b – Calculations at PBE/ma-def2-SVP level. c – calculations at M06-2X/ma-def2-TZVPP level. d – Solvent effect calculated with SMD model. Solvent *tert*-butanol for pentaEG and acetonitrile for the cryptand promoted reactions. e – Gas phase free energy. f - Solution phase free energy. g – Experimental data from NIST. h – Estimated value based on experimental data for CsF and CsCl.



TS1-pentaEG (EtBr + CsF)



TS1-cryp (Etl + KF)

Figure 1S: Transition states for the reaction of ethyl bromide with CsF promoted by pentaEG and reaction of ethyl iodide with KF promoted by [2.2.2]-cryptand. Geometries obtained at PBE/def2-SVP level of theory.

Coordinates of the optimized structures obtained at PBE/ma-def2-SVP level.

EtF

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Coordinates from ORCA-job geom-pbe

F	-4.18297512683942	2.12465769842300	-0.19356357666048
C	-2.77734734004502	2.11926653445647	-0.18185068803257
H	-2.44601727861212	3.17456979887284	-0.29450553917655
H	-2.44541710846215	1.55149591720431	-1.07837968412569
C	-2.25876127376149	1.50051615109574	1.09921678737101
H	-2.60209884884352	2.07122199222585	1.98467002125942
H	-1.14912141456115	1.50214687016814	1.09464452056477
H	-2.60218160887512	0.45225503755366	1.20346815880009

EtBr

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Coordinates from ORCA-job geom-pbe

Br	-4.661244	2.167984	-0.286360
C	-2.688033	2.116952	-0.176490
H	-2.369179	3.169724	-0.288299
H	-2.367840	1.550848	-1.070599
C	-2.199619	1.492925	1.115024
H	-2.543862	2.062903	2.000057
H	-1.088097	1.488526	1.119968
H	-2.546047	0.446268	1.220398

EtI

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Coordinates from ORCA-job geom-pbe

I	-4.84095663629389	2.18710621792878	-0.32425819651263
C	-2.66672818760224	2.11680661469687	-0.17644221979205
H	-2.33102233880723	3.16572017386188	-0.28397577947585
H	-2.33052157599225	1.54927139592512	-1.06482893278342
C	-2.17788529425149	1.49058709052703	1.11974976167395
H	-2.52504116794807	2.05810977742110	2.00607818166330
H	-1.06585938344045	1.48456515164712	1.12997389341892
H	-2.52590541566438	0.44396357799210	1.22740329180778

tri-tert-butanolamine

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Coordinates from ORCA-job geom-pbe

N	-3.29110364554799	-1.60391973847607	0.35269078229853
C	-2.32908175502393	-0.63250260244916	-0.14505703481675
C	-4.04573253853502	-1.24130567025977	1.54741984571806
C	-3.90072594361314	-2.46739180864696	-0.65069145182155
H	-2.45038139648056	-0.48514327862753	-1.24349203470164
C	-0.82460499536664	-0.93410980465101	0.13671987572616
H	-2.53467886405466	0.36637129461886	0.29811527826296
C	0.02709770696493	0.19842530918807	-0.45902676232581
C	-0.38826865175685	-2.28926994046940	-0.41874334816481
O	-0.59878828171618	-1.01549921607720	1.55797922753425

H	-3.34915615781363	-0.71346410470479	2.23111125690764
H	-4.32567919218695	-2.17206950325136	2.08584198456977
C	-5.34938541007436	-0.38367668684546	1.43086194272366
C	-5.12257441163562	0.98098210894050	0.76849733767264
C	-5.90317050664621	-0.19096191977524	2.85731258019748
O	-6.33649599071142	-1.03990776185140	0.62126249401420
H	-3.13943674208825	-2.63449337428596	-1.43854257545602
H	-4.78237587096644	-1.99775307554666	-1.15527308108250
C	-4.35092658310095	-3.88279935129637	-0.20106451864769
C	-3.28107702714279	-4.62281679757032	0.60841665365144
C	-4.75763647501816	-4.68229421564065	-1.44874609581448
O	-5.53505528465595	-3.70369247400333	0.62968998476179
H	-6.26363931363270	-2.01163120004701	0.75808695486979
H	-5.89555179222008	-4.58133713731381	0.85159435085972
H	-0.79762985421968	-0.14154358864409	1.94108050698049
H	-5.20010064859524	0.37460918982735	3.50408825265526
H	-6.09530330073723	-1.17242882579662	3.33770375831179
H	-6.86260457156176	0.36121541940820	2.81434673731884
H	-3.88765237212995	-4.87724597957928	-2.10758427910209
H	-5.52602025895941	-4.13358911067207	-2.02959228699515
H	-5.18152445886771	-5.66676568106962	-1.15937320076395
H	-2.39316299035798	-4.84469077126390	-0.01590461395160
H	-3.67538981628138	-5.59317495030654	0.97558180804707
H	-2.95058684773878	-4.01871431111714	1.47449298343256
H	-0.51143540160506	-2.32552536457632	-1.51986895310160
H	-0.99183327940862	-3.09454544525350	0.03789248609966
H	0.67684650554428	-2.47474376511364	-0.17649314927390
H	-0.08169880701787	0.25750371831045	-1.56170837119898
H	1.09764593147962	0.03680393442223	-0.22204426353356
H	-0.27155686791033	1.18478458272802	-0.04257716818472
H	-4.75099955690477	0.86330231661352	-0.26802928824809
H	-4.40580184090074	1.60169415861150	1.34385473217589
H	-6.08579244080383	1.52722542251353	0.71554066239523

KBr-tri-tert-butanolamine

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Coordinates from ORCA-job geom-pbe

N	-3.44231018355362	-2.14746964139025	0.45060663287279
C	-2.24726970129697	-1.48427164840747	-0.10023984542742
C	-4.21645279420169	-1.16431907659048	1.23645319729403
C	-4.26785020174704	-2.83081338044053	-0.55652408356648
H	-2.08071434016222	-1.82202066854151	-1.14137769389769
C	-0.90277460109362	-1.70163102355529	0.67495444958869
H	-2.42650829225593	-0.38320369153031	-0.17974020406163
C	0.05668406355505	-0.54896627462766	0.35000242265705
C	-0.24713552693875	-3.04451502955797	0.32897060262919
O	-1.12192066014464	-1.75198354755081	2.10745584727967
H	-4.69744735633025	-0.40930362767663	0.55692363182776
H	-3.47178767731023	-0.59599509261921	1.83068091782092
C	-5.29673084046620	-1.61389156319530	2.27848825421062
C	-6.63956591760426	-2.06989742363053	1.67459522635614
C	-5.55774499919418	-0.38085997579931	3.16642482119747
O	-4.76284471094601	-2.63402841353687	3.13220128727039
H	-4.46049275726383	-2.17256831928499	-1.44434760697498
H	-5.25239397003620	-2.99810673414179	-0.08902617252823
C	-3.80249046317396	-4.23669882131107	-1.07428064617850

C	-2.71893022873656	-4.17050396416743	-2.15991468039026
C	-5.04833192005634	-4.93076588145614	-1.65745397815565
O	-3.26120628957567	-5.02114539635897	-0.00403203435866
H	-5.18126763192954	-3.51803577685494	2.91410797520173
H	-4.01110139971007	-5.35426150006790	0.57064450551886
H	-1.42760649220774	-0.87603169977151	2.40707332742565
K	-2.57700575927332	-4.08697463500709	2.56073162155458
Br	-5.32581674269497	-5.73011233996722	2.39291756590823
H	-6.98531940299049	-1.37058509019074	0.88734056089265
H	-7.41081930170296	-2.10319975289030	2.47028065449356
H	-6.58439445989179	-3.09138197451637	1.24912042462918
H	-5.91795655755106	0.48294972272911	2.57114113432103
H	-4.63325785782728	-0.07834287623245	3.69942698591439
H	-6.32374712393588	-0.62613680621446	3.92687214917662
H	0.15459699414740	-3.02346727216509	-0.70267567131497
H	-0.96445668620089	-3.88830747481447	0.37578637847224
H	0.59872326896697	-3.23870374094260	1.01795508402155
H	0.21800125090583	-0.45829235053755	-0.74322839498876
H	1.03918417643157	-0.70857313993193	0.83562584145429
H	-0.35463194165316	0.41964224604678	0.70423440837467
H	-3.04460931152230	-3.53353117023977	-3.00669071533647
H	-2.51961907814658	-5.18911513790598	-2.54646758729490
H	-1.76223958553256	-3.77880193827595	-1.77254909100966
H	-5.51536267580699	-4.31503455479824	-2.45360249473017
H	-5.80218463547540	-5.10878042161373	-0.86318591479226
H	-4.77157967786568	-5.91037312046708	-2.09396909335727

KF-tri-tert-butanolamine

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Coordinates from ORCA-job geom-pbe

N	-3.41882708620862	-2.13400994010051	0.44450525416846
C	-2.23657736467732	-1.45655283702385	-0.11199007602155
C	-4.20060508614114	-1.16845693859347	1.24574874672206
C	-4.23960534801499	-2.82121715535118	-0.56514201745227
H	-2.07135694508804	-1.79498508188064	-1.15364742462328
C	-0.88271923374727	-1.65291249071838	0.65120915295297
H	-2.43023017867638	-0.35731873093811	-0.19255120777253
C	0.06150062411806	-0.49425564699362	0.30150602352177
C	-0.21985303132073	-2.99418193955144	0.31441251973007
O	-1.08254121411496	-1.68896940596976	2.08720010750501
H	-4.69186235650473	-0.41028030328737	0.57662445687426
H	-3.45997954834956	-0.59911589090302	1.84546761067778
C	-5.26906764590028	-1.65228376370576	2.29144976425206
C	-6.61993536529433	-2.08280046199318	1.67821918511468
C	-5.52067516305683	-0.44231030156551	3.21253701702391
O	-4.75276439169360	-2.69466435283869	3.10816205413726
H	-4.39503611090975	-2.17949288574801	-1.47164362175884
H	-5.23837783860107	-2.95318036187349	-0.11803907707991
C	-3.79235807010338	-4.25180388753798	-1.03310024087216
C	-2.69463151271539	-4.23274902571375	-2.10694695740246
C	-5.04578165400596	-4.93155487028669	-1.62621290920858
O	-3.29717258544095	-5.01627274695481	0.06081982847049
H	-4.96810289367997	-3.60665807134720	2.68112424718563
H	-4.03518614704811	-5.09331106846551	0.76723276252381
H	-1.45693536971408	-0.83427474936953	2.37025993106182
K	-2.49924902047382	-4.05133030788609	2.57098613347558

F	-4.84526793893278	-4.97128842742799	2.05896510709983
H	-6.97288196273118	-1.36345578840301	0.91185948716016
H	-7.38269967438465	-2.13986607384862	2.48059176887561
H	-6.56244709434791	-3.09188717656052	1.22615955169741
H	-5.87835311075169	0.44044616997671	2.64382987241133
H	-4.59137580396463	-0.16121944861279	3.74946331194578
H	-6.28411773068086	-0.70462295875109	3.96998720173550
H	0.17241579696733	-2.98199928654015	-0.72087932371883
H	-0.93570373971418	-3.83848394191814	0.37544842636287
H	0.63270241474775	-3.17616456771131	0.99867261414518
H	0.21175287344714	-0.41659630208588	-0.79443886105516
H	1.04995555372904	-0.63619660241950	0.78044927078321
H	-0.35749609037974	0.47394889146473	0.64731659583005
H	-3.01304566068433	-3.64936686127859	-2.99435197019191
H	-2.47910665271421	-5.26952847633429	-2.43213242021172
H	-1.74795347107347	-3.80832189198026	-1.72889527815086
H	-5.48619408870564	-4.32946502489869	-2.44838687331592
H	-5.81772405206758	-5.07149289014757	-0.84233697381259
H	-4.78131903039521	-5.92913612592549	-2.02806277079598

TS1-tri-tert-butanolamine

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Coordinates from ORCA-job geom-pbe

N	-3.26644730024512	-2.28278648972091	0.50120923261953
C	-2.27449182498261	-1.47554483681536	-0.22455202662840
C	-4.05848753218240	-1.39809746424789	1.37782679657889
C	-4.09815017589936	-3.12844881342554	-0.36922778050035
H	-2.12225127699245	-1.90890169820148	-1.23244725595606
C	-0.85096603166496	-1.32502020151646	0.42413600093212
H	-2.68222646970556	-0.44839434385487	-0.40687436572120
C	-0.22328092307915	-0.00899559347295	-0.05230888463559
C	0.07224984347687	-2.49654646822987	0.07036591176608
O	-0.91821004675083	-1.33194526512926	1.87130303347453
H	-4.70098828507554	-0.70638258269400	0.76846171501983
H	-3.32257366189128	-0.74702340132531	1.88901361770217
C	-4.95565254709661	-1.99622727099368	2.52500371891636
C	-6.37712573353202	-2.39052429670540	2.07606444616117
C	-5.07584080356685	-0.88836802641275	3.58930094907817
O	-4.30933906892767	-3.10649132867233	3.14747288816073
H	-4.28750972598905	-2.64124584425090	-1.35941429077599
H	-5.09156807307743	-3.20938580967712	0.10521971262477
C	-3.61842073483637	-4.59694155510160	-0.61815530751149
C	-2.43374758877068	-4.68956807647480	-1.58589973850068
C	-4.81034778078582	-5.37834653602883	-1.20265425845527
O	-3.19478086502166	-5.19673853767774	0.61012721911720
H	-4.74471109787564	-3.96648712471856	2.87041333882451
H	-3.99132278758105	-5.35830259492062	1.19466412592092
H	-1.21739048022831	-0.45650690118843	2.17674946660494
K	-1.75180136121845	-3.89002178802877	2.66707565705642
H	-6.85792699826414	-1.57106906517052	1.50431970197228
H	-7.00118400584840	-2.60149102392838	2.96714606036427
H	-6.39142621402723	-3.30683862857542	1.45410219760951
H	-5.47143822110477	0.05265023211067	3.15578699637683
H	-4.08460146522540	-0.67767912839924	4.03943849632356
H	-5.75587076802378	-1.21205570220253	4.40095339384380

H	0.28706944104237	-2.51210277585366	-1.01614915454120
H	-0.38086847029927	-3.47429993491910	0.32325328859622
H	1.03335167082361	-2.40263174870432	0.61240888264802
H	-0.18582914934667	0.03632949091293	-1.15931173129196
H	0.80902162349472	0.09901978137841	0.33519202654758
H	-0.82086097714767	0.86175321404693	0.29214001773599
H	-2.67865929549814	-4.22448949244188	-2.56204448046839
H	-2.17693413678072	-5.75221631625638	-1.76285645461601
H	-1.53376162399354	-4.19695779466369	-1.17881505517332
H	-5.17836628481879	-4.91371446125412	-2.14019896644826
H	-5.65323612561449	-5.41591178419373	-0.48203470188789
H	-4.50800512375067	-6.41955629092918	-1.42811059761695
H	-3.77307146353313	-8.28185601834215	4.42803552454456
H	-3.07323611171428	-6.44933319258994	2.84863061270955
C	-4.45946389726713	-7.42293983728504	4.29944564935494
Br	-1.36599356287308	-6.26414325158885	4.91011614568677
C	-3.74074068638988	-6.26547845796322	3.69556829427145
H	-5.26485304621797	-7.73544582282982	3.60217065380707
F	-5.03761627095847	-5.53741255357890	2.48690726475601
H	-4.91062079117850	-7.17254031805971	5.27635455900380
H	-3.72246571198470	-5.29992626923382	4.20511745401839

pentaEG

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Coordinates from ORCA-job geom-pbe

O	-1.36787086140797	-1.59454708138037	-0.31710536410333
C	-2.64463719494228	-1.24558526213544	0.18285883311900
H	-2.71994103618580	-1.49263092794121	1.27005069098699
H	-3.44721881333799	-1.81389369351156	-0.35021422252768
C	-2.88279852137568	0.23827586022304	-0.01863537730861
O	-2.04658902938688	0.96892867066810	0.85855804778506
H	-3.96114175382577	0.45672115985029	0.18853804704490
H	-2.67502959828313	0.49482901424480	-1.08312401040287
C	-1.01828082869155	-2.94662699043437	-0.11193274601729
C	0.42878544757580	-3.14693862430337	-0.51868548004341
H	-1.66585326754022	-3.62938748103960	-0.71744195950153
H	-1.14465967281690	-3.23145630334819	0.96135372235714
H	0.58691156439586	-2.72586719605662	-1.53973781966971
H	0.65642867566503	-4.24013734284615	-0.55985469091081
O	1.26513209708188	-2.49152580231107	0.41909657859014
C	-2.20764343957006	2.37481891878373	0.82998126204647
H	-3.23347868336736	2.67356467318619	1.16777728636994
C	-1.96515807722796	3.03945296646617	-0.53721086978981
H	-1.49473244370941	2.75953971191182	1.58737655733540
H	-2.82213062050352	2.85669930850913	-1.21805662392128
O	-0.83133122822948	2.57529843400401	-1.23653838115627
H	-1.91796518123447	4.14529068480088	-0.36160456421439
C	2.59804682293934	-2.24864110895393	-0.00258693368399
C	0.41143517822534	2.72130204519523	-0.56386863562974
C	1.51764083850961	2.18487740124900	-1.47790579579463
H	1.19840119587880	1.18142307687837	-1.84908589762750
O	2.77002953744654	2.14047453523142	-0.82385557738186
H	1.62504103627781	2.84106528357242	-2.36652329988666
H	0.41975292824764	2.14081102277907	0.38789386371997
H	0.60349638629111	3.79205098422770	-0.30654460873294
H	2.71668920616760	1.42017956670141	-0.15081132803147

C	3.15486970883923	-1.19582790899650	0.94495412508598
H	2.60409796627110	-1.86397861647795	-1.05108340888325
H	3.21778935880048	-3.17781022150797	0.03064573169058
H	4.17513342514680	-0.89720205141536	0.63093745575956
H	3.22039342176690	-1.61678411571743	1.97515040517942
O	2.34063511561176	-0.02724780910268	0.94076098190780
H	1.40989034049773	-0.33817478100304	0.97399400624069

KBr-pentaEG

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Coordinates from ORCA-job geom-pbe

O	2.32323935719504	0.88597539060040	-0.48783777190507
C	3.12941136042388	0.22795138492443	0.47918029641851
H	2.93370996184433	0.64515055122482	1.49636007044731
H	4.21336479731479	0.37399988506972	0.25259690045893
C	2.82828832861520	-1.25705482176742	0.46354454543357
O	1.49878719521790	-1.47360272186246	0.91508105640689
H	3.55459390429241	-1.77777146301548	1.13267308127480
H	2.97812916739214	-1.65074851916700	-0.56962669353178
C	2.56418327996068	2.28459559153380	-0.58260499656400
C	1.57166010943765	2.88794929910303	-1.56885211439593
H	3.60505110972246	2.47903515452708	-0.94167725568888
H	2.46597958450597	2.76142995435110	0.42208226377358
H	1.64124553552608	2.34297576713484	-2.53340196323803
H	1.84852043408919	3.95003944407206	-1.76400976671075
O	0.22298078585708	2.77781080856109	-1.13763986832704
C	1.08722577851800	-2.84173847198563	0.94854850125657
H	1.90371098831653	-3.48595199270577	1.35450422231408
C	0.64860621239738	-3.37285326487518	-0.41905799622128
H	0.24250844660856	-2.88277382987804	1.66694077462609
H	1.47427813204588	-3.27729173091310	-1.15662304122723
O	-0.45670499115808	-2.67781281520185	-0.97196969825762
H	0.42188210319484	-4.46234757249128	-0.32000914159272
C	-0.22218906201056	3.82943941007233	-0.27180499548338
C	-1.74452618389541	-3.05435047374344	-0.45358139951808
C	-2.82473443016962	-2.60431429122025	-1.44689225366881
H	-2.58120562820499	-1.56731415914335	-1.78462917030324
O	-4.11018796370435	-2.67648164516109	-0.88119178159913
H	-2.80569861559246	-3.25249592942694	-2.34847978165896
H	-1.94411318824800	-2.56375460715805	0.52831784759318
H	-1.78471212046225	-4.15789626773621	-0.30203648205407
H	-4.20621821619950	-1.87792626505881	-0.30247256442968
Br	-3.51325393970275	0.18110197559795	0.74211869841668
K	-0.46835765116658	0.16771128182795	-0.29677225275927
C	-1.51315516663400	3.41413173183909	0.40771474372983
H	-0.38108501417200	4.76146508126553	-0.86454241303213
H	0.54481914433510	4.04256446593139	0.50783554773012
H	-2.26245113864478	3.11227910807225	-0.36102150645220
H	-1.92498381803162	4.30998876757665	0.93315266369673
O	-1.25349425237802	2.35377371582302	1.30927061351357
H	-2.08287433643610	1.79746207340277	1.37987308152885

KF-pentaEG

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Coordinates from ORCA-job geom-pbe

O	2.49582120127521	0.84187918504194	-0.34228046950948
C	3.39280245981847	-0.01662027674874	0.34711197768644
H	3.38969119269225	0.21275340450902	1.44007573837602
H	4.43620103988148	0.12524781811245	-0.02569991446621
C	2.98339908318467	-1.45953116644005	0.13063978989097
O	1.76167690673221	-1.70938682999120	0.81386378584353
H	3.78765947536064	-2.12619176213051	0.52503909089482
H	2.88844600235768	-1.65258873682391	-0.96347444303051
C	2.70901294662175	2.22120944559723	-0.06590779761518
C	1.73047739472633	3.06855490003163	-0.86080884559241
H	3.75084191059319	2.51978528649614	-0.33791751121158
H	2.57539257488221	2.41329804212148	1.02695598199557
H	1.92811994077786	2.97334268328798	-1.95600814404849
H	1.90247706051525	4.13385756283112	-0.57838257227461
O	0.40694908399455	2.67031996074796	-0.56068061736016
C	1.28607610310439	-3.05413653682466	0.73750603476268
H	2.11677026927142	-3.77385972968410	0.93483816892304
C	0.62633295668864	-3.40197296519787	-0.60171929690781
H	0.55600177093121	-3.15712386160154	1.56672948853532
H	1.35854564161650	-3.30923399037656	-1.43235673143399
O	-0.46143864237378	-2.56524239374449	-0.94359075904496
H	0.31117523715156	-4.47358211257086	-0.56259728673801
C	-0.59225841098417	3.69017227683508	-0.65303989216239
C	-1.69902945330115	-2.83011657429532	-0.26227816881445
C	-2.85099389139126	-2.16516453405830	-1.04377497433257
H	-2.41825689230665	-1.27280282862172	-1.56377600281275
O	-3.93032454879310	-1.82767162781008	-0.22411851633641
H	-3.20565644991531	-2.85153675194436	-1.84423971860287
H	-1.69097085237968	-2.40328853071463	0.76831218129069
H	-1.84648151557073	-3.93135551700860	-0.16552864083190
H	-3.63075881832879	-1.00054003796866	0.27696310450416
F	-2.72454198216965	0.19280796242867	0.80514922340520
K	-0.29414175545190	0.17220546707046	0.20235372215855
C	-1.95106115890182	3.08308733661289	-0.32345008128821
H	-0.61014359398086	4.12741888487253	-1.67992346719611
H	-0.35283908672480	4.50397218633403	0.07231793898603
H	-2.18426970189256	2.29075526791288	-1.07859290701346
H	-2.71371711406174	3.88870557226081	-0.47863222916774
O	-1.97351812926688	2.57396179648650	0.98149451386819
H	-2.44288825438261	1.66171172496537	0.97713824667104

TS1-pentaEG (KF)

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Coordinates from ORCA-job geom-pbe

O	2.47120885280593	0.74543842933190	-0.06616272834607
C	3.45844162801509	-0.07785126864311	0.54162058240833
H	3.57650277094035	0.18530967233890	1.62066107017422
H	4.44957450029923	0.06262002629774	0.04720245613193
C	3.03280749283529	-1.52846326448136	0.41313847021153
O	1.86490125160280	-1.72240451310780	1.19530007107794
H	3.86053750910686	-2.18773659905825	0.77026772958602
H	2.85170276104697	-1.75917338590635	-0.66242393655131
C	2.67744056429444	2.13716113584000	0.11724929781391
C	1.60703087041358	2.91340790356997	-0.63095025826719
H	3.67862430513449	2.44930049356572	-0.26801188889964
H	2.64602801951639	2.39175354900602	1.20588921189516

H	1.70968847492200	2.75302752593903	-1.73152573160318
H	1.76533800862685	3.99999152135983	-0.42735337619649
O	0.32719750285585	2.49096175428449	-0.19425565742126
C	1.22434733645100	-2.99545467265528	1.08530357600630
H	1.97081066718842	-3.82032721390516	1.18184986602666
C	0.44688219158647	-3.16761977213634	-0.22352805886283
H	0.54189194945055	-3.04978898368236	1.95933740664866
H	1.13410692914114	-3.09313018600578	-1.09485551920132
O	-0.55692828754631	-2.18072122677222	-0.41840330429092
H	0.00786654713372	-4.19223606840534	-0.24407960931384
C	-0.75767220972986	3.34091386740986	-0.57613718422753
C	-1.88759318652118	-2.51624640022381	-0.00678461856302
C	-2.85578272279161	-1.57662224498068	-0.74445895713936
H	-2.44177180731455	-0.54082730681786	-0.69417342308026
O	-4.16111470755102	-1.64704342826080	-0.22826899348307
H	-2.86235004418944	-1.85212252502420	-1.82368913166101
H	-2.00554112699274	-2.40708580533660	1.09884791294028
H	-2.11195185997675	-3.57899053189157	-0.25572059882049
H	-4.32779124298504	-0.82959845041653	0.31878721979251
K	-0.11649543844439	0.18720491553289	1.22826512858498
C	-2.05813131604423	2.55196023598437	-0.53161949676988
H	-0.60620232614150	3.72567122187381	-1.61129821249153
H	-0.80246334344063	4.21307021539644	0.11808384404845
H	-2.03579867106678	1.77733935055999	-1.33995102044594
H	-2.88759896326321	3.25648726069304	-0.77891596655387
O	-2.21590323028586	1.96660736753881	0.74079004858961
H	-3.11685295196352	1.51484615911646	0.83765387385410
H	-3.01085814170441	-0.94803626993630	2.14906637318902
Br	-1.20730738884133	-1.04555429592909	4.07309809287618
F	-4.29057216441049	0.55543992077981	1.27810815205273
C	-3.31791699373669	-0.13601430944286	2.80798050699915
C	-4.40249646442534	-0.34249086043197	3.80933911897215
H	-4.65154530486412	-1.41124514016178	3.93857214977931
H	-5.30646382711039	0.18900269266116	3.44439146150475
H	-4.12784034157237	0.08890604739732	4.79034792910600
H	-2.73641607045367	0.79017345713579	2.82087612192011

CsBr-pentaEG

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Coordinates from ORCA-job geom-pbe

O	2.46663925431224	0.83565912830640	-0.24706687351681
C	3.40303235151546	-0.03895836297805	0.36270388190966
H	3.45448520090170	0.14138668697188	1.46495929443146
H	4.42654018063406	0.13524239570196	-0.05103005611361
C	3.01372680286021	-1.47983408379460	0.09862409848121
O	1.85197984253294	-1.81123885508745	0.84834402161954
H	3.86383163963451	-2.14178094529601	0.39476712082149
H	2.84432653493898	-1.61064881340950	-0.99530926255286
C	2.74542614214498	2.20865205917969	-0.01705841772248
C	1.77906459810978	3.08536068280536	-0.79123123339431
H	3.78505170222864	2.45782420348626	-0.34297869668397
H	2.67453127857081	2.43989143543163	1.07507644123009
H	1.88641837001914	2.90331248747559	-1.88865309357792
H	2.06349401073810	4.14805568887244	-0.59654394507800
O	0.45091321400200	2.83315678932825	-0.37466700972615
C	1.37777843760689	-3.14496078879907	0.66430021892266

H	2.22045721593591	-3.87358552805669	0.75115015629973
C	0.65463307770638	-3.37666040925330	-0.66735891895796
H	0.68878188627710	-3.33601746874146	1.51307563475708
H	1.33485458431729	-3.15736698069672	-1.51790647068533
O	-0.48801334144017	-2.56435239614684	-0.85736819381565
H	0.38952101974519	-4.46036891459009	-0.73132700563604
C	-0.48132881117497	3.86116567521075	-0.71660318100922
C	-1.70069655381557	-3.01859108494025	-0.24877582972637
C	-2.88373854688459	-2.37771716137046	-0.98979714090608
H	-2.66099259659697	-1.29506230086753	-1.13958909160113
O	-4.09195866018211	-2.55929695314860	-0.29372168761643
H	-2.96686930234469	-2.83569446501328	-2.00062045444205
H	-1.75105543952555	-2.73660513703316	0.83297961717047
H	-1.76379072524829	-4.13172241052772	-0.29523030696143
H	-4.26403163856170	-1.71901762968512	0.20475420935650
Br	-3.98953956204853	0.49166751042526	1.02014778869857
Cs	-0.54226910034700	0.28042928228669	1.04681490423963
C	-1.89919730298784	3.38404040301368	-0.45560544559370
H	-0.38419864516364	4.12798459667121	-1.79560972828686
H	-0.26177435505574	4.77456515240542	-0.11323897518285
H	-2.11488951064202	2.49529474201119	-1.09737212527626
H	-2.59105140992659	4.19464854255038	-0.79333467512622
O	-2.06839725994817	3.08087080186145	0.91259666201515
H	-2.84946458283812	2.46262242544043	1.00076376923645

CsF-pentaEG

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Coordinates from ORCA-job geom-pbe

O	2.32317360124880	0.79115143118347	-0.25955608511149
C	3.32137525742087	-0.10183117754925	0.20267791142295
H	3.54181855586535	0.07321549780548	1.28552307729543
H	4.27535878486423	0.05011835378230	-0.35936052810557
C	2.85922933318611	-1.53078795360414	-0.00662237683756
O	1.79274457181253	-1.82419692819909	0.88440474469429
H	3.72201004894394	-2.21683039829291	0.17897084433478
H	2.54236327175601	-1.65237033691217	-1.06716954883894
C	2.65667928240623	2.16163831174630	-0.11645865726745
C	1.58715186515719	3.01964726897398	-0.76692473508910
H	3.63827137782617	2.38540630081825	-0.60122002345767
H	2.75491453244126	2.42812100963156	0.96628555027841
H	1.52817773825094	2.78502115079202	-1.85788173251290
H	1.89764598465459	4.08989744590724	-0.66907678251794
O	0.34251758140189	2.78535128181174	-0.14276426297987
C	1.30947387038633	-3.16369511537177	0.83811548548391
H	2.12209690370078	-3.88453537153072	1.10628898595421
C	0.71520192524235	-3.59479898612982	-0.51293149552311
H	0.54479001068474	-3.22332651388955	1.63973878253165
H	1.51794587022262	-3.69121179905377	-1.27459142381143
O	-0.22736415561446	-2.70093953528503	-1.05526941226910
H	0.28387257554355	-4.61825739737602	-0.37189113510098
C	-0.72420616510153	3.621173308606278	-0.61151131774329
C	-1.50369709566614	-2.67420585188298	-0.41907744429357
C	-2.43511171784734	-1.73993427834056	-1.20628779014219
H	-1.88312618313486	-0.78289498983464	-1.38769469831437
O	-3.65360189424965	-1.54030595175176	-0.54878430779468
H	-2.62774783603052	-2.18743974230749	-2.20693833989409

H	-1.43346514529898	-2.30234623973390	0.63292930626667
H	-1.93582842084691	-3.70287811849121	-0.36801623188339
H	-3.49485773056341	-0.82991299490380	0.15438031118179
F	-2.93908594770288	0.27821379815640	1.13171487342104
Cs	-0.26078515452428	0.46712191426272	1.82058420287888
C	-2.06633917790194	2.93681128852411	-0.39244258337545
H	-0.59805398374219	3.82398652303578	-1.70113053733054
H	-0.68803012062098	4.59713026842944	-0.07236784499905
H	-2.07897768643609	1.98722110787245	-0.97971657128044
H	-2.84487486088116	3.60228033813610	-0.84669786228962
O	-2.31350999814686	2.69523952925731	0.96867728531224
H	-2.74756966870630	1.76705377425113	1.04980236770755

TS1-pentaEG (CsF)

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Coordinates from ORCA-job geom-pbe

O	2.12092128367001	0.55517450683244	-0.28673067372772
C	3.23824583750372	-0.30193153309700	-0.11224190771379
H	3.90926897533926	0.08022062487652	0.69686695258200
H	3.84282284714499	-0.35335442496741	-1.05102565345893
C	2.75245527598728	-1.69951082929758	0.22347992598996
O	2.13584058976265	-1.68450930954605	1.50111295175813
H	3.62253571710319	-2.40060341783800	0.21087054100057
H	2.03420686499948	-2.02044920204356	-0.56388460855109
C	2.44027163460326	1.84022619014558	-0.79625275119953
C	1.16638242687426	2.63280854726806	-1.01864756087510
H	2.97708782202653	1.74902381375101	-1.77255662298212
H	3.11205476662349	2.39218059269372	-0.09363418939914
H	0.45702377073425	2.01616696347431	-1.62065750721999
H	1.41384113877930	3.54371109656106	-1.61775920720490
O	0.60348589209523	3.00520261334706	0.22960973454306
C	1.40059628578603	-2.85064667193340	1.86692852442476
H	2.07606511059939	-3.73503227229675	1.96377795368770
C	0.25761095589180	-3.20654719775593	0.91469240594345
H	0.98521083852352	-2.62841997029501	2.87109956989796
H	0.63212529031744	-3.69810321381334	-0.01833365646901
O	-0.45705302508589	-2.03266522676283	0.58689598440778
H	-0.38843380714859	-3.95398369077215	1.43594500945514
C	-0.60156364428637	3.77318458727281	0.13618905601014
C	-1.66186632120731	-2.25121482850765	-0.14827972048076
C	-2.04096867505109	-0.93781166152635	-0.85843092400155
H	-1.65470873655418	-0.10020402184033	-0.23099808729850
O	-3.42096999131904	-0.81420567528734	-1.09998308118742
H	-1.50550414976885	-0.87806067279362	-1.83167578907311
H	-2.48361524036240	-2.55563425260436	0.54277172554667
H	-1.52446191946999	-3.07991950414623	-0.88206231456544
H	-3.81563032183738	-0.36902522330913	-0.30119341279453
Cs	0.26745575398746	0.64376483103899	2.42064404778500
C	-1.86837846734070	2.94006474939027	-0.02934008713949
H	-0.52189239434677	4.51014641843689	-0.69844628210224
H	-0.66902431691315	4.33969674060794	1.08822194771628
H	-1.80713420388230	2.32037737659405	-0.95880095295193
H	-2.71390759240521	3.65403051129909	-0.18328585170532
O	-2.05730303234065	2.14085428643734	1.11707059018138
H	-2.91764417995305	1.61026986313695	1.05138353695563
H	-2.70771860286710	-0.89429588850515	2.05529251575197

Br	-1.77386936028488	-1.36288277693282	4.48727567962875
F	-4.06422031490178	0.53444481524250	1.13635826960023
C	-3.43044570069074	-0.41394376767020	2.71551513079882
C	-4.68415792950466	-1.11068742129760	3.12750532877255
H	-4.66263685171863	-2.18694681061347	2.87503753188307
H	-5.53016431274854	-0.63564155261282	2.58855126693783
H	-4.86453547006425	-0.99965206470191	4.21356789512526
H	-3.17412551629906	0.55414495436139	3.15701476571753

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Coordinates from ORCA-job geom-pbe E -921.221055026178

O	-2.574374	-0.623683	-2.858662
C	-3.883925	-0.849880	-2.382656
C	-3.888525	-2.002867	-1.397695
O	-3.358480	-1.582660	-0.158202
O	-1.164364	-1.966061	1.809122
C	-0.475133	-1.385717	2.896901
C	0.974983	-1.145740	2.524806
O	1.078303	-0.019819	1.679400
C	2.387783	0.206756	1.203395
C	2.391845	1.359058	0.217653
O	1.862074	0.937743	-1.021628
C	1.736656	1.981793	-1.964003
C	1.054369	1.470946	-3.218309
O	-0.331026	1.321624	-2.989824
C	-1.021084	0.741564	-4.077168
C	-2.471084	0.502122	-3.704226
H	-4.940635	-2.366555	-1.274533
H	-3.291479	-2.848268	-1.818643
H	-0.943485	-0.415012	3.191277
H	-0.511069	-2.058738	3.791686
H	1.381556	-2.057666	2.022529
H	1.568015	-0.992127	3.462800
H	3.443801	1.723114	0.094268
H	1.794390	2.204521	0.637883
H	1.515166	0.497403	-3.515107
H	1.241081	2.196891	-4.050915
H	-0.985420	1.414525	-4.972013
H	-0.553368	-0.229372	-4.371817
H	-3.064742	0.348657	-4.641842
H	-2.876987	1.414310	-3.201854
H	-4.575710	-1.095337	-3.229156
H	-4.286763	0.063416	-1.880543
H	1.142496	2.828914	-1.542069
H	2.743616	2.386064	-2.241698
H	3.079319	0.453293	2.049795
H	2.791169	-0.706701	0.702053
C	-2.549564	-2.117386	2.037652
C	-3.231378	-2.627663	0.782857
H	-3.011632	-1.144802	2.335603
H	-2.735140	-2.844543	2.869449
H	-4.237657	-3.033853	1.060264
H	-2.636032	-3.473346	0.359669

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Coordinates from ORCA-job geom-pbe E -4094.453685716042

O	-2.557700	-0.554485	-2.787899
C	-3.860392	-0.912129	-2.338788
C	-3.771149	-2.144091	-1.458786
O	-3.021956	-1.817421	-0.306799
O	-1.145701	-1.896441	1.843265
C	-0.535960	-1.179342	2.912404
C	0.944707	-1.032936	2.628905
O	1.127821	-0.137129	1.540224
C	2.472515	0.044571	1.144688
C	2.546754	1.200775	0.167254
O	1.832323	0.876562	-1.018318
C	1.778748	1.951820	-1.943445
C	1.031723	1.523972	-3.189380
O	-0.327037	1.273344	-2.870815
C	-1.121096	0.932562	-3.997882
C	-2.539134	0.641197	-3.552958
H	-4.809246	-2.450131	-1.182694
H	-3.304052	-2.993308	-2.015712
H	-1.010068	-0.173204	3.020564
H	-0.659158	-1.735519	3.873888
H	1.390277	-2.029725	2.391277
H	1.453232	-0.638641	3.541721
H	3.618598	1.412112	-0.067759
H	2.113410	2.113847	0.640506
H	1.504573	0.610079	-3.624026
H	1.113678	2.340914	-3.948005
H	-1.138563	1.776362	-4.730688
H	-0.696097	0.038834	-4.516216
H	-3.182848	0.539190	-4.460765
H	-2.932956	1.496316	-2.951785
Br	-2.756195	1.818498	1.443260
H	-4.528112	-1.127236	-3.208600
H	-4.306583	-0.074558	-1.751836
H	1.273501	2.835139	-1.483788
H	2.809063	2.267599	-2.238659
H	3.116800	0.289863	2.024215
H	2.879972	-0.886475	0.679527
K	-0.970983	0.075340	-0.331343
C	-2.552550	-2.052147	2.020038
C	-3.141179	-2.711489	0.788678
H	-3.028570	-1.052925	2.170748
H	-2.761944	-2.696430	2.909232
H	-4.215858	-2.936861	0.989645
H	-2.623379	-3.677112	0.568247

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44

Coordinates from ORCA-job geom-pbe E -1620.635532007206

O	-2.515700	-0.603091	-2.811160
C	-3.815863	-1.080426	-2.490923
C	-3.709235	-2.218672	-1.494044
O	-3.143050	-1.718236	-0.304338
O	-1.193834	-1.927301	1.883367
C	-0.544555	-1.140757	2.885815
C	0.935174	-1.069353	2.578630

O	1.144099	-0.186976	1.478252
C	2.484592	-0.046820	1.067511
C	2.579375	1.145143	0.134530
O	1.810429	0.898108	-1.035074
C	1.716966	2.022298	-1.890456
C	0.973045	1.644006	-3.153522
O	-0.383154	1.346552	-2.858198
C	-1.111243	0.931014	-4.003845
C	-2.528092	0.558276	-3.621739
H	-4.736929	-2.620652	-1.314504
H	-3.093377	-3.051644	-1.914884
H	-1.000554	-0.113600	2.879872
H	-0.676083	-1.614622	3.890020
H	1.338123	-2.084286	2.339392
H	1.478604	-0.687500	3.476667
H	3.649742	1.327223	-0.131513
H	2.197327	2.052546	0.660409
H	1.466013	0.760851	-3.626623
H	1.038676	2.495413	-3.875469
H	-1.149468	1.752734	-4.761323
H	-0.610885	0.053946	-4.481371
H	-3.107567	0.381500	-4.561562
H	-3.018214	1.407706	-3.085175
F	-2.185158	1.074936	1.762953
H	-4.338950	-1.438350	-3.411693
H	-4.427791	-0.259791	-2.045996
H	1.196450	2.866803	-1.375606
H	2.733291	2.386645	-2.180514
H	3.156857	0.140600	1.941110
H	2.850730	-0.972414	0.557571
K	-1.078712	0.170511	-0.193776
C	-2.615183	-1.893150	2.025364
C	-3.251331	-2.572609	0.831570
H	-2.940412	-0.820383	2.086806
H	-2.924132	-2.438833	2.951357
H	-4.327727	-2.770178	1.053480
H	-2.757086	-3.553285	0.625220

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Coordinates from ORCA-job geom-pbe E -4273.146443812740

C	-1.202093	-1.728957	-0.925089
C	-1.058038	-1.055089	-2.272804
O	-2.427035	-1.352681	-0.320309
O	-2.056722	-1.538499	-3.158901
C	-1.949160	-1.005951	-4.471129
C	-2.618462	-1.962054	0.954459
C	-3.099751	-1.508976	-5.319774
O	-4.311851	-1.025738	-4.776219
C	-5.455113	-1.220338	-5.598714
C	-3.959639	-1.572455	1.534227
C	-6.670994	-0.645454	-4.903007
O	-7.001797	-1.460006	-3.782512
O	-4.999702	-2.104292	0.717412
C	-8.101790	-0.937364	-3.041595
C	-6.295922	-1.892960	1.276021
C	-8.328566	-1.784814	-1.807877

O	-7.273378	-1.562709	-0.883771
C	-7.348572	-2.356296	0.292051
H	-0.337807	-1.427013	-0.283863
H	-1.155884	-2.837963	-1.052263
H	-0.037862	-1.277508	-2.671860
H	-1.141572	0.052987	-2.158926
H	-0.984092	-1.315778	-4.942187
H	-1.971812	0.109807	-4.438496
H	-1.815834	-1.637062	1.659663
H	-2.555726	-3.072731	0.850702
H	-2.953906	-1.137525	-6.363530
H	-3.097527	-2.625955	-5.356017
H	-5.605623	-2.307300	-5.806664
H	-5.317408	-0.701109	-6.577794
H	-4.021110	-1.994404	2.566661
H	-4.062542	-0.464207	1.622128
H	-7.520733	-0.620362	-5.629299
H	-6.457552	0.394470	-4.560186
H	-9.028782	-0.954948	-3.665554
H	-7.883326	0.116499	-2.748208
H	-6.438188	-0.813897	1.524341
H	-6.408161	-2.477786	2.221275
H	-9.308338	-1.504309	-1.350525
H	-8.381783	-2.865557	-2.086587
H	-8.350508	-2.250700	0.775127
H	-7.206971	-3.435380	0.037299
K	-4.748625	-0.943480	-1.987397
F	-5.861426	1.299369	-2.474404
C	-6.718633	3.160547	-0.776818
C	-5.980693	1.873045	-0.580254
H	-7.707840	3.142659	-0.282574
H	-6.865347	3.302814	-1.867717
H	-6.146453	4.020929	-0.381791
H	-4.887707	1.861616	-0.581702
H	-6.520068	0.935969	-0.420274
Br	-5.746698	1.902784	1.930675

cryptand

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Coordinates from ORCA-job geom-pbe

C	2.18128602839373	-1.24157519785638	0.77560539329549
C	2.01102842476690	-0.06200139897035	-0.18680386960237
O	2.66804914835654	-2.43295004605705	0.14622833003541
N	3.26373596185792	0.41882692252849	-0.76427371623979
C	3.82458027561157	1.66386988610269	-0.30285568927581
C	1.73446313993306	-3.46537901488236	-0.09761732690467
C	3.16887374545142	2.96491321147852	-0.80103251618951
O	1.86252043424977	3.06973276487466	-0.25643151634493
C	0.97732510449793	3.89212449707245	-0.97981670072429
C	0.84458466519032	-3.30624793789820	-1.32782271892482
C	-0.44365822441107	3.65849512460685	-0.50119027869516
O	-0.84072775607563	2.34016991810807	-0.82249266794456
O	-0.26326274463732	-2.46495767833385	-1.06009824927994
C	-2.16265859087118	2.03460245927244	-0.42670960306368
C	-1.14875782284112	-2.37293547242479	-2.16949632585130
C	-2.44099927989631	0.53747206275199	-0.52716915962897
N	-2.18185533326112	-0.08996720693775	-1.81618658145797
C	-2.37281910977777	-1.54009021478894	-1.79463693801206

H	1.21098705405173	-1.44899373463752	1.28502526060347
H	2.92895285740351	-0.97641842900413	1.55593922562219
H	3.79217230928001	3.84573865371676	-0.49571536470656
H	3.11468811119273	2.96709380288466	-1.91520724669724
H	-2.33168625297704	2.32579028339386	0.63966981941632
H	-2.89444625650802	2.63142005422927	-1.02877452983233
H	-1.48523406868647	-3.40255066477137	-2.45629149538662
H	-0.62893418479148	-1.92180111513280	-3.04533328608562
H	-3.50948792577057	0.40817880491066	-0.19132396343821
H	-1.80914297342444	0.02115825508164	0.22450225056202
H	-2.69276839109569	-1.86023937860813	-0.77950560703916
H	-3.21073109600720	-1.83542658528149	-2.47249921436186
H	3.80746465693991	1.69446446926194	0.81216807909286
H	4.90053808872441	1.70678448664261	-0.59109179256396
H	1.53322774324466	0.76916202929193	0.36943187864253
H	1.28207283582677	-0.32269943644802	-0.98058290712084
H	2.34088273166413	-4.38445832655925	-0.24282165357322
H	1.07898206614288	-3.63148172712781	0.79241807714331
H	0.47942291823359	-4.32267349661861	-1.62773200561641
H	1.44648330273904	-2.91139453198158	-2.18286132765996
H	1.22504365335736	4.97761951631442	-0.85213994755692
H	1.03957858874652	3.66278320931112	-2.07222367068864
C	3.75265191490253	-0.18412562609349	-1.98313795409912
C	-2.75514078758890	0.57782236174731	-2.96873088346572
C	3.28948800994810	0.43279452617076	-3.31362677073777
H	3.46060870117144	-1.25436327611816	-1.97213092048041
H	4.86904475248516	-0.170744446160457	-1.99250611367996
H	-2.54573398487367	1.66309399720203	-2.88236971317174
H	-3.87936991571475	0.48272307101223	-3.02290670615616
C	-2.22720989407943	0.08598519007576	-4.32836261271224
O	-0.82139948966615	0.04608012182629	-4.47334226380483
H	-2.69010457794202	0.73414959890387	-5.11583924649179
H	-2.56804196887737	-0.95049448587384	-4.52868285965685
O	1.87775044275281	0.42712872137255	-3.36713521446457
H	3.72934316621745	-0.15131079120044	-4.16343092478348
H	3.66986425082037	1.48148213961131	-3.42164036075089
C	1.33134594128897	1.11560965342968	-4.47067487864262
C	-0.16335146489383	1.28798681517331	-4.28001434264754
H	-1.11306315011205	4.41127452185066	-0.98857982621664
H	-0.50287740281220	3.82521849789372	0.60291615703350
H	1.53893239604824	0.57525188957062	-5.42794436303199
H	1.79099608022696	2.13284596510780	-4.55934239192600
H	-0.34337400785780	1.67795376242665	-3.25225472306112
H	-0.53522284626788	2.04173899000130	-5.02004353099824

KBr-cryptand

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Coordinates from ORCA-job geom-pbe

C	3.30217937450832	-1.89659908391994	0.01000946215506
C	3.60833929761960	-0.45410549700309	0.40958876710393
O	2.04109190844018	-1.99766977157368	-0.63063334200504
N	3.41125366725173	0.57234573431869	-0.62228194988602
C	3.70794040346770	1.90063828243879	-0.08213913262851
C	1.44916478140597	-3.28561523306804	-0.54522969115516
C	2.84099122285761	3.06194399284678	-0.57191044656156
O	1.48362483850554	2.79037383475638	-0.29546463206986
C	0.63180398703725	3.92254712784179	-0.39078748075485

C	0.20096707520968	-3.33391926066952	-1.41061067161621
C	-0.81445474383919	3.48646226358656	-0.29831131993126
O	-1.17644908057996	2.82324108522381	-1.51608133589711
O	-0.67757171518359	-2.30306995768685	-1.01253771439443
C	-2.56718992407825	2.55662477170009	-1.66152052594111
C	-2.03464281585107	-2.46952868206792	-1.38898430302852
C	-3.02560679330562	1.18657058149605	-1.15948204348204
N	-2.43107656464100	0.01542597191689	-1.83323075041525
C	-2.80787874662596	-1.19208028092180	-1.08501652933363
H	3.31446088196792	-2.49664276046793	0.94963348994862
H	4.09624757848394	-2.32535432667749	-0.65097223227309
H	3.18029523733466	3.97542968262313	-0.02332149081339
H	2.97734694989058	3.27499021335660	-1.65861266069884
H	-3.16577799294607	3.32633924551847	-1.12198664594953
H	-2.79302455061213	2.69317665772934	-2.74231291965788
H	-2.49686812318825	-3.29614586738323	-0.79591416846291
H	-2.11201435265972	-2.76861588163290	-2.46072944901981
H	-4.14852389641438	1.17402801237140	-1.23076558994693
H	-2.76533898066756	1.10004142065849	-0.07872037271546
H	-2.65172965942800	-0.96706625074850	-0.00620756734251
H	-3.89839949815270	-1.42607901556972	-1.22600898017098
H	3.56231638560472	1.85086825937152	1.01590942764270
H	4.78350321783607	2.18005751370038	-0.24543560658465
H	4.66038472572167	-0.46247340944813	0.80672742141601
H	2.94852615371039	-0.18520423770115	1.26214631265882
H	2.15611092604305	-4.07535139897752	-0.89871981368280
H	1.18437829393668	-3.50732492476340	0.51626983933346
H	-0.26635243260290	-4.34003197916121	-1.27702682173775
H	0.46903278747872	-3.22262057612814	-2.49039865740989
H	0.85060806569600	4.63761859624230	0.43971777994255
H	0.80352567865234	4.45686721553649	-1.35778330874980
K	0.39110489992904	0.27671194705296	-0.88806826164850
C	4.04375633601106	0.26499721092430	-1.89818311404226
C	-2.70774265015082	-0.03284571126108	-3.26646589912734
C	3.50414743683791	1.03504663939987	-3.10640719657836
H	3.87529400367587	-0.80871133289888	-2.10825929805495
H	5.15803596473520	0.42284870362512	-1.87286197779186
H	-2.85102616257591	1.00574930781049	-3.62434199170361
H	-3.67765223289508	-0.55501820689479	-3.49397294877336
C	-1.63441862786938	-0.68353240730847	-4.16378857820578
O	-0.29799056052902	-0.26184930028960	-3.95758305442434
H	-1.93826533132869	-0.50192086363599	-5.22644962887092
H	-1.60701132628812	-1.78129374030824	-4.02528235974098
O	2.09414431197545	0.92861449915724	-3.15234129648384
H	3.96342259585806	0.58766272172312	-4.02128239014795
H	3.81413735624903	2.10863813247985	-3.09058924070068
C	1.51945111522016	1.21843144310598	-4.41394867155016
C	0.00944850775245	1.07366427162307	-4.32625367574545
H	-1.44822601881440	4.39514717811549	-0.16384535380912
H	-0.95715865633443	2.81175564913641	0.58336808413025
H	1.92579792586821	0.52201165476190	-5.18775505085567
H	1.75857766361852	2.26228163120290	-4.73524347345927
H	-0.39512527765671	1.80371557561755	-3.58711647907459
H	-0.42195038543237	1.31910504940717	-5.32844993602188
Br	-1.06167445573999	0.50279787978988	1.99822744679630

KF-cryptand

Coordinates from ORCA-job geom-pbe

C	3.35690925715470	-1.89540823439679	-0.00823730706342
C	3.71444548759751	-0.46254327344182	0.38530589650761
O	2.05463290234122	-1.96079211763151	-0.55728567143462
N	3.46439486771175	0.57421771381493	-0.62066493306141
C	3.76443632884542	1.90382167004486	-0.08549129289846
C	1.49712040981917	-3.26643453939851	-0.57409343252659
C	2.83415461548977	3.04790618546139	-0.49599817796439
O	1.50635924145597	2.73994938345789	-0.13002600551573
C	0.60814131609074	3.84731522734627	-0.19112904712339
C	0.21992234785275	-3.26927518744258	-1.39866000675570
C	-0.82599154403335	3.36251526695860	-0.23180619207603
O	-1.10274325975825	2.88033823467860	-1.55653446669548
O	-0.66078008566021	-2.29251304696793	-0.88995012625384
C	-2.47616282493369	2.60207302708679	-1.80999329506989
C	-2.01681765450149	-2.40535251143125	-1.31068366510203
C	-2.98938653820281	1.26533049779372	-1.27509798185294
N	-2.41141581106366	0.05576438740053	-1.89681968967175
C	-2.75432314742909	-1.09726407857038	-1.05163281606395
H	3.42757429090931	-2.51338407407402	0.91887982456651
H	4.09616950198412	-2.32616694519539	-0.72967787229559
H	3.19155509189124	3.96464747360701	0.03638661518231
H	2.88965735954410	3.27207978593664	-1.58760949319279
H	-3.11276040704756	3.40594040078568	-1.36716251715826
H	-2.59337983144215	2.68791513297146	-2.91388841363698
H	-2.52328354822126	-3.20814570550488	-0.72143043764681
H	-2.06357285595777	-2.71862205202656	-2.37854174448767
H	-4.11011302039221	1.27583368609634	-1.37166857189111
H	-2.71800108192164	1.19950386017896	-0.19067999408107
H	-2.52353161129572	-0.78391418940101	-0.00531742934916
H	-3.85369534522006	-1.32584309814298	-1.11779310347243
H	3.70701306740348	1.83897945477056	1.02021869545504
H	4.81674937429155	2.21390178662142	-0.32524377372830
H	4.78962423958220	-0.49154367570772	0.71513449204876
H	3.11903282527572	-0.19276287015022	1.28323407860246
H	2.21030497455981	-3.99927266273393	-1.02454231784055
H	1.28169736978666	-3.59652411795008	0.47087198061890
H	-0.22196944835073	-4.29456275935549	-1.33401620147682
H	0.45180421629813	-3.06482756797045	-2.47313088167057
H	0.75575766215020	4.49984436154878	0.70362971977353
H	0.82190520554627	4.45781325831614	-1.10158125960099
K	0.34367655063716	0.29832633603547	-0.73738285208848
C	4.04997261231710	0.28426014509991	-1.92264381493517
C	-2.74219636886749	-0.07310577323038	-3.31022329292099
C	3.44882546260599	1.03759090631942	-3.10951026842951
H	3.90201887612041	-0.79313852143631	-2.12907472595355
H	5.16039212398916	0.46955249230141	-1.93894807056950
H	-2.90304318560552	0.94728899779480	-3.71259769919588
H	-3.71928489556902	-0.60670828119593	-3.47507478293987
C	-1.69861159929686	-0.76495275960371	-4.21429489566937
O	-0.34760050104700	-0.38062309128867	-4.02655957640273
H	-2.00843503019197	-0.58467597349573	-5.27625755429581
H	-1.70040223817745	-1.86229083414938	-4.06691054972174
O	2.04849699602722	0.85007238133022	-3.14564344030498
H	3.92523016419077	0.62973739649537	-4.03474757892983
H	3.69808120046528	2.12719753569389	-3.08262268248002
C	1.46018398132967	1.14481833609579	-4.40129434594817

C	-0.04505032712857	0.97408324492101	-4.31796933896021
H	-1.49380618795530	4.22995082989072	-0.00897142719885
H	-1.00966295026258	2.54819518580682	0.52486297184407
H	1.88130110722331	0.47006198260891	-5.18680667600786
H	1.67711047669258	2.19847866322995	-4.70554156570722
H	-0.44803937041849	1.65913742365120	-3.53772723870394
H	-0.48029094992022	1.27397149395530	-5.30439926709379
F	-1.35771988530834	0.69635379578686	1.07087548851698

TS1-cryptand (EtBr)

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Coordinates from ORCA-job geom-pbe

C	3.20250976510503	-1.95492057469626	0.08396904880976
C	3.56488209196295	-0.53817916941163	0.51480275581283
O	1.89559069279378	-2.01170305399623	-0.47995018425544
N	3.32277942111961	0.53949048095016	-0.45946596512637
C	3.62899228132050	1.84042201690281	0.13809662904317
C	1.25585613980108	-3.26936604434957	-0.28738137268969
C	2.74227764540236	3.01595746813384	-0.27146277316635
O	1.39003762679234	2.73233178397642	0.03993120576485
C	0.52953209335088	3.85916179060203	-0.06510324210427
C	-0.01580635338987	-3.33056258706159	-1.11176653159354
C	-0.91590891817971	3.41042681134799	-0.11901547025840
O	-1.17798265796435	2.85637328216924	-1.41459523711918
O	-0.87919080860285	-2.26436716840291	-0.74825556610164
C	-2.55271148735443	2.63206700288372	-1.70165144935060
C	-2.20208425965887	-2.38606794033523	-1.24649982806945
C	-3.11828272349965	1.29778288017512	-1.21080159396018
N	-2.52917133647509	0.08771113227785	-1.81395702412866
C	-2.96372408151636	-1.08223622003844	-1.03819726491029
H	3.24764792179385	-2.57076742476247	1.00980706123296
H	3.93748162207999	-2.38014347807454	-0.64435944881015
H	3.09561461530602	3.91102131245820	0.29772617733275
H	2.83568904483167	3.26778674511311	-1.35399012718321
H	-3.17452865155742	3.44559338862841	-1.25742813645616
H	-2.65012276827479	2.73623658732370	-2.80481781569424
H	-2.74459537988160	-3.19121665941318	-0.69305784338020
H	-2.18608556198419	-2.69909733292316	-2.31639098273999
H	-4.23147073506990	1.33530233019050	-1.36944367848597
H	-2.93728477839265	1.22161473556459	-0.11690779596128
H	-2.85335720442656	-0.80886123491182	0.03239678023887
H	-4.05007787150151	-1.30330806457167	-1.22351336245106
H	3.52286358818952	1.73374630813637	1.23669338127441
H	4.69671283462432	2.13840087102548	-0.04281329227432
H	4.64046292097191	-0.57619504246891	0.83721697583727
H	2.97214285441778	-0.31244415135091	1.42650261386378
H	1.91736314717208	-4.10583267756871	-0.62002701205087
H	1.03734818530379	-3.41056888699136	0.79843814327730
H	-0.50237397403301	-4.31746429324753	-0.91836605829386
H	0.21856591577853	-3.27340086666044	-2.20347262852964
H	0.67391027620015	4.53449221714280	0.81374117079350
H	0.76965192855040	4.44342595758952	-0.98627641606189
K	0.30305920516461	0.28009642372716	-0.81106063421115
C	3.95423302168274	0.29310936451512	-1.74979252908198
C	-2.75920170011817	-0.00579594391433	-3.25407730057244
C	3.43472029999884	1.12130874295444	-2.92569484511483
H	3.78064081823380	-0.76924713011103	-2.00918253190453

H	5.06985108750101	0.43847766850995	-1.70865692851468
H	-2.89403441632358	1.02142832619980	-3.64779597353184
H	-3.71959419626499	-0.53794204744710	-3.49550738367254
C	-1.65148955005032	-0.67987705793876	-4.08874875252771
O	-0.32861640286461	-0.23552176001739	-3.84474392008080
H	-1.91483549808152	-0.54110296011717	-5.16818932562316
H	-1.62080498855731	-1.77138821494026	-3.90687504090461
O	2.02420590422740	1.01090766821093	-3.01317360238086
H	3.91634502313551	0.72193308802642	-3.85022675901715
H	3.73535582229752	2.19492623675608	-2.85205993073083
C	1.49002491222932	1.24502389163986	-4.30303694031190
C	-0.01996780902889	1.08686184737956	-4.25803600527802
H	-1.56927702060497	4.30075621767877	0.04390566002905
H	-1.12116378998978	2.65598742698405	0.67934998653970
H	1.92738073248048	0.52327221106287	-5.03531607529170
H	1.72775925957827	2.27829285106225	-4.65787784432262
H	-0.45158573695306	1.84162327920495	-3.56037043956113
H	-0.42313723091266	1.28815032685435	-5.28121575162194
H	-0.81619242858058	-0.12077154773938	4.55688951445346
H	0.42623913668826	0.20636968002379	2.39764173597007
Br	1.41665093281788	-2.04928634654764	3.42232081755804
C	-1.30355112001847	-0.52736248956332	3.65101138307383
C	-0.37106171927069	-0.53666710646226	2.47964479095295
H	-2.16733073321041	0.11977319014751	3.39293987159959
F	-1.40873154537638	0.64612164667884	1.27310495215239
H	-1.67591392409220	-1.54300018153365	3.88176829470924
H	-0.46539940684283	-1.28872953263967	1.69201766514347

KI-cryptand

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Coordinates from ORCA-job geom-pbe

C	3.28567356080692	-1.88302771599333	0.03089417909737
C	3.57697485988881	-0.43398157282354	0.41725674643578
O	2.04320319562687	-2.00317852972082	-0.64462356159011
N	3.40628360386376	0.57832726932476	-0.63393428476701
C	3.70781146641297	1.91199810667248	-0.11161655802340
C	1.42625853060419	-3.27444626325995	-0.49900216944574
C	2.83876343048535	3.06678519957185	-0.61276808934534
O	1.48239621152018	2.79553116860763	-0.32748557982366
C	0.63008313546197	3.92625547009938	-0.41422664934469
C	0.19885712825375	-3.35516667008389	-1.39075886323826
C	-0.81431964102033	3.48917285549685	-0.29358984414973
O	-1.19645477860136	2.81410583614979	-1.49698961318092
O	-0.67768280493323	-2.29616494407986	-1.06977810427926
C	-2.58979081783326	2.54719892276174	-1.61848951822643
C	-2.03213416173916	-2.48167339788826	-1.43840995057968
C	-3.03208389147087	1.16445805581967	-1.13706499954062
N	-2.43700510729132	0.00986255480344	-1.83724025895491
C	-2.81989547612834	-1.21544676375919	-1.12246969918076
H	3.27304423499657	-2.46590452997128	0.98053850653163
H	4.09923526743468	-2.31962062895648	-0.60019045769719
H	3.17702459113896	3.98781280382371	-0.07657403470861
H	2.96992980555949	3.26587421554774	-1.70274294827006
H	-3.17885506729381	3.30175479221414	-1.04850255412066
H	-2.84137206909200	2.70675926098850	-2.69017668621651
H	-2.48125423997389	-3.31556284188509	-0.84493455182612

H	-2.11433729029338	-2.77965930436004	-2.51094976660294
H	-4.15568537446124	1.14652304884140	-1.19671914874542
H	-2.76127866885929	1.06159436193386	-0.06018812612162
H	-2.67994373370870	-1.01483915332093	-0.03668234511135
H	-3.90643844155545	-1.45233555886699	-1.28699707134222
H	3.56729682115809	1.87688050309739	0.98760446918841
H	4.78268272886402	2.18820640247854	-0.28384738523144
H	4.61874382361827	-0.43503482074769	0.84057459313961
H	2.89251058943300	-0.15492988757725	1.24751968877572
H	2.12784476394403	-4.09443278867804	-0.78813097825707
H	1.12983728232558	-3.42719830881308	0.56627489801961
H	-0.28407535606238	-4.34699661940403	-1.21401195163637
H	0.49231278659292	-3.30582926914063	-2.46852634870365
H	0.86173417622259	4.64712190814646	0.40800882665023
H	0.78311661404853	4.45596041335915	-1.38697343397042
K	0.41093788550870	0.27158540536558	-0.92392622921103
C	4.04301792606701	0.24780485617045	-1.90128468008850
C	-2.70097725553499	-0.00453177529687	-3.27339301234487
C	3.52329718841920	1.01919335363134	-3.11810788325759
H	3.85655189178043	-0.82455679112479	-2.10299463531943
H	5.15981472244047	0.38712552663753	-1.87162933554571
H	-2.83225424630976	1.04226876849128	-3.61121146144687
H	-3.67195854029204	-0.51543974240678	-3.52110097989738
C	-1.62332947434282	-0.64575829552856	-4.17188809598142
O	-0.28898504819699	-0.22300428607984	-3.95584603724978
H	-1.92254249083331	-0.45601286229360	-5.23425256038360
H	-1.59525832605731	-1.74432985597870	-4.04137530133135
O	2.11084148664861	0.94515504163229	-3.16480726851203
H	3.97319930038599	0.55432869110481	-4.02883440268504
H	3.85743042279260	2.08575406287595	-3.11002047999280
C	1.54091106864592	1.23351694997723	-4.42845906096520
C	0.02910285457100	1.10574700970304	-4.33878827389349
H	-1.44752073643351	4.39732989638566	-0.15327517187186
H	-0.93799134234466	2.82323957076448	0.59758302149789
H	1.93793732942515	0.52639187193601	-5.19729050125383
H	1.79294366445988	2.27201506342219	-4.75744160804489
H	-0.36952396707878	1.84707370376901	-3.60726783076403
H	-0.40082119708141	1.34446860055668	-5.34306366972218
I	-0.92356480458287	0.31798165587746	2.20856908265878

TS1-cryptand (EtI)

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Coordinates from ORCA-job geom-pbe E -2342.014408170963

C	3.220047	-1.958339	0.061749
C	3.590264	-0.543766	0.493027
O	1.906001	-2.009097	-0.485741
N	3.335267	0.537621	-0.473557
C	3.640777	1.836942	0.128002
C	1.276936	-3.275637	-0.319513
C	2.753638	3.013861	-0.276821
O	1.401334	2.730924	0.035278
C	0.541730	3.858350	-0.071247
C	-0.000430	-3.326086	-1.136297
C	-0.904662	3.411842	-0.120672
O	-1.170569	2.852874	-1.413178
O	-0.864932	-2.268928	-0.749936

C	-2.546249	2.629377	-1.697073
C	-2.191358	-2.388365	-1.240269
C	-3.111687	1.295625	-1.204408
N	-2.522937	0.085202	-1.807217
C	-2.951114	-1.084189	-1.026835
H	3.275300	-2.578316	0.985289
H	3.945057	-2.382434	-0.677292
H	3.108404	3.906970	0.294562
H	2.845876	3.269124	-1.358612
H	-3.166452	3.443684	-1.252118
H	-2.645912	2.732781	-2.800141
H	-2.731204	-3.193552	-0.684354
H	-2.182409	-2.700253	-2.310483
H	-4.224984	1.333083	-1.362176
H	-2.929874	1.220584	-0.110647
H	-2.832366	-0.809415	0.042531
H	-4.038851	-1.305691	-1.203357
H	3.535567	1.726283	1.226293
H	4.708193	2.136391	-0.052744
H	4.670195	-0.584055	0.800210
H	3.011827	-0.320156	1.414995
H	1.941869	-4.098790	-0.677751
H	1.068234	-3.446873	0.764109
H	-0.482370	-4.317959	-0.957044
H	0.227169	-3.249541	-2.228275
H	0.688879	4.536224	0.805185
H	0.780662	4.439586	-0.994652
K	0.311364	0.278986	-0.805901
C	3.960241	0.298682	-1.768586
C	-2.760102	-0.010871	-3.246006
C	3.431458	1.127851	-2.939506
H	3.790215	-0.763734	-2.030202
H	5.075412	0.448505	-1.732583
H	-2.898741	1.015715	-3.640103
H	-3.720928	-0.544722	-3.481891
C	-1.655547	-0.683829	-4.085741
O	-0.332011	-0.238558	-3.847455
H	-1.923871	-0.544873	-5.163951
H	-1.623184	-1.775389	-3.904513
O	2.020958	1.012804	-3.020378
H	3.909788	0.732136	-3.867335
H	3.728916	2.202294	-2.865272
C	1.481212	1.247982	-4.307880
C	-0.028044	1.085684	-4.258047
H	-1.555865	4.304143	0.040085
H	-1.110115	2.661352	0.681209
H	1.918057	0.528959	-5.043157
H	1.714862	2.282614	-4.661420
H	-0.458968	1.837427	-3.556824
H	-0.435217	1.288850	-5.279310
H	-0.969676	-0.084046	4.587863
H	0.378998	0.220819	2.484903
I	1.489504	-2.138634	3.640410
C	-1.410634	-0.501663	3.663429
C	-0.426492	-0.516746	2.534181
H	-2.263707	0.141052	3.359401
F	-1.408695	0.650461	1.271677
H	-1.793165	-1.515048	3.887513

H -0.473161 -1.283717 1.755883

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Coordinates from ORCA-job geom-pbe

C	-6.59984767050027	5.08236547861785	1.70641462215890
C	-6.87503430604370	5.76909171735843	0.38315464727610
O	-5.21270430921424	4.80144579899015	1.80679255205490
O	-6.84910549060284	4.83090395823796	-0.67255676449558
C	-7.04484073743034	5.41825129939013	-1.94172499791236
C	-4.76588201450587	4.09801480099892	2.88621825797532
C	-6.93837260365723	4.36872065793145	-3.03065809202956
O	-5.57214630177911	4.03948220067508	-3.22715037205531
C	-5.25586083939898	3.06435488832167	-4.12462273177189
C	-3.37728423461702	3.75993498425129	2.87324256737992
C	-3.86899457592492	2.72862933883321	-4.20688161496319
O	-3.05002042633844	3.43224664437233	-3.37678761402512
O	-2.67701826668211	4.19584622394255	1.79070742197765
C	-1.68717080081912	3.05128730896440	-3.24972906154705
C	-1.35362556440879	3.71016726238294	1.58400676429623
C	-1.13349725778556	3.80996518166717	-2.05694450244711
O	-1.64226223031802	3.29612461019644	-0.81109063972485
C	-0.96394352010009	4.10776292991547	0.17455850709791
C	-5.56088480683815	3.69847145308223	3.97252060504067
C	-2.83355784731162	3.02775221528172	3.94053749662254
C	-5.00153773685330	2.96488769801495	5.03811730967285
C	-6.17476532813315	2.39305041047623	-4.94667334703696
C	-3.44814243317855	1.73549238645562	-5.10366174538053
C	-5.73860206433850	1.39578813822730	-5.84187924994466
C	0.38884723776020	3.87204459953957	-1.83453174761304
C	0.52148730885674	4.15401852484655	-0.28592966926084
C	-4.38272481109426	1.06797060478558	-5.91963212200783
C	-3.64531137794547	2.62977435095155	5.02122401322015
C	1.32084946331108	2.64738338763135	-2.03038408955643
C	1.65270721805612	3.17596673136038	0.16817601016178
C	0.89179372930208	1.35386328259392	-1.26580149704884
C	1.30192264219312	1.67313345253338	0.22851988770797
C	2.49930596989630	3.11995046610314	-1.13555824768872
O	-0.45442104211609	0.91996324195909	-1.34108733518635
O	0.32748120630937	1.25592187268086	1.15756068137664
H	-7.19665478751500	4.14434890497825	1.77043718837879
H	-6.92064694127184	5.75495650972186	2.53660005170710
H	-7.52260562704208	3.46602205119383	-2.73775731262179
H	-7.37855885092958	4.77812308405569	-3.97076411911871
H	-1.58653332739557	1.95289080283174	-3.11547029860680
H	-1.10963288235212	3.34170465237429	-4.15968060283760
H	-1.29557813651193	2.61396643357589	1.72425201339889
H	-0.64307652241549	4.17944595153588	2.30385985160372
H	-1.50155577329605	4.85946428583857	-2.15646062786563
H	-1.35670465770661	5.14421516856774	0.04083738066395
H	-6.62844390905541	3.95549441969988	3.99533649233756
H	-1.76805971340019	2.76008072469945	3.93337616657421
H	-5.64248888798651	2.65734063990497	5.87793795118493
H	-7.24322065484696	2.64118110176192	-4.89203850428376
H	-2.38336932680099	1.47135938723338	-5.16907504430219
H	-6.47481771137199	0.87751624463619	-6.47420318377681
H	0.80638404188752	4.70437661625887	-2.43715143543421

H	0.89566995022660	5.18141946297247	-0.10047478436628
H	-4.03475363658753	0.28759567801354	-6.61316319886805
H	-3.20184605476259	2.05483445250088	5.84819444758032
H	1.56617353168164	2.45539270622772	-3.09368754714416
H	2.18563855125765	3.53255948914221	1.07110589984453
H	1.49052400675705	0.50427659769010	-1.65199439409837
H	2.25460447755472	1.14326292003502	0.46336218097624
H	3.34045984289446	2.39911162655865	-1.07856763159081
H	2.90455789269865	4.10344650861511	-1.44640081627049
H	-1.03495368583063	1.67555142632341	-1.04367706461693
H	-0.28961236320769	0.68417420353413	0.64440552716116
H	-7.87850435771785	6.26208241012353	0.44449770915007
H	-6.11698896188291	6.57322618060375	0.22025291765481
H	-8.05837174059548	5.88999169371842	-2.00466673738536
H	-6.29152996222456	6.22161956350179	-2.12960837735165

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Coordinates from ORCA-job geom-pbe

C	-6.69609428933204	4.86168351087346	1.78219965817501
C	-7.06311316048179	5.48087593664713	0.45132892366061
O	-5.30462791937684	4.57190962227547	1.78236320855733
O	-6.89150046280246	4.53719016914932	-0.59589554957926
C	-7.24652024681874	5.06558407115449	-1.86485519066566
C	-4.72646094634700	4.15186882662664	2.96038084412353
C	-7.03393278070181	4.02879366744224	-2.94653029271288
O	-5.64299390261603	3.75461336017951	-3.04572700209360
C	-5.19630062797861	3.01057125734637	-4.11584833598732
C	-3.31821664139998	3.93782795338255	2.90862130417191
C	-3.78139483976450	2.87269027613388	-4.21684595393231
O	-3.04865352774986	3.50722045998285	-3.25457629466474
O	-2.71970682657766	4.20476020060871	1.71148507791392
C	-1.62961756015259	3.28002760527496	-3.23977492508583
C	-1.32118984591997	3.89816243881601	1.57484161984831
C	-1.03648141002614	4.02574583593061	-2.06102670381108
O	-1.67359665882178	3.66316302315285	-0.82915826700674
C	-0.88548440470083	4.30592496656400	0.18141229894953
C	-5.42614877950536	3.92351185519691	4.15324438106035
C	-2.65440976809242	3.47548458166767	4.05616203714237
C	-4.74410142901799	3.47413134181856	5.30061311978663
C	-6.03007396080395	2.39739259770097	-5.06093626307719
C	-3.24330318731555	2.10935156653359	-5.26519638680456
C	-5.47482633695328	1.64302003770326	-6.11266885957019
C	0.47893349442109	3.85857033981600	-1.79342450887830
C	0.58528057671458	4.05176405728851	-0.23078625490108
C	-4.08836564769231	1.49967601894980	-6.21054136465791
C	-3.36646256645515	3.24748311005079	5.24827267885274
C	1.28782459834030	2.55051270395681	-2.03823967803701
C	1.44760528424684	2.83338478090910	0.21639462060762
C	0.69007322862825	1.22474172461749	-1.47919638723474
C	0.79983448844070	1.42384253293883	0.09486960252873
C	2.41587568921965	2.76465085675804	-0.99437001404071
O	-0.53697500184031	0.83527052582247	-2.03691091976515
O	-0.33973918286085	1.22862623220234	0.88956888603581
K	-4.27692948075120	3.05798635786835	-0.55137715616517
H	-7.28795853610410	3.93378172777137	1.95624488253657

H	-6.94430654970387	5.58771833611724	2.58941387560052
H	-7.60230367271165	3.09825608968461	-2.71410068561245
H	-7.42126995961794	4.44006988705985	-3.90663294926175
H	-1.41549488717796	2.19582304564745	-3.14790157302025
H	-1.16999256476639	3.68049682024819	-4.17220431918233
H	-1.14448003478345	2.81399121192484	1.72705458258682
H	-0.72841689268308	4.48779845997298	2.31017434937001
H	-1.21989432270246	5.12090822753524	-2.21545128368651
H	-1.06003913340982	5.40893780165801	0.08112650601080
H	-6.51168435658267	4.08512958537107	4.20005056590832
H	-1.57558889030917	3.27605856158397	4.02139770083521
H	-5.30635425860322	3.29299756108880	6.22853705179121
H	-7.12176856928296	2.49015558877679	-4.98068191267260
H	-2.15637375926923	1.97330826516126	-5.34147019042236
H	-6.14034958772692	1.16200132705985	-6.84449155226589
H	1.01467035832687	4.66989932746304	-2.32772109617616
H	1.17083948621743	4.96219974909445	0.01464315196223
H	-3.64565303759078	0.90242912888737	-7.02160712682369
H	-2.82887168755202	2.88085897945894	6.13515461822791
H	1.61943970243751	2.44545711951570	-3.09067160653175
H	1.92444386568584	2.99122469046569	1.20460105716279
H	1.43593665481635	0.43862815795547	-1.74749318513427
H	1.58215161302193	0.71049726091440	0.44849749415830
H	3.13061363226184	1.91794708028568	-0.93947363528343
H	2.99181421791592	3.69889149580554	-1.15250461799527
H	-1.25246054205788	0.57995384569136	-1.38648974352705
H	-1.11060503596228	0.77808359173701	0.44027822832560
H	-8.12672255225960	5.81747807799689	0.50106264151808
H	-6.43113457450580	6.38302843499068	0.26804141340185
H	-8.32091981435304	5.36957496035855	-1.87243044723491
H	-6.63719724446330	5.97334865128535	-2.09191506499466
Br	-3.14575503365849	0.08085254809179	-0.25725908231385

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Coordinates from ORCA-job geom-pbe

C	-6.68856232137549	4.76426702889050	1.79377033675008
C	-7.07182342929911	5.38880414226122	0.47011433962100
O	-5.29351607518091	4.49561545434406	1.78401665608869
O	-6.90126514007525	4.45387449917759	-0.58434219077594
C	-7.24513787088926	4.99857380559324	-1.84892298292820
C	-4.69613388752170	4.10219905324395	2.96060813381792
C	-7.01961976592283	3.97623339930655	-2.94136470716897
O	-5.62705063778033	3.71345562716810	-3.03480202075861
C	-5.16839567164928	2.98488011154910	-4.10939630242518
C	-3.27898395855292	3.95185050329552	2.90520804842430
C	-3.75045601516787	2.88243879662681	-4.21667719490708
O	-3.03088057844243	3.53871809059471	-3.26180219476669
O	-2.69655926631784	4.24837814601879	1.70876737163748
C	-1.60839221612708	3.32958718663523	-3.24062103174320
C	-1.28841361056997	3.99080685114858	1.56550348763767
C	-1.01283129447712	4.09897096262948	-2.07677898022708
O	-1.67554148477615	3.80122128509647	-0.84116016385995
C	-0.85816678687743	4.40337678608885	0.16975094161379
C	-5.38319021305535	3.84065734173047	4.15420247250707
C	-2.59413125079052	3.51590009809787	4.05127884595496

C	-4.68001656572001	3.41903220335061	5.29968157120509
C	-5.99172948375919	2.35473650323638	-5.05280222893997
C	-3.19947546747842	2.12967272244212	-5.26665303758578
C	-5.42337227720624	1.61448730334198	-6.10790059792422
C	0.48857188607989	3.85846236783811	-1.79510590260725
C	0.59391293736320	4.06227820871312	-0.23448337831244
C	-4.03413864740943	1.50162497040967	-6.20933790917135
C	-3.29368933541219	3.25348853953732	5.24394365029629
C	1.21227620053148	2.49734680338519	-2.01996827489787
C	1.35245236970375	2.78646975868149	0.23432487002951
C	0.53256920450669	1.19940967218889	-1.46568935135232
C	0.61196102494295	1.41179541570043	0.11207997127936
C	2.33437870315114	2.64396746732546	-0.95872958425557
O	-0.68527475973737	0.80358032843355	-2.02615875616226
O	-0.55539533535702	1.23887069446498	0.86371391708303
K	-4.16800519392710	2.96811357564127	-0.54755346915544
H	-7.26765307981659	3.82728543715007	1.96381875618875
H	-6.94221428143682	5.47978483876219	2.60868417801195
H	-7.58462515532377	3.04016567223780	-2.72238960077116
H	-7.40397506243371	4.39476390407716	-3.89967627368824
H	-1.38509841110598	2.24559073532201	-3.13496592863260
H	-1.15278415019285	3.72174300327064	-4.17862667854139
H	-1.07988396837945	2.90982930385272	1.71934850279670
H	-0.71342037270639	4.60209168177099	2.29739244327062
H	-1.14808005253557	5.19524004927478	-2.26734843733385
H	-0.98076977022634	5.51370362945894	0.07552123212346
H	-6.47498775088746	3.95458346125951	4.20281720556119
H	-1.50734799799436	3.36595255716564	4.01412081337179
H	-5.23195733455575	3.21210600496711	6.22844382037938
H	-7.08501414796127	2.42433835077146	-4.96897741495142
H	-2.10995463159334	2.01895698294315	-5.34647865162257
H	-6.08026061755377	1.12148036016268	-6.83966686312154
H	1.07386821946584	4.63180407171524	-2.33393137643434
H	1.23859022199758	4.93311875290442	0.00767003733115
H	-3.58062508518242	0.91580211105546	-7.02285070115014
H	-2.73865974708618	2.90977056975691	6.12934940709922
H	1.55483897759473	2.36842364853082	-3.06672449671777
H	1.82406619015808	2.91858423716635	1.22944146606959
H	1.26517259187629	0.39382068166467	-1.71183948901387
H	1.35069121296150	0.67005258064225	0.49906565514804
H	2.98816207070007	1.75085106207760	-0.88617790605753
H	2.97444121320644	3.53686948503279	-1.11183945843629
H	-1.49723777806082	0.84647780207410	-1.39964996875454
H	-1.40907037076174	1.10696389718570	0.31672729517285
H	-8.13768704761817	5.71781843403511	0.53021646307998
H	-6.44742688011527	6.29657965994127	0.28850917575389
H	-8.32004734275997	5.30178178196408	-1.86258385914006
H	-6.63429061330975	5.90938634712786	-2.05844713387144
F	-2.69021283378604	0.94693320049085	-0.49201656714071

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Coordinates from ORCA-job geom-pbe

C	-6.78145389322402	4.29007078169414	1.62196197181538
C	-7.20329597956466	5.08844502485439	0.40798326560415

O	-5.35057114661501	4.24522660981676	1.65649135129886
O	-6.83230451664630	4.40404922530978	-0.78268780575339
C	-7.20649445684109	5.08430828234106	-1.96671518783464
C	-4.73908088924865	3.78742714846642	2.79784519472347
C	-6.97710830239554	4.18559786636733	-3.16411161100432
O	-5.58298565106853	3.90507404304153	-3.26615744667155
C	-5.14185705822250	3.17473590521538	-4.34376779072659
C	-3.31352901092145	3.77590972084359	2.77680153919828
C	-3.73743151592947	2.93273924783333	-4.38893496791460
O	-3.00867996299607	3.46971559003976	-3.36297771601038
O	-2.72270015696751	4.18980024234148	1.60877093198319
C	-1.59739873622231	3.21009548251656	-3.32771012267413
C	-1.31080428103240	3.98114740915787	1.48249817043319
C	-1.01000087827451	3.97457687176337	-2.15797736590068
O	-1.65632366476852	3.64224634947772	-0.92045320136659
C	-0.88596635712799	4.34002058455086	0.07145279392225
C	-5.41878656088239	3.33243135211812	3.93758883319610
C	-2.61140138447555	3.33832367469301	3.91146824075899
C	-4.70239538938831	2.89824523047258	5.06804634803880
C	-5.96853072691829	2.66581351082025	-5.35572592035061
C	-3.20307011541349	2.17486242194255	-5.44243414040200
C	-5.41753810280865	1.91532003067657	-6.41244167295665
C	0.49577425360443	3.80462615372358	-1.87062523216733
C	0.58731313002062	4.07130509333451	-0.31766351840491
C	-4.04252822846592	1.66987256608253	-6.45319536875785
C	-3.30495547954561	2.90694502637851	5.05749188374427
C	1.26673535588809	2.46527612582773	-2.04248220470157
C	1.41836795063111	2.85966414233629	0.19736646809543
C	0.63424789094630	1.17790525576300	-1.42208158056857
C	0.76722545593979	1.44065789182963	0.13959967479745
C	2.39303764157712	2.70473020722202	-1.00127174547326
O	-0.61456122595477	0.75724159255581	-1.91490065705093
O	-0.34729557980404	1.17762444132251	0.95178954002246
K	-4.28347887979514	3.13587239884181	-0.74807913401840
H	-7.18782279878214	3.25160485869266	1.58477601166833
H	-7.17242390902038	4.80638017949223	2.52682017226269
H	-7.55149740526224	3.23885559834813	-3.04777350781158
H	-7.33757834119120	4.70730753319122	-4.07971764544134
H	-1.40686187706685	2.12179197776615	-3.22316980344007
H	-1.11663147833300	3.58429331685548	-4.25987846649887
H	-1.05531458109034	2.92649071126573	1.71001540054862
H	-0.75747460157470	4.64706859145301	2.18422427364018
H	-1.19067224073989	5.06491884674712	-2.34144409774114
H	-1.07435852908312	5.43422295576587	-0.07732595031318
H	-6.51537345293663	3.28020574406216	3.94078226116309
H	-1.51353785659531	3.32140847379396	3.90571819626145
H	-5.25308247580572	2.53708577676165	5.94901514756049
H	-7.05161464442215	2.84454963271341	-5.32705087712512
H	-2.12628884606354	1.96193682510046	-5.47401715807211
H	-6.07953233777009	1.51918854779519	-7.19640532037662
H	1.05322111157903	4.57623818983950	-2.43990636864954
H	1.17895918655856	4.98608956333119	-0.10619659176120
H	-3.60600914838660	1.07590463834111	-7.26996546658848
H	-2.73738052442129	2.56297188832703	5.93485428269875
H	1.60424633411408	2.29922399081394	-3.08510229718342
H	1.89300121625346	3.05740725890542	1.17915230856508
H	1.34504686887953	0.36045549613139	-1.68040509359542
H	1.56523223017803	0.76111145413212	0.51326819816354

H	3.08827559148654	1.84660286248751	-0.89685192296434
H	2.99115411327668	3.61593357597551	-1.20425465774400
H	-1.36461762729960	0.85517280920548	-1.27179809967320
H	-1.21597028854343	1.11930147475670	0.46684552133235
H	-4.80975159398612	0.34731983405766	-0.38064278761986
H	-4.63067275741366	-1.48512663390402	1.74267746791339
C	-4.29896568562308	0.27505361065071	0.58276916365228
F	-2.71596998780275	0.92913581891766	-0.22201149814972
C	-3.84622742115083	-1.05059219129950	1.09163617995417
Br	-6.89520645015252	0.44861424986148	1.21324062224925
H	-3.64803587736898	-1.75469377138244	0.26207517690863
H	-4.32576661983721	1.12640767349285	1.26906396499035
H	-2.92719126983160	-0.92895642405499	1.69858154973912
H	-8.31096493898708	5.22252442900249	0.44383727518192
H	-6.73522826446989	6.10191808799491	0.43121526418916
H	-8.28978311446151	5.35323114346666	-1.94052993073288
H	-6.62713325394121	6.03299789957288	-2.07737271408405

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Coordinates from ORCA-job geom-pbe

C	0.67763367716137	-0.69380337437335	3.96620588352354
C	-0.74616812526175	-0.81322028923866	3.93942056543259
O	-1.25065263323469	-1.53953977805465	2.90176833738830
C	-2.87479839999595	-2.19859719776781	1.31568629674134
O	-2.48213125999667	-1.35796932682450	0.21206276512941
C	-2.83497277231589	-2.15443195813863	-0.94322443178978
C	-2.52679853755024	-1.43814034702959	-2.24305701426209
O	1.33564233262467	-1.32862361601316	2.95819737049899
C	2.73162264401421	-1.09865889783111	2.78857979665494
O	-1.11355438529622	-1.49101008622463	-2.41942737398146
C	-0.54782515114395	-0.76854922541261	-3.42486915778732
C	0.87799304546840	-0.67662763434769	-3.38979387595433
C	3.12605478829853	-1.76147569618335	1.48389388832668
O	2.68706321081345	-0.99655413608824	0.33682349756359
C	3.17712911600621	-1.77264814346518	-0.77451730806690
C	2.86510567518383	-1.12412020253653	-2.11192589432762
O	1.47712307319548	-1.31631729961224	-2.34586204363238
C	-1.51144222732489	-0.20191019466146	4.94365744493553
C	-0.88465730842165	0.53092599511397	5.97170056565958
C	0.50730542462242	0.65357309858288	5.99472131484052
C	1.28837471380232	0.04312014403356	4.99320623007039
C	1.55068159587376	0.03892835891021	-4.39172237840576
C	0.82927249672493	0.66604754133793	-5.42739018295189
C	-0.56524861186954	0.58106319539064	-5.45950953461662
C	-1.25372050614627	-0.13393960454973	-4.45901971058303
C	-4.29260587949073	-2.66468696476166	0.93711248913252
C	-4.25622744460500	-2.70939812889788	-0.63985155408297
C	4.60356208172216	-2.14374599004306	1.17897508920152
C	4.64006885035715	-2.07113160691842	-0.39760689241474
C	-5.56151688677457	-1.81842946969690	1.21833947292180
C	-5.60862691445120	-2.04374666081590	-1.05511311150887
C	-6.49563256860701	-2.45635344764231	0.15384849039737
C	-5.51267273054781	-0.34671985942296	0.69579152623088
C	-5.72565400887340	-0.51691891043220	-0.86239476737478
O	-4.37529299411469	0.44988972378978	0.97186002274946
O	-4.86906620926158	0.30663153566335	-1.62034922219217

C	5.86761025441015	-1.33225293952454	1.61135105509056
C	5.80261723289280	-1.07885515094711	-0.65882430205564
C	6.80052562986688	-1.62014700085278	0.40093606367080
C	5.57654892823373	0.36815717957352	-0.11416377861335
C	5.80700334040607	0.20061931876131	1.44214230218166
O	4.86034593572974	0.90961956826215	2.20885959011018
O	4.34929885211989	1.02164268094771	-0.37892287910081
H	-6.77961164900585	-0.25328400704283	-1.11490602901616
H	6.35453647390586	1.02985123025547	-0.54627276250932
C	-2.65048578979674	-1.53066996790196	2.66143566799712
H	-2.21112600268859	-3.09556773376077	1.30146010230165
H	-2.15379840243049	-3.03830078842999	-0.92717473477897
H	-2.89470387889829	-0.39508314621244	-2.22672311212106
H	-3.04932047607934	-1.96640705586605	-3.07475284951054
H	3.31177386397714	-1.56411055865275	3.61923784947350
H	2.96898494781570	-0.01758038299834	2.78075490482608
H	2.55246590302329	-2.71762722376758	1.45219343319794
H	2.62732432332752	-2.74321423174990	-0.76586714813731
H	3.47224384099531	-1.62760205279098	-2.90133680887782
H	3.12750310195375	-0.04456052486818	-2.11486449219756
H	-2.60684829475437	-0.29189113514244	4.93059467223713
H	-1.49989391614041	1.00621163047488	6.75037773152834
H	1.00397186865606	1.22774176663407	6.79147417046634
H	2.38212661602892	0.15135741678752	5.01464184644932
H	2.64688041471537	0.11786758097321	-4.36839147000996
H	1.37319650415807	1.22394919364469	-6.20451197965755
H	-1.13572992662672	1.07195378856726	-6.26229947905650
H	-2.35103567985334	-0.19175144990197	-4.48984026599215
H	-4.46641994220847	-3.67160565525735	1.36946502932609
H	-4.29122570251367	-3.75561321609835	-1.00475548336020
H	4.75804943335162	-3.18429900718536	1.53034699103026
H	4.93143201571431	-3.04431458603299	-0.84354537831104
H	-5.90390238558959	-1.88716111256307	2.26956754654669
H	-5.96289324108129	-2.38202775578888	-2.04827997354478
H	-7.51141952759447	-2.01223030193857	0.12165424606780
H	-6.59988472375896	-3.55310787994273	0.27471453148207
H	-3.57472714703450	-0.02857275427611	0.62134523930145
H	-4.51894114644259	0.97179610054075	-0.98479517451566
H	6.25544623457164	-1.64250638330387	2.60108676097884
H	6.15552182192204	-1.09137540689314	-1.70873446869081
H	7.03232932539235	-2.69507865018849	0.26411536161359
H	7.75817307213212	-1.06235312119584	0.44474316187409
H	4.42669897940326	1.52820789622047	1.57704631591070
H	3.61398892436582	0.43894459376906	-0.03997693050538
H	-3.18974698552247	-2.11929899041476	3.44153903168651
H	-3.05397385920553	-0.49618421284889	2.67581453578335
H	6.82260949632342	0.58122557812889	1.70169223592924
H	-6.36497582875238	0.20738731496012	1.13910253003501

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Coordinates from ORCA-job geom-pbe

C	-6.49809691081012	4.20370811485258	1.85195718307390
C	-7.01856791586516	4.62142110631324	0.49239935416511
O	-5.08037901475380	4.33819739646087	1.80723544724753
O	-6.51013646140382	3.77431647341239	-0.56324040159804

C	-7.16265732118145	4.31855274508749	-1.73945905638820
C	-4.37984269702455	4.21937897413797	2.97985880835673
C	-6.78807442177555	3.56642811745817	-2.99544255579033
O	-5.38033803574217	3.74111457911984	-3.17490199109207
C	-4.83377823035366	3.39216498413190	-4.38255599973539
C	-2.96963387520017	4.40143007935188	2.87950340902833
C	-3.43603875438196	3.63382929347349	-4.52316217803996
O	-2.79659314482661	4.17518637089018	-3.43761064219267
O	-2.47644602279044	4.67835174118974	1.63115464313152
C	-1.36893064633452	4.12850492759714	-3.46793895013765
C	-1.05709309282170	4.59436197356667	1.48666946444688
C	-0.75172405403477	4.67921155399539	-2.18146274101968
O	-1.49549810926538	4.43621994951493	-0.97865639955924
C	-0.61119386011723	4.88934474718272	0.05532013379518
C	-4.95987110333702	3.92419606674586	4.22260569808198
C	-2.18591838404081	4.28157416576845	4.03933362760476
C	-4.16060170609288	3.81446761929289	5.37587466796466
C	-5.55354103303813	2.81960729104982	-5.44216508143270
C	-2.80785220411488	3.30325467662055	-5.73530155224271
C	-4.90941162754904	2.49917043837641	-6.65165847866402
C	0.66842737083731	4.14335534190219	-1.87853656883877
C	0.76569211324176	4.28834538174408	-0.31604109389626
C	-3.54220692492436	2.74396748096188	-6.79755394310351
C	-2.77882782562127	3.99426452113607	5.28300011844189
C	1.07861007987823	2.65816115969119	-2.12465215886450
C	1.21858069500663	2.86774721920566	0.14552146019537
C	0.09499421216445	1.57034079242671	-1.61587585103719
C	0.19145035038704	1.71656469838776	-0.03418329277565
C	-8.53613157157879	4.66914979355112	0.23806798308473
C	2.17172674552796	2.52411538516869	-1.03100511298471
C	-8.64616357711410	4.51007509828217	-1.33013905307522
C	-9.52244870448834	3.59002427927807	0.75601229744550
C	-9.78870098829545	3.45964036409235	-1.51113509109541
C	-9.13522740240155	2.11402029365600	0.42089273640720
C	-9.47048981895533	2.00030503993150	-1.12151065231816
C	-10.66337720093595	3.80903397779208	-0.27365157958410
O	-7.82572289667671	1.66564365392124	0.70301062795529
O	-8.46112996841725	1.35026595393724	-1.86152004021745
O	-1.20726046865296	1.64472495633260	-2.13889574615978
O	-1.03963204388178	1.90108572366813	0.61963039051622
K	-3.69433938700986	3.04235932118549	-0.73387700153284
Br	-3.23874397969198	-0.18062551767898	-0.45259411675453
H	-6.78888375851055	3.16431618230340	2.11436705273116
H	-6.93414548682855	4.89414838629454	2.60999999737092
H	-6.61606046464853	5.64581207908838	0.30179546028098
H	-6.74272842343095	5.34623431501432	-1.86528896667996
H	-7.05769776056542	2.49413791161143	-2.93104337647733
H	-7.34886514422953	4.02502357179947	-3.84153021699791
H	-1.06406642173610	3.07941834484427	-3.63546072676958
H	-0.98215401479048	4.76004017079206	-4.30025516754185
H	-0.73910512585342	3.58377799771769	1.80192522005887
H	-0.56159836791645	5.35398440301641	2.13405083056660
H	-0.67296627779419	5.79164196294663	-2.28103715419705
H	-0.53213718614125	6.00051402964925	-0.06262022933695
H	-6.04242481072279	3.75505779694823	4.30091003095024
H	-1.09790205021118	4.40934453425944	3.98108191673621
H	-4.63163175789334	3.57394133394339	6.34025012602042
H	-6.62240594924157	2.59690184088734	-5.32506587372657

H	-1.73216010061027	3.47986682744726	-5.86258948290719
H	-5.48851683779493	2.04742414175701	-7.47054950399346
H	1.41637603432674	4.78230919031544	-2.39145640552974
H	1.56493439056143	5.00147593356600	-0.02595455260655
H	-3.02683414793203	2.49176185357989	-7.73618610266237
H	-2.14272063109061	3.90213146225509	6.17577070647293
H	1.41871060183034	2.47481938641116	-3.16377505572136
H	1.68498825744128	2.87313608620964	1.15094070245468
H	0.54991386890926	0.58998054424950	-1.89631749289273
H	0.68548365256180	0.79832696591924	0.36386308679084
H	-8.92130751562193	5.65473751577198	0.57001660994642
H	2.60822491206518	1.50637829372287	-0.96462555353797
H	3.00123311197456	3.25006141288451	-1.14963735824592
H	-9.00189155923462	5.45074075357250	-1.79679138244617
H	-9.79581395434084	3.73065642096930	1.82026746185925
H	-10.29313133121784	3.54393432070812	-2.49339564452567
H	-9.79938341763493	1.44489756466247	1.00406977025522
H	-10.42161398975352	1.43044909924835	-1.24335665115550
H	-11.52329371509607	3.12224984052573	-0.14055960950380
H	-11.04758171076892	4.84866563061255	-0.28144371324685
H	-1.76222528614333	0.90190146885493	-1.75850517861132
H	-1.62577600372642	1.10555438619555	0.45490361641653
H	-7.96132546519890	0.78797870814737	-1.22911771563717
H	-7.20186634453302	2.21184902713354	0.16363980522766

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Coordinates from ORCA-job geom-pbe

C	-6.59646655392257	4.23951259895545	1.84618995148720
C	-7.05133481872029	4.72081307932452	0.48117116697400
O	-5.17446455611709	4.20787838893396	1.81431501763058
O	-6.63972378261462	3.81561847650770	-0.57165823539873
C	-7.21742759605456	4.42777501547838	-1.75708198982031
C	-4.49588143982304	3.91465204155080	2.97370655295488
C	-6.91233553047469	3.62596874161984	-3.00323292927232
O	-5.49397109944145	3.65457331188362	-3.16334314797729
C	-4.95358673878056	3.10644953936699	-4.30172449182049
C	-3.07317394660344	3.94862890221386	2.87514021513498
C	-3.53331103993469	3.18981402137298	-4.40809362388442
O	-2.88812525586011	3.82180220342603	-3.38309326264464
O	-2.56384589219207	4.30293327005586	1.65928846412587
C	-1.45157421033479	3.75485180978319	-3.36630910316364
C	-1.13907187250930	4.20784706665887	1.48130509069384
C	-0.92575544990314	4.50617025728062	-2.15773186629235
O	-1.53727078742505	4.07291258273856	-0.93484602421586
C	-0.77508342271503	4.71209658852371	0.09684827037416
C	-5.10827502055530	3.58259885171529	4.19005018767086
C	-2.30641888967357	3.61806294294733	4.00466085407091
C	-4.32453052117317	3.27045227726694	5.31785119765256
C	-5.697414711335300	2.48290587637862	-5.31365736865454
C	-2.90112371251805	2.62693880542589	-5.52902306570989
C	-5.04879957995176	1.93728855165423	-6.43835918371257
C	0.59584264945875	4.40042028948390	-1.89942022681551
C	0.70085494646377	4.54221115715351	-0.33296770216921
C	-3.65717148632436	2.00757078124399	-6.54168032524215
C	-2.93074051424102	3.28385356405955	5.22110407621875

C	1.44224518505522	3.12635241016525	-2.19265692583083
C	1.59574679036089	3.33346553730791	0.07000137147773
C	0.89160283058456	1.75111606518583	-1.68534709149613
C	0.99670678595468	1.89777954524959	-0.10017681426688
C	-8.54958204774861	4.94232051722071	0.21349966134124
C	2.56395665408426	3.33791587477201	-1.14206732057758
C	-8.66921461270723	4.79926690371407	-1.35633637920249
C	-9.65401678629369	3.98091697408235	0.72416687049915
C	-9.93284163107981	3.89694675191932	-1.54458711474593
C	-9.44310465971559	2.47323926680461	0.37690079598523
C	-9.79815831430078	2.40812460117889	-1.16310895927797
C	-10.76093600717007	4.34043600627264	-0.30415007636175
O	-8.18911253480378	1.87139498654853	0.64032999178722
O	-8.88047493909161	1.63512165809731	-1.90487167062952
O	-0.30850083881225	1.29553644933819	-2.24110906313480
O	-0.11748478007137	1.57420141163052	0.68019736590748
K	-3.87104537864189	2.91558752898309	-0.67686046650947
F	-2.23169461486908	1.04288412298575	-0.60933069459326
H	-7.01469508619850	3.24033000043490	2.09490761447447
H	-6.95756256960308	4.96836428429349	2.60827858657098
H	-6.52665694099826	5.68874183864437	0.29451238362635
H	-6.67698587935541	5.39652132669079	-1.88426570835048
H	-7.29542876427397	2.58934577326374	-2.92839570647672
H	-7.41517864139845	4.12333829491807	-3.86468077261746
H	-1.12226173348896	2.69392030354628	-3.32271005189709
H	-1.03559836432994	4.24711443510210	-4.27486952270255
H	-0.81174268463258	3.15195287942508	1.60270308235240
H	-0.61908163584361	4.85692332063685	2.22178823284880
H	-1.17141009480877	5.59309356901996	-2.27882530480021
H	-1.01265552657429	5.80651114866312	0.04666790571869
H	-6.20415477870861	3.54974778918382	4.26775007825704
H	-1.21085151277898	3.60766382312209	3.93637023375313
H	-4.81830632573803	3.00463786426098	6.26412594400964
H	-6.78991610342342	2.40304919561915	-5.22793933517007
H	-1.80692335627215	2.65942274249200	-5.61394064374938
H	-5.64479011265464	1.44898670584902	-7.22364177928281
H	1.09650687895440	5.25035594067434	-2.40804405319203
H	1.25236222176974	5.46459066181924	-0.05413834124189
H	-3.14013334216727	1.57267612314885	-7.41000551239639
H	-2.30995908749529	3.02489613071050	6.09155189371601
H	1.77652220745139	3.07438652414111	-3.24853661901085
H	2.07040590744181	3.47122988017297	1.06279920848947
H	1.67922644131089	1.01869404641992	-1.98620385041808
H	1.82255799916097	1.21994266846328	0.22450956580116
H	-8.82265517171587	5.96436141161576	0.54670762881888
H	3.30363432140200	2.51113630569394	-1.11691962563351
H	3.11280203603062	4.29388398931614	-1.26740317739646
H	-8.90406471984278	5.77660792017089	-1.82376418389606
H	-9.91056958765142	4.14418573641651	1.78926568424397
H	-10.42205321043623	4.04838505990157	-2.52641710313191
H	-10.17301159370319	1.87870401373366	0.96192585102741
H	-10.81319570619025	1.96204705832901	-1.28245930682059
H	-11.69739503382106	3.76119924120180	-0.17688641121320
H	-11.01786209714375	5.41820476095428	-0.30348138792487
H	-1.07996967639793	1.16999465394822	-1.57918233878366
H	-0.96517254768407	1.33859706005187	0.15703767105210
H	-8.44062710860933	1.04043467425581	-1.25783611872162
H	-7.50678928502131	2.37552323923379	0.12883331150133

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Coordinates from ORCA-job geom-pbe

C	-6.70589688536659	4.56995900545879	1.85855035555169
C	-7.24221355041841	4.95594580357920	0.49442406287440
O	-5.27201563986463	4.63783091870507	1.84073373767679
O	-6.65594773511573	4.20199103967973	-0.57354262672510
C	-7.39830102346008	4.60893363228788	-1.73001876136770
C	-4.62346410449035	4.34126250347822	3.01306458624574
C	-7.04074468669923	3.81931095885400	-2.97377289248131
O	-5.61774011507574	3.85193208320918	-3.16157941350999
C	-5.12321124966508	3.22097783790729	-4.27521619676559
C	-3.20668872521089	4.19145286794494	2.93688242879687
C	-3.70545728445892	3.07707509238183	-4.34745890615598
O	-2.98522974066157	3.58963506336904	-3.29825766390322
O	-2.64035875126421	4.36435368942843	1.69924025697731
C	-1.58163937240629	3.29685162535119	-3.26575374687785
C	-1.25056039941789	4.03386249969023	1.56718728212710
C	-0.95814329124407	3.99704656630162	-2.07541730706950
O	-1.61970437102590	3.68765836644776	-0.83921290833949
C	-0.80440031211904	4.33363958564599	0.15056575341774
C	-5.26637070185073	4.16746954072870	4.24959490627511
C	-2.48530486385952	3.86638902319615	4.09740129597154
C	-4.52919107950064	3.85361823180365	5.40620575474740
C	-5.91891922541288	2.70868342329929	-5.31303975671408
C	-3.13542732829825	2.42238773463299	-5.45154451018987
C	-5.33265953117162	2.06656686398192	-6.41954297097553
C	0.53385364276427	3.71710871329789	-1.79307110863923
C	0.64254749161668	3.95186914759838	-0.23575254522386
C	-3.94513627754046	1.92289848333360	-6.48816312285900
C	-3.14299919882942	3.70193985919291	5.33021271421875
C	1.20038703152509	2.32430275486081	-1.98485465141050
C	1.35740364880415	2.66363046128255	0.26352606361199
C	0.46770115287528	1.07700793672666	-1.39492788572336
C	0.57270084280611	1.31606054070476	0.17220377436963
C	-8.76951931440964	4.83571464042241	0.27473809549907
C	2.32984585808468	2.44905672730430	-0.92777347424833
C	-8.87925435615852	4.59360368477763	-1.27978674380148
C	-9.67042811007792	3.71198363451350	0.87285901584736
C	-9.83051066075620	3.36112224795176	-1.38028548415313
C	-9.18120706446229	2.25068025675745	0.71384452572444
C	-9.29208105581006	2.00652445866685	-0.85558812152688
C	-10.78841840889111	3.70592491615493	-0.20580196654885
O	-7.92290363977494	1.98306026214397	1.27852807713087
O	-8.11752570919766	1.55295382356742	-1.47933117946954
O	-0.78416462293013	0.72365918511650	-1.92901663251906
O	-0.59676692396433	1.18378606137451	0.94205819216780
K	-4.20845770146803	3.26212804787201	-0.59040449639141
H	-7.02520062102556	3.54585984740286	2.13145438008270
H	-7.11722373792292	5.30114537339885	2.59128357435961
H	-6.97408022576780	6.03005601987839	0.31918546646730
H	-7.13252917653522	5.68022488571370	-1.92395244700556
H	-7.37859776522944	2.76856493764027	-2.88661887676669
H	-7.55378715460413	4.31036730801620	-3.83183247594840
H	-1.42493023209040	2.20015518225157	-3.20903670626161

H	-1.08274678547407	3.69432700382957	-4.17884550754516
H	-1.08967151862174	2.96539779141749	1.81685066991099
H	-0.63743538332133	4.66872647582148	2.24666427682225
H	-1.06550310449421	5.10050356326832	-2.23450561977554
H	-0.90924236532657	5.43724385778142	-0.01103960849623
H	-6.35735122572820	4.26636308084292	4.32003692387089
H	-1.39850340446995	3.72261270172351	4.04513967779880
H	-5.05628282322543	3.71696662709114	6.36213799981168
H	-7.01169728367872	2.79853956205146	-5.26237318885618
H	-2.04791187623784	2.28231400959105	-5.50597535666675
H	-5.97682520628614	1.67126410429566	-7.21883495933493
H	1.14687266842556	4.45411047880825	-2.35092340527858
H	1.30974143106773	4.80854401720817	-0.00695367631481
H	-3.47586345691299	1.41234670448993	-7.34233303522552
H	-2.55792531013326	3.44215299932270	6.22464807428039
H	1.53467998640280	2.15111991745608	-3.02728974072122
H	1.83580061185727	2.79901277380911	1.25412778466399
H	1.14009529495910	0.22316786679974	-1.63807710180958
H	1.27942086624253	0.55406227875082	0.57202560264817
H	-9.23839250218591	5.80055195064784	0.55821552336809
H	2.94867298929052	1.53374176288801	-0.83227668733568
H	3.00358651034468	3.31119574836233	-1.10554065105338
H	-9.40123320673682	5.43778667991489	-1.77462888505964
H	-10.00069830793016	3.94070611678002	1.90568045973124
H	-10.30653992466351	3.27300266558496	-2.37722761840972
H	-9.95018879130581	1.61239355961354	1.21053252860354
H	-10.10820136862552	1.26349345239573	-1.02597275735366
H	-11.56756696065177	2.93632027209121	-0.02991554455272
H	-11.28926609574771	4.68791550397105	-0.32264699745996
H	-1.55797937276019	0.87485656570465	-1.32177041616316
H	-1.43787831290069	1.12409856992914	0.41637606674789
H	-7.82952902909196	0.69870780869991	-1.06410154965673
H	-7.67469749976309	1.03838354336452	1.10486763793449
H	-4.85265301246646	0.09062550060237	-1.07573309961751
H	-4.30303222235306	-2.32492048608531	-0.55600735616115
C	-4.47611517213403	-0.22879787408759	-0.09854339957508
F	-2.94846123194915	0.94680511176991	-0.36182146850197
C	-3.79133551374649	-1.54737902237624	0.04169615331802
Br	-6.94822025574778	-1.01428287611256	0.24907686893599
H	-2.75916036795641	-1.44917559597931	-0.35346948079471
H	-4.72396683831237	0.37989841524086	0.77553586200195
H	-3.73656237062260	-1.87648654256461	1.09508628070205

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Coordinates from ORCA-job geom-pbe E -5534.807377736982

C	-3.401268	-3.051398	2.117303
C	-3.163873	-3.830905	0.840633
O	-4.821652	-3.068393	2.339664
O	-3.823228	-3.193918	-0.260171
C	-3.399787	-3.932092	-1.410822
C	-5.319506	-2.512796	3.484236
C	-3.900791	-3.270969	-2.677379
O	-5.335885	-3.306150	-2.608684
C	-6.063361	-2.873086	-3.680430
C	-6.730217	-2.640117	3.661172

C	-7.479150	-3.000716	-3.550956
O	-7.916704	-3.540312	-2.369844
O	-7.392939	-3.303813	2.661915
C	-9.327496	-3.586670	-2.134566
C	-8.821027	-3.366363	2.727110
C	-9.563378	-4.183274	-0.759448
O	-8.869425	-3.466211	0.274487
C	-9.324435	-4.085227	1.488796
C	-4.556353	-1.838883	4.449037
C	-7.334979	-2.093621	4.802753
C	-5.176379	-1.297629	5.591849
C	-5.520067	-2.319997	-4.849682
C	-8.309656	-2.575274	-4.598441
C	-6.365697	-1.900682	-5.895128
C	-11.020876	-4.274629	-0.257795
C	-10.853981	-4.204931	1.309916
C	-7.751920	-2.028488	-5.771008
C	-6.556863	-1.425736	5.768573
C	-12.101987	-3.193979	-0.545251
C	-11.856922	-3.089131	1.718895
C	-11.716350	-1.698570	-0.308126
C	-11.540960	-1.625272	1.267902
C	-1.721903	-4.120946	0.356521
C	-12.992771	-3.402894	0.708845
C	-1.886349	-4.185262	-1.211914
C	-0.486235	-3.193011	0.546045
C	-0.730429	-3.278903	-1.726465
C	-0.660904	-1.707830	0.160900
C	-0.838756	-1.767894	-1.423280
C	0.352710	-3.657324	-0.677902
O	-1.675280	-1.025254	0.851534
O	-1.997004	-1.141791	-1.917105
O	-10.702918	-1.127876	-1.094225
O	-10.381811	-1.000497	1.755800
K	-6.437711	-2.358124	-0.026007
F	-8.351457	-0.542146	0.045842
H	-3.021255	-2.015566	2.011838
H	-2.878052	-3.557261	2.959913
H	-3.649706	-4.831391	0.982846
H	-3.891844	-4.937904	-1.358660
H	-3.526939	-2.229721	-2.743044
H	-3.547006	-3.852147	-3.558443
H	-9.769054	-2.572172	-2.206735
H	-9.821650	-4.250072	-2.881955
H	-9.254660	-2.347738	2.790016
H	-9.142443	-3.954829	3.617916
H	-9.149093	-5.223489	-0.768689
H	-8.905962	-5.124016	1.505281
H	-3.474351	-1.716462	4.304600
H	-8.421006	-2.177505	4.944526
H	-4.563847	-0.768521	6.337039
H	-4.432488	-2.195085	-4.945364
H	-9.400484	-2.660102	-4.504276
H	-5.922507	-1.465668	-6.803312
H	-11.443162	-5.251799	-0.570980
H	-11.195559	-5.145324	1.790034
H	-8.418050	-1.697391	-6.581636
H	-7.048070	-1.002074	6.657148

H	-12.604886	-3.343033	-1.521689
H	-12.137696	-3.140777	2.789658
H	-12.638743	-1.130672	-0.566852
H	-12.385830	-1.022850	1.671483
H	-1.430130	-5.113155	0.758353
H	-13.846483	-2.696665	0.768294
H	-13.389909	-4.434337	0.799281
H	-1.669300	-5.207848	-1.585002
H	-0.004744	-3.324228	1.535658
H	-0.469391	-3.486777	-2.783412
H	0.318826	-1.213435	0.369960
H	0.058064	-1.286507	-1.881224
H	1.299196	-3.092539	-0.799242
H	0.591490	-4.740114	-0.663868
H	-1.737564	-0.119146	0.444053
H	-1.987440	-0.211370	-1.568859
H	-9.827899	-1.024033	-0.625587
H	-9.634226	-0.951390	1.098251
C	-6.293341	4.048261	1.834545
C	-6.731668	4.631361	0.507869
O	-4.856454	4.076957	1.830970
O	-6.249738	3.823374	-0.571689
C	-6.853728	4.386364	-1.741705
C	-4.182860	3.677196	2.949779
C	-6.549705	3.533249	-2.955677
O	-5.120675	3.555989	-3.112189
C	-4.564997	3.013981	-4.236196
C	-2.761563	3.790199	2.881641
C	-3.152418	3.177976	-4.358568
O	-2.545910	3.862511	-3.338225
O	-2.264686	4.284677	1.703580
C	-1.116702	3.938724	-3.337814
C	-0.844327	4.312890	1.532098
C	-0.676142	4.698996	-2.100192
O	-1.186346	4.118523	-0.889421
C	-0.542670	4.869015	0.153155
C	-4.783555	3.166257	4.110300
C	-1.983455	3.393561	3.979288
C	-3.990316	2.773374	5.205707
C	-5.273007	2.320006	-5.228330
C	-2.490114	2.645968	-5.474975
C	-4.595978	1.797901	-6.347589
C	0.843484	4.832244	-1.853508
C	0.936192	4.950932	-0.283053
C	-3.213290	1.960199	-6.470416
C	-2.598826	2.888188	5.141535
C	1.870446	3.710884	-2.180459
C	2.006164	3.885620	0.088348
C	1.540869	2.259394	-1.700907
C	1.638218	2.381956	-0.120929
C	-8.233063	4.870704	0.216222
C	2.955548	4.061501	-1.127321
C	-8.317961	4.697494	-1.350566
C	-9.418562	4.004451	0.732524
C	-9.537906	3.749100	-1.536830
C	-9.299793	2.475133	0.549878
C	-9.379494	2.297375	-1.033563
C	-10.442704	4.299836	-0.399108

O	-8.182681	1.884559	1.163647
O	-8.318660	1.577380	-1.609122
O	0.409771	1.612329	-2.224354
O	0.588154	1.831785	0.630940
K	-3.617589	3.010454	-0.640371
F	-1.702118	1.201683	-0.621553
H	-6.675961	3.013879	1.945053
H	-6.683871	4.681460	2.662582
H	-6.235334	5.632600	0.417968
H	-6.364060	5.379059	-1.921630
H	-6.923213	2.499778	-2.808028
H	-7.037564	3.984306	-3.848780
H	-0.673226	2.922638	-3.352079
H	-0.758684	4.504869	-4.229009
H	-0.415638	3.297030	1.652931
H	-0.378379	4.993053	2.282330
H	-1.095638	5.735281	-2.170867
H	-0.959737	5.907692	0.112183
H	-5.875467	3.053053	4.159071
H	-0.888665	3.467180	3.932562
H	-4.477457	2.367540	6.104887
H	-6.355347	2.164363	-5.123274
H	-1.402066	2.757194	-5.575032
H	-5.166030	1.256525	-7.117453
H	1.202044	5.759815	-2.345757
H	1.340751	5.939175	0.018835
H	-2.677817	1.550055	-7.339589
H	-1.973123	2.577738	5.991563
H	2.201731	3.731731	-3.237689
H	2.459824	4.068106	1.082988
H	2.407517	1.650083	-2.044028
H	2.548200	1.826657	0.201256
H	-8.463814	5.917238	0.505024
H	3.814086	3.358418	-1.123899
H	3.352819	5.091761	-1.229912
H	-8.593126	5.657739	-1.833891
H	-9.737051	4.290171	1.754788
H	-9.964478	3.803689	-2.558341
H	-10.229070	2.034168	0.983712
H	-10.340904	1.777540	-1.264347
H	-11.394520	3.742004	-0.287156
H	-10.680826	5.377276	-0.508267
H	-8.171963	0.929767	0.882231
H	-8.266275	0.711002	-1.123838
H	-0.370942	1.582455	-1.603712
H	-0.258631	1.704796	0.119845

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Coordinates from ORCA-job geom-pbe

C	-0.42812175398039	-4.90122921363106	-0.65382418161665
C	-0.27426471202354	-5.52413480438017	-2.02518885405933
O	-1.14049866144383	-5.84169205406028	0.16614082429856
O	-1.55204464459688	-5.81533691470496	-2.61199857092091
C	-1.23315703531659	-6.27383529409150	-3.93309608681837
C	-1.37766052440119	-5.50393942374967	1.47431537599525

C	-2.48689082075458	-6.49278048263759	-4.75279645179918
O	-3.26992491467559	-7.48568465660257	-4.07076710333126
C	-4.41983980053972	-7.93107411443937	-4.66597510680343
C	-2.14349655994439	-6.44150910324744	2.22832506212417
C	-5.16369648578799	-8.90215413968078	-3.93128517545533
O	-4.63584207760405	-9.27339889978808	-2.72018477679163
O	-2.55350005999997	-7.56619679471603	1.55229018277660
C	-5.41761725529034	-10.14744085829642	-1.89782229606123
C	-3.40725492917792	-8.48204642712025	2.24533772483073
C	-4.66414953450863	-10.39645426343501	-0.60508171540087
O	-4.31663138697665	-9.17707682016313	0.07220540957607
C	-3.74079325864290	-9.62886837428698	1.30872057429577
C	-0.93299613899869	-4.32132961292809	2.08513385726373
C	-2.44000294668428	-6.16975093867244	3.57297408735279
C	-1.23853488017196	-4.06252303353487	3.43470113235488
C	-4.89598935899281	-7.49083968131902	-5.91043077792693
C	-6.36077550739036	-9.40230749802725	-4.46634901421683
C	-6.09522049529125	-8.00619862894392	-6.43777527848763
C	-5.36146234530075	-11.25212580504719	0.47667454678415
C	-4.72179347348450	-10.70817275558677	1.81370133277253
C	-6.82412543866468	-8.95699058435066	-5.71914521522774
C	-1.98704726909352	-4.98071458857481	4.17592433830890
C	-6.88916453212798	-11.19354274753358	0.76879048251434
C	-5.96405353223995	-10.39238089731996	2.69298838763977
C	-7.55124353532930	-9.78446912312572	0.90937224851054
C	-6.89406386425550	-9.22101609683683	2.23983243497344
C	0.51940553133566	-4.77416691523527	-3.12246254833864
C	-6.86643972611993	-11.58342869524456	2.27127384319250
C	-0.14841883070484	-5.30093776952747	-4.45305016578120
C	0.54890541608003	-3.23172766652566	-3.32530733005318
C	-0.42533445618439	-3.99517865232456	-5.25005107352508
C	-0.82377296830774	-2.50237203779817	-3.34243092291668
C	-1.49602264785745	-3.02799690265539	-4.67211482049361
C	0.84480576120180	-3.19163370670203	-4.85067392919229
O	-1.71715604526700	-2.69819181451961	-2.27284811138126
O	-2.78929085102683	-3.53182691059408	-4.42891813922561
O	-7.57817157559075	-8.93327965169293	-0.20812209160789
O	-6.37484870505984	-7.91395558002964	2.19166379665277
K	-3.54507515896123	-6.94484609356117	-1.18597404235566
H	-0.98426515024435	-3.94750193696482	-0.71591874443871
H	0.58356594517561	-4.70820177430613	-0.23205172030952
H	0.24660999123017	-6.50542294644140	-1.87707906483194
H	-0.73677600845359	-7.27285190635735	-3.82456883247825
H	-3.05359961682497	-5.54463504864357	-4.85534171775947
H	-2.19143939149007	-6.86477656119303	-5.76013118956303
H	-6.41302694210359	-9.70242528445986	-1.69497909938567
H	-5.55564807524698	-11.13181118056611	-2.40260047221937
H	-4.32732254710627	-7.96788621829339	2.59087134814938
H	-2.87892646869062	-8.90984610010670	3.12874696777860
H	-3.70337680103653	-10.90976189399881	-0.86579494372661
H	-2.77975581324267	-10.14445245351825	1.05426029710293
H	-0.35651130736180	-3.57308264948299	1.52327478969989
H	-3.03930281363457	-6.87950936847231	4.15841569904966
H	-0.88772161717125	-3.12249157038505	3.88446039776946
H	-4.34044079069589	-6.72772110845294	-6.47096744294518
H	-6.94922223987232	-10.13856646446146	-3.90340076654188
H	-6.45446657403807	-7.64550489625382	-7.41222089286575
H	-5.09712235888307	-12.31761542168686	0.31335635625246

H	-4.14353663971427	-11.50139074174091	2.33064112780826
H	-7.76768850634510	-9.35658356815859	-6.11775582744823
H	-2.23930904914457	-4.77989704711599	5.22772224361619
H	-7.47500411264741	-11.86302151755292	0.10793966124194
H	-5.71874837291695	-10.33511902929535	3.77225843495218
H	-8.61957381088256	-10.00238089893324	1.13319220222121
H	-7.69034114176102	-9.17539345521171	3.01546655177353
H	1.57660936017178	-5.10504481121140	-3.05852054224619
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H	0.57785335158743	-5.89167436307843	-5.04874552692287
H	1.28436469123517	-2.72057831965712	-2.67295643328657
H	-0.55271519086754	-4.17688407904060	-6.33603962181554
H	-0.60648950606372	-1.41571965852002	-3.44730871709484
H	-1.58236149075250	-2.18548763359816	-5.39729395338041
H	0.86066930419932	-2.16417705569951	-5.26788612186308
H	1.79097838363022	-3.69746983125674	-5.13083806924803
H	-1.50267455064279	-2.03826478792715	-1.52768011872247
H	-2.92230255865406	-3.37564940025556	-3.45975087411114
H	-6.92469613892489	-8.18336352310991	-0.17147318451857
H	-6.09238593865009	-7.62507743334862	1.28452069385706
C	-6.31190804005030	1.40760286600234	1.53147147463260
C	-6.30609677130200	2.28584803180461	0.29744667735353
O	-4.95029664104780	1.32006754013852	1.98048512185030
O	-5.49851487570398	1.69879583083020	-0.72906378069169
C	-5.70764212890629	2.53445705414568	-1.87262052183112
C	-4.67836612463815	0.60479230768373	3.11246055898634
C	-5.01931459850460	1.95433987740388	-3.09162065019449
O	-3.61243883608459	1.94701285016598	-2.79411130157202
C	-2.72468817494275	1.64752414495278	-3.78754988058398
C	-3.30170529622085	0.54089495142619	3.48258928403944
C	-1.34637116492069	1.77035101563514	-3.43707058680406
O	-1.09026181772866	2.16940073548612	-2.15296586134137
O	-2.43657124885329	1.20758127410197	2.65479687323323
C	0.26197072993958	2.09152037763141	-1.69221916302125
C	-1.03449052462957	1.10194266210353	2.91781536449267
C	0.29875613746207	2.43345546558016	-0.21446817429220
O	-0.59642657094319	1.62249508860824	0.55966401251512
C	-0.29535741702517	1.97098932128257	1.91843002225015
C	-5.63756651325201	-0.05217703768891	3.89798631993991
C	-2.92591884070494	-0.17810242475070	4.62707793095429
C	-5.24736261237278	-0.76602682648774	5.04743892896906
C	-3.07823206768680	1.22591157628197	-5.07800790291848
C	-0.36348369679150	1.48037699694936	-4.39661034280172
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C	1.66368648571422	2.30765777224649	0.50479250190590
C	1.24419410671179	1.96827493667472	1.98676555829872
C	-0.73153552203743	1.06991314006509	-5.69358250300057
C	-3.89929436034780	-0.82866451804870	5.41009421005521
C	2.72305442208387	1.21265321487120	0.18049781043328
C	2.08498373219007	0.70156865481809	2.30949675889739
C	2.24205970619050	-0.26920812212642	0.05101528221516
C	1.75655225029020	-0.61292804662864	1.52456287166046
C	-7.64258159434953	2.66556635359875	-0.38832062875143
C	3.39430036908780	1.09949060062062	1.57648818945916
C	-7.22555119924367	2.83051739955253	-1.90082096984964
C	-8.92056571866257	1.77859098222617	-0.46851795713470
C	-8.30770822474849	2.00914485151324	-2.66005205529327

C	-8.73633832099028	0.31678791651871	-0.93285105455499
C	-8.29226543581478	0.47787990905515	-2.45638629716408
C	-9.53446542593066	2.36158019599758	-1.77314078397700
O	-7.88182722340027	-0.45934130322087	-0.13128885421550
O	-7.07926655418965	-0.14427327309675	-2.80295591143259
O	1.39486527577127	-0.62892269068092	-1.00724645039334
O	0.47881814496704	-1.18377488170009	1.66275045541993
K	-3.00014323515628	0.68381168099096	-0.21866983906444
F	-1.12305182741732	-1.06121189683915	-0.44859667779682
H	-6.71554798079001	0.40484827016312	1.28624035654315
H	-6.94421142961868	1.88419418020570	2.31502479519024
H	-5.82011008019996	3.25369841755259	0.58767803987615
H	-5.20557661358493	3.51512723761425	-1.66392276952701
H	-5.39053039808817	0.93120544679407	-3.30003203164067
H	-5.21851627314163	2.61034873279420	-3.96830253383593
H	0.67177711301683	1.07724340252041	-1.87292246557653
H	0.89734893989592	2.83596381350165	-2.22635081338983
H	-0.70330813129900	0.04483730403556	2.84385884838662
H	-0.80346152087028	1.48881174896778	3.93738556122582
H	-0.03829408277230	3.49552035596708	-0.10059098527007
H	-0.63680642594838	3.02676646214114	2.07239678638581
H	-6.69644676469487	-0.01846074099716	3.60891739156794
H	-1.86747671359989	-0.24120828536279	4.91422734018244
H	-6.01199382730584	-1.27724858797174	5.65046887345272
H	-4.13712561962416	1.09865176374783	-5.34116821890543
H	0.69940057098057	1.57169336153400	-4.13763202671333
H	-2.37847505526488	0.60909164944310	-7.03751588116150
H	2.18028044576570	3.28816917137218	0.45237898435253
H	1.57169235599990	2.76500708162339	2.68621422662708
H	0.05279442898505	0.85313714119358	-6.43439442654162
H	-3.58614216509877	-1.38756713683370	6.30418559909447
H	3.39451591857326	1.50359388095414	-0.65173658718185
H	2.18134254665768	0.52167543203183	3.39904491195400
H	3.18123821976424	-0.84104376301089	-0.12450486171804
H	2.45945461197059	-1.36984243310800	1.94064844698656
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H	4.18525505939183	0.32267292798056	1.62472877094126
H	3.82323166476900	2.05530221513267	1.93928407056266
H	-7.35353193834660	3.88370652935947	-2.22592096798893
H	-9.55248651283888	1.86170717492787	0.43778564990593
H	-8.38755701918778	2.29836709609085	-3.72705206920241
H	-9.75431715736457	-0.14160377190593	-0.93082858671127
H	-9.11154467321533	0.06598980415542	-3.09161760435840
H	-10.46777380565472	1.85076472020855	-2.08586449579969
H	-9.73490846981777	3.45018017153761	-1.71544583303629
H	-7.89080010450698	-1.38100598049370	-0.49971581764237
H	-7.19355382746562	-1.11985823349243	-2.68756753240589
H	0.42775188400974	-0.72432129892026	-0.75100139287829
H	-0.12777305413406	-1.03851492592198	0.87973072449454
H	-9.08954678230589	-5.55993782433965	0.13852422047068
H	-7.31454029350445	-5.73298649000034	-1.60169016099841
H	-7.74067061936382	-6.00732555460969	1.23706829158770
C	-8.07975987926025	-5.26772640625531	0.48059300475873
Br	-8.11396144155761	-3.19827477037982	-1.93154083514567
C	-7.10183444248004	-5.24131886280502	-0.64747129236181
F	-5.98740636068866	-6.76817555804803	-0.21449954249969
H	-8.13742770182301	-4.28330728579335	0.98192368777872
H	-6.21060264797619	-4.60706561873649	-0.59731228939081

